A THEORETICAL CONSIDERATION OF THE DIRECT CAPTURE PROCESS $O^{16}(p,\gamma)F^{17}$ AT LOW ENERGIES

BY

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ABSTRACT

The cross sections for the $O^{16}(p, \gamma)F^{17}$ transitions to the ground d-state and to an excited s-state of F^{17} have been measured in this laboratory and elsewhere, at different energies in the range from about 100 kev to 2.5 Mev incident proton energy. In this thesis an attempt is made to calculate these cross sections at several energies in the above range on the hypothesis of direct proton capture. Similar calculations have been made at the California Institute of Technology but have not been published.

The standard formula for the cross section for an electric dipole transition from an incident p state to a final d-or s-state has been used. The matrix element appearing in this formula was split up into an angular part which can be evaluated exactly, and a radial integral which has to be calculated approximately.

In the case of transitions to the excited s-state numerical calculations using tabulated wave-functions were made at center of mass proton energies of 150, 378 and 940 kev. The cross section at 150 kev was also calculated by the saddle point method using WKB approximations to the wave-functions, but this method was found to break down at energies above 200 kev due to difficulties with the WKB functions. Reasonably good agreement between the two methods was obtained at 150 kev.

For transitions to the ground d-state the numerical method could not be used since tabulations of the required d-state

wave-function are unavailable. Calculations were made only by the saddle point method at center of mass proton energies of 150, 378 and 500 kev. This method can not be used above 500 kev.

The calculated ratio of $\frac{\sigma_s}{\sigma_d} \approx 9$ at energies of 150 and 378 kev, and the absolute values of the cross sections agree reasonably well with the experimentally observed values. Some discrepancies are noted between these calculations and those carried out at the California Institute of Technology which are very briefly referred to in a preprint of an experimental paper, but a detailed comparison was not possible,as the details of those calculations are unavailable.

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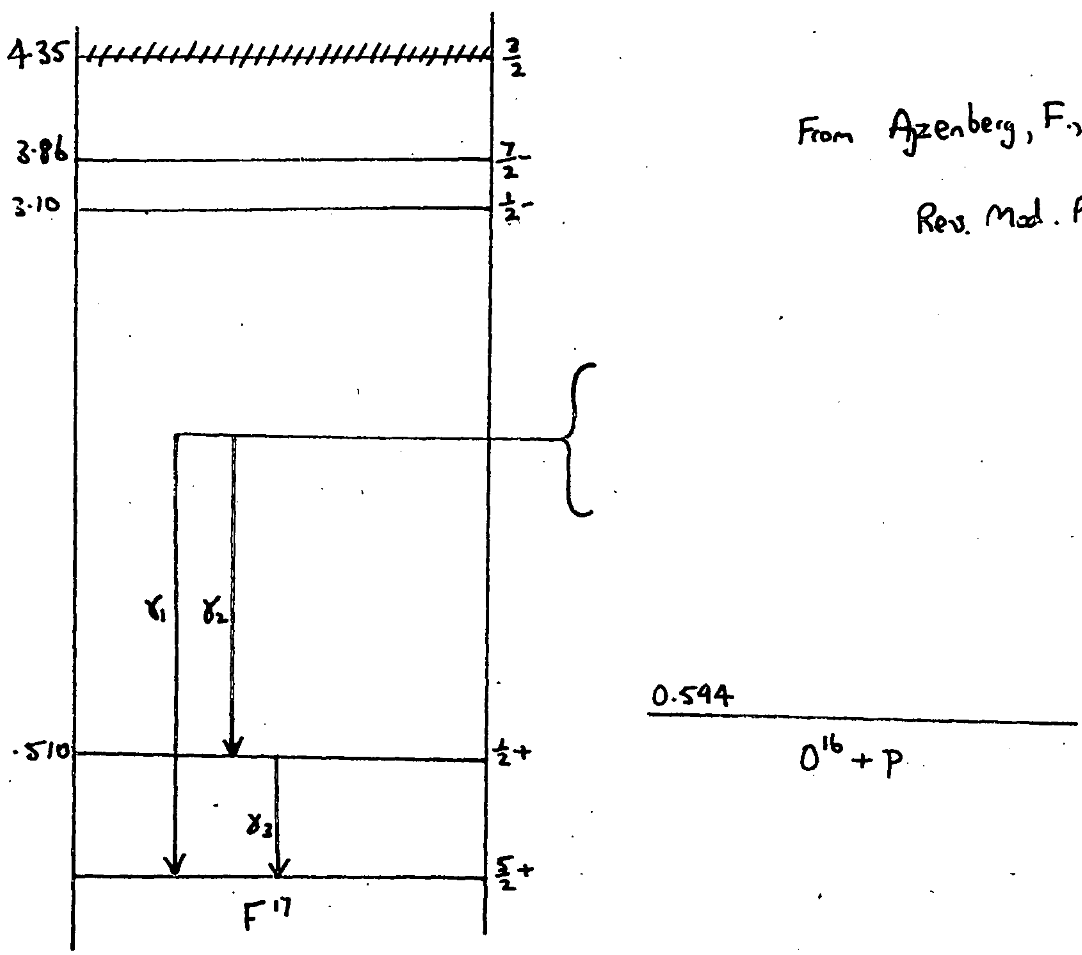
INTRODUCTION

The $O^{16}(p, \gamma)F^{17}$ reaction has been studied experimentally in this laboratory (Warren et al 1954, Riley 1956, Robertson 1957), and elsewhere (Tanner 1958). In these papers experimental reasons are given for supposing that this process is one of direct radiative capture. Calculations of the magnitude of the total cross section, based on the hypothesis of direct radiative capture, and of its dependence on energy have been made at the California Institute of Technology (Christy and Duck 1959). These calculations are briefly referred to by Tanner but have not been published in detail, and correspondence with the authors indicates that they are not likely to be published in the near future. In view of the interest in the theory of the direct capture process by the experimental group in this laboratory it was decided to repeat the calculations and to complement them as far as possible.

The shell model predicts that the F^{17} nucleus consists of a single proton moving in the potential of the doubly closed core. The lower energy levels of this system are shown in fig. 1. (Ajzenberg and Lauritsen 1955). According to the shell model (Blatt and Weisskopf 1952) the additional proton outside the second shell may be in a $1d_{5/2}$, $1d_{3/2}$ or a $2S_{1/2}$ state. That the two lowest levels are in fact $1d_{5/2}^{+}$ and $2S_{1/2}^{+}$ has been shown experimentally by stripping experiments (Ajzenberg 1951). For direct radiative capture the selection rules for radiative processes lead us to expect electric dipole transitions between p wave incident protons and these final single particle states.

Fig 1. Level diagram for $O^{16}(p,\gamma)F^{17}$



From Ajzenberg, F., and Lauritsen, T., 1955 Rev. Mod. Phys. 27, 77.

Shell Model Predictions.

Level	No in level	No in shell.
$1s\frac{1}{2}$	2	2
$1p\frac{3}{2}$	4	
$1p\frac{1}{2}$	2	6
$1d\frac{5}{2}$	6	
$1d\frac{3}{2}$	4	
$2s\frac{1}{2}$	2	12.

For a single particle transition the cross section is given by

$$\sigma(\ell m) = \frac{8\pi(\ell+1)}{\ell[(2\ell+1)!!]^2}\,\frac{K^{2\ell+1}}{\hbar v}\,|Q_{\ell m}|^2$$

(see Appendix A).

The matrix elements $Q_{\ell m}$ may be reduced to a radial and an angular part. The latter may be evaluated exactly (see Appendix B).

Three methods are available for computing the radial integral.

(i) the 'exact' method.

(ii) W.K.B. method and counting squares.

(iii) W.K.B. method and 'saddle point'.

The free particle wave functions known as Coulomb wave functions, and the bound state wave functions, Whittaker functions, are investigated in Appendix C. The saddle point method theory is given in Appendix D. In Appendix E a W.K.B. approximation to the Whittaker function has been worked out. Finally in Appendix F two auxiliary functions used in the saddle point method are written down explicitly. The calculations were carried through using methods (i) and (iii) for transitions to the s state, and by (iii) to the d state. In one case only was it possible to compare the two methods, and here good agreement was found. The absolute value of the cross section was computed in each case, and the ratio of the two transitions found at two energies. The results were compared with the experimental results of Riley (1956) and fair agreement found.

CHAPTER I

The Radial Integral

It is shown in Appendix A that for direct radiative capture, the total cross section in terms of the matrix element of the transition is given by

$$\sigma(Lm) = \frac{8\pi(L+1)}{L[(2L+1)!!]^2} \frac{K^{2L+1}}{\hbar v} |Q_{Lm}|^2 \qquad 1.1$$

where L is the angular momentum of the multipole
K is the wave number of the incident radiation
v is the velocity of the incident particle

We have found it convenient to introduce

$$Q^{\dagger}_{Lm} = Q_{Lm} / \sqrt{4\pi(2l+1)} \qquad \text{(Appendix A)}$$

The matrix element $Q^{\dagger}_{Lm}$ can be reduced into a radial part and an angular part

$$Q^{\dagger}_{Lm} = e\,a^L\, I_L (-1)^m (l's'j'm'|Y_L^{-m}|l s j m) \qquad 1.2$$

where

$$I_L = \int R_b \left(\frac{r}{a}\right)^L R_a\, r^2\, dr \qquad 1.3$$

and R_b and R_a are the radial parts of the final and initial state wave-functions ϕ_b and ϕ_a, and "a" is the nuclear radius. The angular part is defined by

$$(-1)^m (l's'j'm'|Y_L^{-m}|l s j m) \equiv \int \Omega_b^* Y_L^{m*} \Omega_a\, d\omega \qquad 1.4$$

Fig 2. Diagram of Functions assuming a square well.

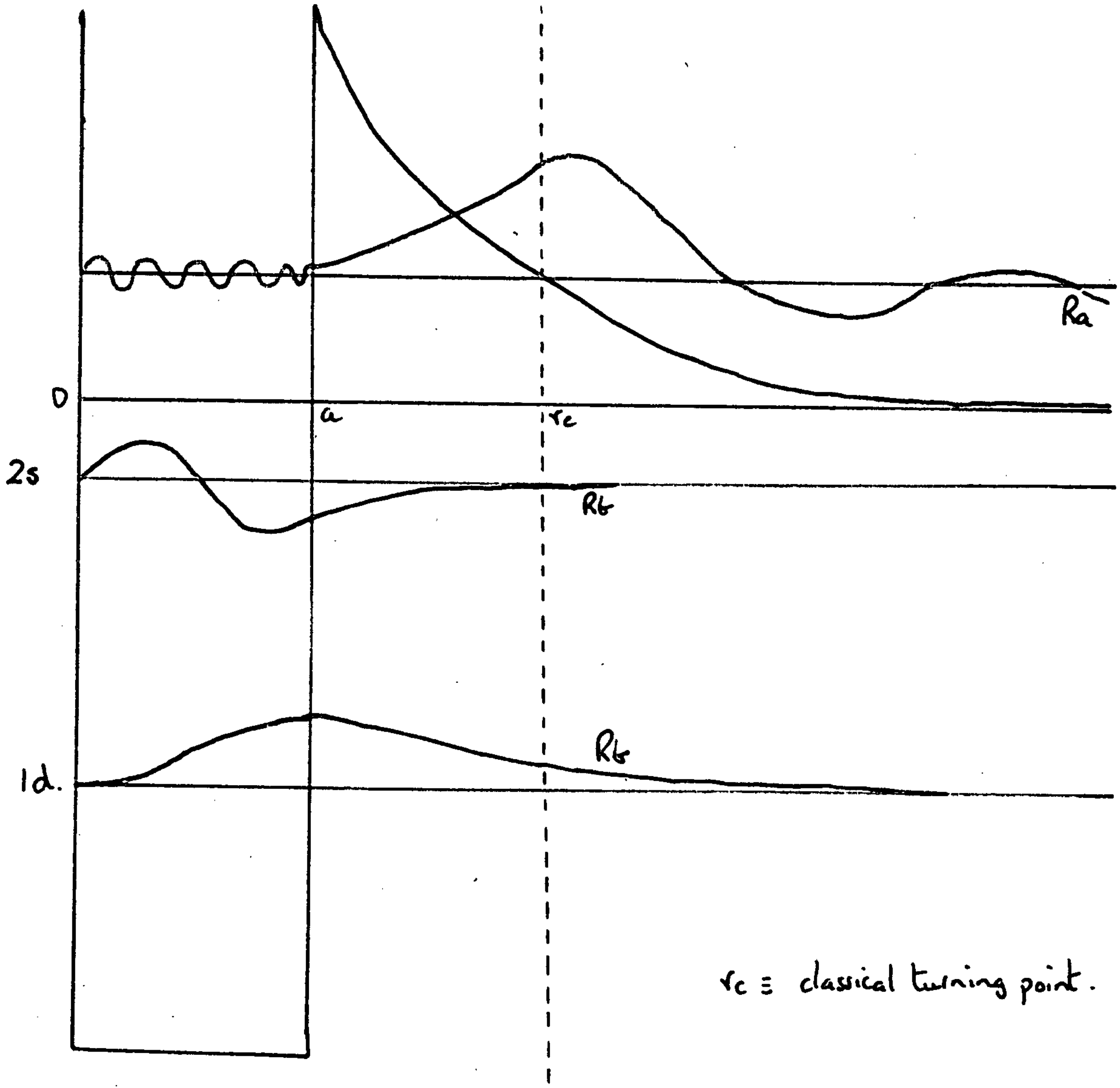
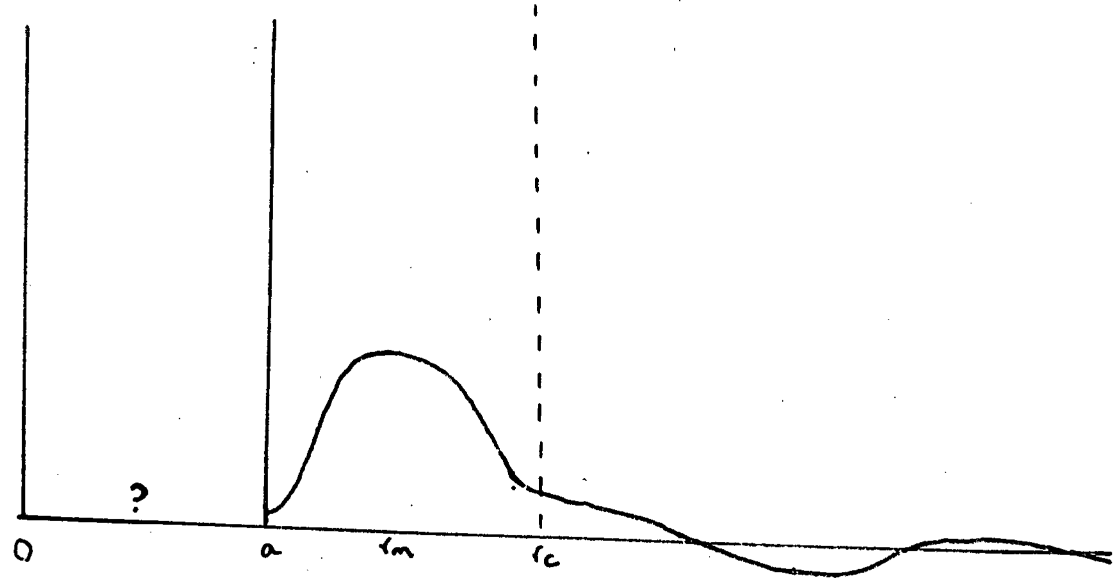


Fig 3. Radial Integrand.



where Ω_b and Ω_a are the spherical harmonics multiplied by spin functions contained in ϕ_b and ϕ_a, and the integration over $d\omega$ in 1.4 implies a scalar product of spins. To obtain the experimental cross section averaging over the initial magnetic quantum numbers m and summation over the radiation and final state quantum numbers M and m', must be performed. This enables us to reduce the angular contribution to a statistical factor $\bar{S}$ which is a number (Appendix B). We find that for a transition from a p state to an s state this factor $\bar{S} = 1$, and to a d state $\bar{S} = 9/5$.

We are left with the problem of evaluating the radial integral. For a dipole transition this is

$$I_I = \int_0^\infty R_b \frac{r}{a} R_a r^2 dr \qquad 1.5$$

The wave-functions outside the nucleus are investigated in Appendix C. For positive energies they are the Coulomb functions $\frac{F(\alpha r)}{\alpha r}$ and $\frac{G(\alpha r)}{\alpha r}$ (Bloch et al 1951), and for negative energies the normalized Whittaker functions $\frac{N\,W(\beta r)}{\beta r}$ where α and β are related to the center of mass energy E of the incident particle, and to the binding energy E_b of the bound states by:

$$\alpha^2 = \frac{2\mu E}{\hbar^2} \qquad \beta^2 = \frac{2\mu E_b}{\hbar^2} \qquad 1.6$$

Hence outside the nucleus

$$R_a = \frac{\mathcal{F}(\alpha r)}{\alpha r} = \frac{\cos\delta\, F(\alpha r) - \sin\delta\, G(\alpha r)}{\alpha r} \qquad 1.7$$

where δ is the nuclear phase shift.

Inside the nuclear surface little is known about the wave-functions. If a square well is assumed the wave-functions are approximately as shown in fig. 2.

The radial integral is then made up of two parts viz.,

$$I_I = \int_0^a R_b \frac{r}{a} R_a r^2 dr + N \int_a^\infty \frac{F(\alpha r)}{\alpha r} \frac{r}{a} \frac{W(\beta r)}{\beta r} r^2 dr \qquad 1.8$$

Not much is known about the first part except that the interior portion of the wave-function R_a is small due to the small penetrability through the Coulomb barrier. In this calculation it was neglected completely. It has been estimated as some 10% of the total at 600 kev (Duck 1959).

A rough estimate of the effect of the nuclear phase shift δ can be obtained by assuming an extreme case, for instance if hard sphere phase shift is assumed

$$\tan \delta = \frac{F(\alpha a)}{G(\alpha a)} \qquad 1.9$$

which at 940 kev and a = 3.6 x 10^{-13} cm becomes tan δ = .003. Hence the contribution to the whole from

$$N \int_a^\infty \frac{W(\beta r)}{\beta r} \frac{G(\alpha r)}{\alpha r} \frac{r}{a} r^2 dr \sin \delta \qquad 1.10$$

is small in spite of the large value of $G(\alpha r)$ at small r . Duck estimated this to be 20% at 600 kev. It was neglected in this calculation.

The integral then reduces to

$$I_I = \frac{N}{\alpha\beta a}\int_a^\infty F(\alpha r)\,W(\beta r)\,r\,dr \equiv \frac{N}{\alpha\beta a}\,d. \qquad 1.11$$

$\cos\delta$ being approximately unity.

CHAPTER II

Methods for Computation of the Radial Integral

Three methods are available:

Method 1: The 'exact' method (using 'exact' tabulated values for both the initial and final state functions).

Since the Coulomb wave-functions are tabulated, and in the case of an s state Whittaker functions may be tabulated for integer and half integer values of the parameter η (see Appendix C), the value of d in 1.11 may be computed numerically by plotting the integrand and either counting squares or using Simpson's rule.

Method 2: W.K.B. and counting squares method

W.K.B. approximations for the positive and negative energy solutions are available (Schiff 1955).

Using the tabulated free particle solutions and a W.K.B. expression for the bound particle solution, (see Appendix E) an integration by counting squares is feasible.

Method 3: W.K.B. and 'steepest descents' method

The wave equation for the free state given by C.7 is

$$\frac{d^2F}{d\rho'^2} + \left[1 - \frac{2\eta_2}{\rho'} - \frac{\ell(\ell+1)}{\rho'^2}\right]F = 0 \qquad 2.1$$

where $\rho' = \alpha r.$

and for the bound state

$$\frac{d^2W}{d\rho^2} - \left[1 + \frac{2\eta_1}{\rho} + \frac{n(n+1)}{\rho^2}\right] W = 0 \qquad 2.2$$

where $\rho = \beta r$.

The W.K.B. approximations to the solutions of 2.1 (suitably normalized by proper choice of C) and 2.2 (normalised to unity at the nuclear surface $r=a$) are:

$$F(\rho') = C\left[\frac{P(\alpha a)}{P(\rho')}\right]^{\frac{1}{2}} e^{\int_a^r P(\rho')\,d\rho'} = C\left[P(\alpha a)\right]^{\frac{1}{2}} e^{\int_a^r P(\rho')\,d\rho' - \frac{1}{2}\ln P(\rho')} \qquad 2.3$$

$$W(\rho) = \left[\frac{Q(\beta a)}{Q(\rho)}\right]^{\frac{1}{2}} e^{-\int_a^r Q(\rho)\,d\rho} = \left[Q(\beta a)\right]^{\frac{1}{2}} e^{-\int_a^r Q(\rho)\,d\rho - \frac{1}{2}\ln Q(\rho)}$$

(see Schiff 1955)

where $P(\rho') = \left[-1 + \frac{2\eta_2}{\rho'} + \frac{l(l+1)}{\rho'^2}\right]^{\frac{1}{2}}$

$$Q(\rho) = \left[1 + \frac{2\eta_1}{\rho} + \frac{n(n+1)}{\rho^2}\right]^{\frac{1}{2}}.$$

If as before

$$d = \int_a^\infty W(\rho)\, r\, F(\rho')\, dr$$

$$\approx \int_0^\infty W(\rho)\, r\, F(\rho')\, dr$$

$$= \int_{-\infty}^\infty W(\beta e^x)\, F(\alpha e^x)\, e^{2x}\, dx \qquad \text{where } r = e^x$$

$$d' = \frac{d}{C\left[Q(\beta a)\, P(\alpha a)\right]^{\frac{1}{2}}} = \int_{-\infty}^\infty e^{-\psi(x)}\, dx$$

where $\psi(x) = \int^{x} Q\alpha e^{x}dx + \frac{1}{2}\ln Q + \frac{1}{2}\ln P - \int^{x} P\beta e^{x}dx - 2x$

This form of $\psi(x)$ is due to Christy and Duck (1959).

Then by the method of steepest descents (D.10)

$$d' = \sqrt{\frac{2\pi}{\gamma_m}}\, e^{-\psi(x_m)}$$

where x_m is determined from the condition that the exponent be a minimum ie $\frac{d\psi}{dx} = 0$ at $x = x_m$ (this equation must be solved numerically), and $\gamma_m = \left|\frac{d^2\psi}{dx^2}\right|_{x_m}$ is evaluated at $x = x_m$.

Hence substituting back

$$d = \sqrt{\frac{2\pi}{\gamma_m}}\, W(\beta r_m)\, F(\alpha r_m)\, r_m^2$$

$F(\alpha r_m)$ may be evaluated from the tables and for $W(\beta r_m)$ the W.K.B. expression (Appendix E) is used.

The expressions for $\frac{d^2\psi}{dx^2}$ and $\frac{d\psi}{dx}$ are worked out in Appendix F.

Normalisation of the Whittaker Function:

We are now left with the problem of normalising the Whittaker Function. Various methods are available. We could assume a square well and integrate over all space. We could use experimentally obtained reduced widths if they were available. In this thesis the following procedure was adopted, which though crude is simple and fairly accurate.

The Whittaker functions were tabulated normalised to unity at the nuclear surface. Normalised to unity over all space they then become

$$\frac{N\,W(\rho)}{\rho} = \frac{N\,W(\beta r)}{\beta r} \qquad \text{where } W(\rho_0) = W(\beta a) = 1$$

We then assume that the internal wave-function is constant and equal to its value at the nuclear surface, and also that most of the contribution comes from the interior of the nucleus.

Hence $$\frac{N^2\,[W(\rho_0)]^2}{\beta^2 a^2}\,\frac{4\pi}{3}\,a^3 \sim 1.$$

i.e. $$N^2 = \frac{3\beta^2}{4\pi a}$$

Limitations of Methods of Calculation:

The W.K.B. approximation for the free particle fails at the classical turning point r_c, since in (2.3) $P(\rho') = 0$ at that point. The radial integrand is $W(\beta r)\,r\,F(\alpha r)$ an exponentially decaying function, a linear one, and an exponentially increasing one (for $r < r_c$). The overlap integrand then takes the form of a hump as suggested in Fig. 3 if the W.K.B. approximation holds good. In method 3 to this hump we then fit a Gaussian curve. However, if the actual saddle point of the hump is near the classical turning point, the free state wave-function may have already ballooned up, and in this approximation the integrand may not have a saddle point but always increase. The method then fails. At low energies both the saddle point and the classical turning point r_c are some way from the nuclear radius and $r_c > r_m$ as suggested in Fig. 3. However, as the energy increases, the saddle point moves in, and the classical turning point also moves in at an even greater rate, so that eventually $r_c \approx r_m$. Hence there is an energetic upper limit above which the method fails. In the O^{16} nucleus this was 200 kev for the s state, and 550 kev for the d state.

Our neglect of the contribution from the interior of the nucleus will become less and less justified as $r_m \to a$. However, at the highest value of E = 940 kev $r_m \approx 5a$.

The contributions from successive humps of the Radial Integral

The radial integrand in Fig. 3 consists of a series of humps alternatively positive and negative becoming progressively smaller as the bound state decays. In method 3 only the first hump is considered. An estimate was made of the contributions of successive humps at 378 kev for transitions to the s state.

The free state wave-function is only tabulated out to $\rho' = 6$. For larger values of ρ' the asymptotic form was used

$$F_1 = \sin(\rho - 1.995 \ln 2\rho - .3387)$$

This function had been tabulated to large ρ by Dr. G. Griffiths. The Whittaker functions were found using the W.K.B. expression

(Appendix E), and interpolation. The integrand was then plotted.

The areas under the successive humps were found to be in the following ratio

$$\frac{3\text{ hump}}{2\text{ hump}} = 6.3\ 10^{-2}$$

$$\frac{2\text{ hump}}{1\text{ hump}} = 3.8\ 10^{-2}$$

Consequently only the first hump need be considered in the calculation.

CHAPTER III

Calculations

Evaluation of the radial integral

s state ('exact' method)

Here the Whittaker functions were tabulated using C42 from Appendix C and the experimentally determined energy level. The value E_b = .094 Mev was adopted for the binding energy. This was supplied by Dr. G. Griffiths on the basis of experimental data more recent than Fig. 1.

The bound state parameter η_1 was found to be 4.006, and thus taken, for purposes of calculation, to be 4.

The unnormalised value of $W(\rho)$ is given by

$$W(\rho) = \frac{e^{\rho}}{2}\left\{E_2(2\rho) - 3E_3(2\rho) + 3E_4(2\rho) - E_5(2\rho)\right\} \tag{3.1}$$

The radial integral $d = \int_0^{\infty} F(\rho') W(\rho)\, r\, dr$ was then evaluated using the method of counting squares for three values of the incident proton energy - 150 kev, 378 kev and 940 kev. (These values were chosen so as to give tabulated values of the Coulomb function). The W.K.B. method was found to fail at energies higher than 200 kev, however a value was obtained at 150 kev for comparison of the W.K.B. method with the more exact method using Whittaker functions.

d state

Here the Whittaker functions were not available and the W.K.B. method was used at 150 kev, 378 kev and 500 kev, the latter energy being the highest at which the method was found to work.

The results for d are collected in Table 1.

Table 1

Values of the Reduced Radial Integral d (sq. cm.)

Energy (c of m) kev.	s state 'exact'	s state W.K.B.	d state W.K.B.
150	$2.0 \; 10^{-27}$	$2.4 \; 10^{-27}$	$1.5 \; 10^{-28}$
378	$3.5 \; 10^{-26}$	-	$3.0 \; 10^{-27}$
500	-	-	$9.4 \; 10^{-27}$
940	$7.3 \; 10^{-26}$	-	-

The values of d/a for the d state are 2.03, 2.61, 2.82, and for the s state 4.25. The value of a was taken as $(16)^{\frac{1}{3}} \times 1.45 \; 10^{-13} = 3.65 \; 10^{-13}$ cm.

Agreement between the two methods in the one case where comparison was possible (s state, 150 kev) was fairly good.

Now the cross section for dipole radiation is given by B17

$$\sigma = \left(\frac{16\pi}{3} \frac{K_\gamma{}^3}{\alpha} \frac{e^2}{\hbar^2} \frac{16M}{17} \right) N^2 \frac{d^2}{\beta^2 \alpha^2} \bar{S} \qquad 3.2$$

where d is defined by 1.11.

The values of k_γ were obtained from

$$\hbar c k_\gamma = E + E_b$$

where E is the incident proton energy (c of m), and E_b is the binding energy.

Substituting into 3.2 we obtained the following cross sections.

Table 2

Cross Section (sq. cms.)

Energy kev	s state (exact)	d state (W.K.B.)	σ_s/σ_d.
150	4.5 10^{-35}	5.0 10^{-36}	9.0
378	2.3 10^{-32}	2.6 10^{-34}	8.8
500	-	2.4 10^{-32}	-
940	2.9 10^{-31}	-	-

Most of the variation could be taken out of these figures by calculating S where $\sigma = S\,E^{-1} \exp(-2\pi\eta)$ (Blatt and Weisskopf 1952). Table 3 contains these S values.

Table 3

S kev (sq. cms.kev)

Energy kev	s state	d state
150	2.7 10^{-24}	1.4 10^{-25}
378	2.5 10^{-24}	1.6 10^{-25}
500	-	3.1 10^{-25}
940	7.4 10^{-25}	-

CHAPTER IV

Comparison with Experiment

The experimental results from the thesis of Peter Riley (U.B.C. 1956) were reduced to total cross sectional form. As he tabulated them as cross sections at ninety degrees, there was a multiplicative factor in each case, necessary for conversion.

The angular distributions are for transitions from p states to s and d states respectively (Blatt and Weisskopf 1952, particular case of B.W. 3.16).

$$\sin^2\theta \qquad \text{and} \qquad \left(1 + \tfrac{1}{6}\sin^2\theta\right)$$

If the latter is taken to be isotropic, the multiplicative factors are

$$\int_0^{\pi}\int_0^{2\pi} \sin^2\theta \sin\theta \, d\theta \, d\phi = \frac{8\pi}{3}$$

and

$$\int_0^{\pi}\int_0^{2\pi} \sin\theta \, d\theta \, d\phi = 4\pi$$

Riley's results then became

Table 4

Cross Sections (sq.cms.)

E (c of m)	s state ($\sin^2\theta$)	d state (isotropic)	σ_s/σ_d
583	$3.45\ 10^{-31}$	-	-
793	$8.71\ 10^{-31}$	$2.69\ 10^{-31}$	3.2
1110	$24.8\ 10^{-31}$	$8.06\ 10^{-31}$	3.1

Table 5

S (kev sq.cms.)

E (c of m) in kev.	s state	d state
583	4.2 10^{-24}	-
793	4.0 10^{-24}	1.2 10^{-24}
1110	1.8 10^{-24}	6.1 10^{-25}

Conclusion

The only energies in Table 3 which lie close to the experimental values of the energy in Table 5 are 940 kev for the s state and 500 kev for the d state. The S values corresponding to these energies in the two tables are of the same order of magnitude.

The calculated value of $\frac{\sigma_s}{\sigma_d} \approx 9$ agrees with the value of ≈ 10 at higher energies reported by Ajzenberg and Lauritsen (1955), and is not too far off Riley's value of ≈ 3 in Table 4.

Over the energy range investigated our calculated values of S remain fairly constant in agreement with the results of Christy and Duck reported by Tanner. However, our values of S for transitions to the s state are lower than those of Christy and Duck by about a factor 2. The reason for this discrepancy could not be ascertained as the details of their calculation are unavailable to us.

APPENDIX A

Determination of the Cross Section in Terms of the Matrix Element of the Transition

The derivation given below is a somewhat expanded version of the one given by Blatt and Weisskopf (1952).

The Maxwell Equations for a periodically varying field with a source containing a distribution of currents $\underline{j}(\underline{r})$ and charge $\rho(\underline{r})$ and magnetisation $\underline{M}(\underline{r})$ are

$$c\,\nabla\times\underline{H} = -i\omega\underline{E} + 4\pi\underline{j} \qquad \text{A.1}$$

$$c\,\nabla\times\underline{E} = i\omega(\underline{H} + 4\pi\underline{M}) \qquad \text{A.2}$$

$$\operatorname{div}\underline{j} = i\omega\rho \qquad \text{A.3}$$

for $$\underline{E}(\underline{r},t) = \underline{E}(\underline{r})e^{-i\omega t} + \underline{E}^{*}(\underline{r})e^{i\omega t} \qquad \text{A.4}$$

and a similar expression for $\underline{H}(\underline{r},t)$

Eliminating $\underline{E}$ and $\underline{H}$ in turn and putting $K = \frac{\omega}{c}$ A.5

$$\nabla\times(\nabla\times\underline{H}) - K^2\underline{H} = \frac{4\pi}{c}(\nabla\times\underline{j} + cK^2\underline{M}) \qquad \text{A.6}$$

$$\nabla\times(\nabla\times\underline{E}) - K^2\underline{E} = \frac{4\pi iK}{c}(\underline{j} + c\nabla\times\underline{M}) \qquad \text{A.7}$$

The solutions of the corresponding sourceless equations are, for electric multipoles

$$\underline{H} = r^{-1} f_e(lm;r)\, \underline{X}_{lm}(\theta\phi) \qquad \text{A.8}$$

where $\underset{\sim}{X}_{lm}(\theta\phi)$ is a vector spherical harmonic (defined in Blatt and Weisskopf 1952, Appendix B),

and $f_e(lm;r)$ satisfies

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right] f(lm;r) = 0 \qquad \text{A.9}$$

We set

$$\underline{H}(\underline{r}) = a_e(lm)\, \underline{H}_e(lm;\underline{r}) \qquad \text{A.10}$$

where $$\underline{H}_e(lm;r) = \frac{u_e^+(r)}{\kappa r}\, \underline{X}_{lm}(\theta\phi) \qquad \text{A.11}$$

the function $u^+(r)$ is that solution of (A.9) which for large r behaves like

$$u_e^+(r) \approx \exp i(\kappa r - \tfrac{1}{2} l\pi) \qquad \text{A.12}$$

and $a_e(lm)$ is a normalising constant to be determined later.

Similarly $\underline{E}(\underline{r}) = a_e(lm)\, \underline{E}_e(lm;r)$ A.13

$$\underline{E}_e(lm;r) = \frac{i}{\kappa} \nabla \times \underline{H}_e(lm;\underline{r}) \qquad \text{A.14}$$

Substituting A,8 into A.6, taking the scalar product with $\underline{X}^*_{lm}(\theta\phi)$, and integrating over all angles, we obtain

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - k^2\right] f_l(lm;r) = K_l(lm;r) \qquad \text{A.15}$$

$$K_l(lm;r) = \frac{4\pi r}{c} \int \left[\underline{X}^*_{lm}(\theta\phi)\right] . \left[\nabla \times \underline{j} + c k^2 \underline{M}\right] d\Omega \qquad \text{A.16}$$

A similar equation is obtained for magnetic multipoles.

The Green's function for A.15 leading to outgoing radiation is

$$G_T(rr') = k^{-1} F_l(r_<) u_l^+(r_>) \qquad \text{A.17}$$

where $r_<$ denotes the smaller of r and r' and $r_>$ the larger, while $\frac{F_l}{r}$ is the solution of A.9 which is regular at the origin and for large r behaves like $\sin(kr - \frac{1}{2}l\pi)$. Outside the source $r' < r$ hence we may put $r_< = r'$ and $r_> = r$ giving for the solution of A.15 outside the source

$$f_l(lm;r) = k^{-1}\left[\int_0^\infty F_l(r') K_l(r') dr'\right] u_l^+(r) \qquad \text{A.18}$$

Comparison of A.18, A.8 and A.11 yields the normalisation constant

$$a_l(lm) = \int_0^\infty F_l(r) K_l(r) dr = \frac{4\pi}{c}\int r^{-1} F_l(r) X^*_{lm} . (\nabla \times j + c k^2 M) dV \qquad \text{A.19}$$

the integral extending over the source volume.

We now assume the wave length of the radiation is large compared to the dimensions of the source, i.e. $Kr \ll 1$ for all r which contribute to the integral. We can then replace $F_l(r)$ by its asymptotic form for small r

$$\frac{(Kr)^{l+1}}{(2l+1)!!} \qquad \text{A.20}$$

and using the identity $\underline{X}_{JM}(\theta\phi) = \underline{L} \cdot \frac{Y_{JM}(\theta\phi)}{\sqrt{J(J+1)}}$

$$\underline{L} = -i\underline{r} \times \nabla \qquad \text{A.21}$$

where Y_{JM} is a scalar spherical harmonic, we have the approximate form

$$a_e(lm) \approx \frac{4\pi}{c} \frac{K^{l+1}}{(2l+1)!!\sqrt{l(l+1)}} \int r^l Y_{lm}^*(\theta\phi) \left(\underline{L} \cdot \nabla \times \underline{j} + cK^2 \underline{L} \cdot \underline{M}\right) dV \qquad \text{A.22}$$

Using the vector identities

$$\underline{L} \cdot \nabla \times \underline{j} = -i\left[(\underline{r} \cdot \nabla + 2)(\nabla \cdot \underline{j}) - \nabla^2(\underline{r} \cdot \underline{j})\right] \qquad \text{A.23}$$

$$\underline{L} \cdot \underline{M} = i\nabla \cdot (\underline{r} \times \underline{M}) \qquad \text{A.24}$$

and A.3 the integral in A.22 becomes

$$\int r^l Y_{lm}^*(\theta\phi)\left[\omega(r \cdot \nabla)\rho + 2\omega\rho + i\nabla^2(r \cdot j) + icK^2 \nabla \cdot (r \times M)\right] dV \qquad \text{A.25}$$

Now

$$\int r^l r \frac{d}{dr} \rho r^2 dr = \left[r^{l+3}\rho\right] - \int (l+3) r^{l+2} \rho dr \qquad \text{A.26}$$

and

$$\int r^l \nabla^2 (\underline{r} \cdot \underline{j})\, dV = 0 \qquad \text{A.27}$$

$$\therefore a_e(lm) = -\frac{4\pi}{(2l+1)!!} \left(\frac{l+1}{l}\right)^{\frac{1}{2}} k^{l+2} \left(Q_{lm} + Q'_{lm} \right) \qquad \text{A.28}$$

$$Q_{lm} = \int r^l Y_{lm}^{*}(\theta, \phi)\, \rho(\underline{r})\, dV \qquad \text{A.29}$$

$$Q'_{lm} = \frac{-ik}{(l+1)} \int r^l Y_{lm}^{*}(\theta, \phi)\, \mathrm{div}(\underline{r} \times \underline{M})\, dV \qquad \text{A.30}$$

with an analogous solution for the magnetic radiation.
Replacing the operator div by $\frac{1}{a}$ to obtain an estimate of the relative sizes of Q and Q' where a is the nuclear radius $a \sim \frac{\hbar}{Mv}$

$$\frac{Q'_{lm}}{Q_{lm}} \sim \frac{k\hbar}{Mc} = \frac{\hbar\omega}{Mc^2} \sim 10^{-3}$$

for transition of a few Mev. We thus neglect Q'_{lm} in comparison with Q_{lm}.

To change to quantum mechanics we replace in A.29

$$\rho(ab, r) \quad \text{by} \quad e\, \phi_b^{*}(\underline{r})\, \phi_a(\underline{r}) \qquad \text{A.31}$$

where a and b refer to the initial and final states, obtaining

$$Q_{lm}(ab) = e \int r^l Y_{lm}^{*}(\theta\phi)\, \phi_b^{*}(r) . \phi_a(r)\, d\tau . \qquad \text{A.32}$$

In A.31 and A.32 the final bound state ϕ_b is normalised to unity over all space, while the normalisation of the initial state ϕ_a in the continuum is discussed later.

The energy emitted is determined by the Poynting vector $\underline{S}$.

Far from the source $\underline{E}$ and $\underline{H}$ are perpendicular, so that

$$|\underline{S}|_{av} = \frac{c}{4\pi} \underline{E}^2_{av} \simeq \frac{c}{4\pi} \underline{H}^2_{av} \qquad \text{A.33}$$

where

$$E^2_{av}(r,t) = 2\underline{E}^*(r) \cdot \underline{E}(r) \qquad \text{A.34}$$

Using A.11 we get for the energy emitted per second per unit solid angle

$$U_e(lm;\Omega) = \frac{c}{2\pi K^2} Z_{lm}(\theta\phi) \, |a_e(lm)|^2 \qquad \text{A.35}$$

where $\qquad Z_{lm}(\theta\phi) = \underline{X}^*_{lm} \cdot \underline{X}_{lm}$

For example, in the case of dipole radiation with $m=0$

$$Z_{10}(\theta,\phi) = \frac{3}{8\pi} \sin^2\theta$$

Integrating over the full solid angle

$$\int Z_{lm}(\theta\phi)d\Omega = 1$$

The total energy emitted per second is then

$$U_e(lm) = \frac{c}{2\pi K^2} |a_e(lm)|^2 \qquad \text{A.36}$$

Here we see that the total number of quanta emitted per second, which equals the rate of emission of energy divided by $\hbar\omega$, is given by

$$T_e(lm) = \frac{8\pi(l+1)}{l[(2l+1)!!]^2} \frac{K^{2l+1}}{\hbar} |Q_{lm}|^2 \qquad \text{A.37}$$

This is related to the cross section $\sigma^{e}_{cap}(lm)$ by

$$\sigma^{e}_{cap}(lm) = \frac{T_e(lm)}{Flux} \qquad A.38$$

Therefore if the wave-function for the incident particle used to evaluate Q_{lm} in $T_e(lm)$ in A.37 is normalised to unit flux then

$$\sigma^{e}_{cap} = T_e(lm) \qquad A.39$$

In the case of incident plane waves or of plane waves modified by a Coulomb field, which will be discussed later, the wave-function normalised to unit incident flux is obtained by multiplying the wave-function normalised to unit incident amplitude, by the factor $\frac{1}{\sqrt{v}}$ where v is the velocity of the particle. Therefore the final form of A.39 is

$$\sigma^{e}_{cap}(lm) = \frac{8\pi(l+1)}{l\left[(2l+1)!!\right]^2}\frac{K^{2l+1}}{\hbar v}|Q_{lm}|^2 \qquad A.40$$

where the free wave-function is normalised to unit incident amplitude, and the bound wave function is normalised to unity over all space. This well known formula appears in this notation for example in Blatt and Weisskopf (1952). To transfer to notation used by Kennedy and Sharp (1954), and in the body of this text, we replace $l \rightarrow L$ and $m \rightarrow M$.

In A.32 the angular part of the final bound state ϕ_b is a spherical harmonic. The initial state ϕ_a consists of a space wave-function which should be taken as a positive energy solution for a particle in a Coulomb field modified by a nuclear potential at the origin. As discussed in the main text the effects of the nuclear potential are neglected in this thesis, and the space part of $\tilde{\phi}_\alpha$ is taken to be the Coulomb wave-function regular at the origin. This may be written as the sum of an incident and a scattered wave of the form

$$I + S f(\theta) \tag{A.41}$$

where the asymptotic formsof I and S may be found, for example in Mott and Massey (1949) for the case of I normalised to unit amplitude. There also Gordon's expression for the expansion of the space part of ϕ_α so normalised, into partial waves, is recorded. This is

$$\Phi_\alpha = \sum_{l=0}^{\infty} (2l+1)\, i^l\, e^{i\delta_l}\, \frac{F_{l\eta}(kr)}{kr}\, P_l(\cos\theta). \tag{A.42}$$

where $F_{l\eta}(kr)$ is defined by C30 and δ_l by C32 .
If $\phi_\alpha = \Phi_\alpha \chi$ where χ is the appropriate spin function, is substituted into A.32 in which the replacement $l \to L$ and $m \to M$ has been made, the integral Q_{lm} reduces to a sum of integrals each involving one of the partial waves from A.42.

Due to angular momentum selection rules (properties of integrals of three spherical harmonics), all but a small number of these integrals vanish, and of these the one with the smallest value of l is dominant (see form of A20). We can then conveniently replace Q_{LM} by $\sqrt{4\pi(2l+1)}\, Q^{\dagger}_{LM}$, where $Q^{\dagger}_{LM}$ has the form of A.32, but $\phi_a(r)$ is replaced by $\phi_{al}(r)$, where

$$\phi_{al}(r) \equiv \chi_c\, i^{l}\, e^{i\delta_l}\, \frac{F_{l\eta}(kr)}{Kr}\, Y_{l0}(\theta) \qquad \text{A.43}$$

In the above l has the lowest value consistent with the angular momentum selection rules and χ is an appropriate spin function. In terms of $Q^{\dagger}_{LM}$ the cross section is given by

$$\sigma^{e}_{cap}(LM) = \frac{32\pi^2 (L+1)(2l+1)}{L[(2L+1)!!]^2}\, \frac{K^{2L+1}}{\hbar v}\, |Q^{\dagger}_{LM}|^2 \qquad \text{A.44}$$

In the case of electric dipole transitions (L = 1) to an s or d state from a continuum p state $l=1$ this reduces to

$$\sigma^{e}_{cap}(1M) = \frac{64\pi^2}{3}\, \frac{K^3}{\hbar v}\, |Q^{\dagger}_{1M}|^2 \qquad \text{A.45}$$

APPENDIX B

Reduction of Matrix Element. (See Kennedy and Sharp 1956)

For a single particle transition

$$Q^{\dagger}_{LM} = e \int \phi^*_{b}(r)\, \phi_{al}(r)\, r^L\, Y^*_{LM}(\theta\phi)\, d\tau \qquad \text{B.1}$$

If we define the radial integral by

$$I_L = \int R_b \left(\frac{r}{a}\right)^L R_a\, r^2 dr \qquad \text{B.2}$$

where R_b and R_a are the radial parts of ϕ_b and ϕ_{al} and if the initial and final states are denoted by $l s j m$ $l' s' j' m'$

$$Q^{\dagger}_{LM} = e\, a^L I_L (-1)^M \left(l' s' j' m' \,|\, Y_L^{-M} \,|\, l s j m\right) \qquad \text{B.3}$$

$$= e a^L I_L (-1)^M \frac{(L j -M m | j' m')}{(2j'+1)^{\frac{1}{2}}} \left(l' s' j' \| Y_L \| l s j\right) \qquad \text{B.4}$$

$$= e a^L I_L (-1)^{M+L+s-j-l'} (L j -M m | j' m') (2j+1)^{\frac{1}{2}} (2j'+1)^{\frac{1}{2}} \times W(l j\, l' j', s L)\, (l' \| Y_L \| l) \qquad \text{B.5}$$

$$= e a^L I_L (-1)^{M+L+s-j-l'} \frac{(L j -M m | j' m')}{(2j'+1)^{\frac{1}{2}}} \left[\frac{(2j+1)^{\frac{1}{2}} (2j'+1)^{\frac{1}{2}} (2l+1)^{\frac{1}{2}} (2l'+1)^{\frac{1}{2}}}{\sqrt{4\pi}}\right] \qquad \text{B.6}$$

$$\times W(l j\, l' j', s L)\, (l l' 0 0 | L 0)$$

Using Clebsh-Gordan coefficients, the Wigner-Eckart Theorem and the Racah coefficients (see Wigner 1959) setting $s=\frac{1}{2}$, and introducing the Z^{0} coefficient

$$Z^{0}(l_j l'_{j'}, sL) = \left[(2j+1)(2j'+1)(2l+1)(2l'+1)\right]^{\frac{1}{2}} W(l_j l'_{j'}, sL)\,(ll'00|L0) \qquad \text{B.7}$$

we get

$$Q^{+}_{LM} = e a^{L} I_L (-1)^{m-j+\frac{1}{2}} \frac{(Lj-Mm|j'm')}{(4\pi)^{\frac{1}{2}}(2j'+1)^{\frac{1}{2}}} Z^{0}(l_j l'_{j'}\tfrac{1}{2}L) \qquad \text{B.8}$$

Now
$$\sum_{mMm'} \frac{(Lj-Mm|j'm')^{2}}{2j'+1} = 1 \qquad \text{B.9}$$

hence
$$\sigma^{l}(L) = \frac{8\pi(L+1)(2l+1)}{L[(2L+1)!!]^{2}} (ka)^{2L} \frac{ke^{2}}{\hbar v} I_L^{2} \frac{Z^{0\,2}(l l'_{j'}\tfrac{1}{2}L)}{2j+1} \qquad \text{B.10}$$

is the value of $\sigma^{l}_{cap}(LM)$ from A.44 averaged over the magnetic substates of the initial state and summed over the magnetic substates of the radiation field and the final state.

Now the Racah coefficients are defined by (Racah 1942)

$$W(abcd;ef) = \left[\frac{(a+b-e)!\,(a+e-b)!\,(c+d-e)!\,(b+e-a)!\,(d+e-c)!\,(c+e-d)!\,(a+c-f)! \times (a+f-c)!\,(c+f-a)!\,(b+d-f)!\,(b+f-d)!\,(d+f-b)!}{(a+b+e+1)!\,(c+d+e+1)!\,(a+c+f+1)!\,(b+d+f+1)!}\right]^{\frac{1}{2}} \times \omega(abcd;e \qquad \text{B.11}$$

$$w(abcd;ef) = \sum_z (-1)^z \frac{(a+b+c+d+1-z)!}{(a+b-e-z)!\,(c+d-e-z)!\,(a+c-f-z)!\,(b+d-f-z)!\,z!\,(e+f-a-d+z)!\,(e+f-b-c+z)!} \qquad \text{B.12}$$

For transition from a p state to an s state

$l = 1 \quad j = \frac{3}{2} \qquad l' = 0 \quad j' = \frac{1}{2}.$

$$Z(1\tfrac{3}{2}0\tfrac{1}{2},\tfrac{1}{2}1) = 24^{\frac{1}{2}} W(1\tfrac{3}{2}0\tfrac{1}{2},\tfrac{1}{2}1)(1000|10)$$
$$= 2 \qquad \text{B.13}$$

and $\dfrac{Z^2}{2j+1} = 1$ B.14

and to a d state

$l = 1 \quad j = \frac{3}{2} \qquad l' = 2 \quad j' = \frac{5}{2}$

$$Z(1\tfrac{3}{2}2\tfrac{5}{2},\tfrac{1}{2}1) = 360^{\frac{1}{2}} W(1\tfrac{3}{2}2\tfrac{5}{2};\tfrac{1}{2}1)(1200|10)$$
$$= \frac{6}{\sqrt{5}} \qquad \text{B.15}$$

$$\therefore \frac{Z^2}{2j+1} = \frac{9}{5} \qquad \text{B.16}$$

A table of these statistical factors may be found in the article by Moszkowski in 'Beta- and Gamma-Ray Spectroscopy' edited by

Kai Siegbahn. Alternatively they may be calculated by integrating the respective spherical harmonics correctly normalised.

The general formula B.10 in the case of electric dipole transitions (L = 1) from an incident p state ($l = 1$) to a final s or d state reduces to

$$\sigma = \frac{16\pi}{3} (R_a)^2 \frac{e^2}{\hbar v} K I^2 \bar{S} \qquad \text{B.17}$$

where $\bar{I}_s$ and $\bar{I}_d$ are given by B.2 with L = 1, R_b is chosen to correspond to an s or a d state, $R_a = \frac{F_{0\eta}(kr)}{kr}$ as defined by C.30, and the statistical factor has the values $\bar{S}_s = 1$, $\bar{S}_d = \frac{9}{5}$.

APPENDIX C

Coulomb Wave Functions

The wave equation for the relative motion of a pair of particles interacting only by a Coulomb field is

$$\frac{\hbar^2}{2\mu}\nabla^2\psi + \left(E - \frac{ZZ'e^2}{r}\right)\psi = 0 \qquad \text{C.1}$$

μ is the reduced mass of the pair, E is their relative energy, Ze and $Z'e$ are the charges on the pair, and r is their separation distance.

The radial dependence is given by

$$\frac{\hbar^2}{2\mu}\frac{d^2(r\psi_\ell)}{dr^2} + \left(E - \frac{ZZ'e^2}{r} - \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}\right)(r\psi_\ell) = 0 \qquad \text{C.2}$$

where ℓ is the relative angular momentum quantum number, (see Blatt and Weisskopf 1952).

Define $$W_\ell(r) = r\psi_\ell \qquad \text{C.3}$$

$$K^2 = \pm\frac{2\mu E}{\hbar^2} \qquad \text{C.4}$$

$$\rho = Kr \qquad \text{C.5}$$

$$\eta = \frac{ZZ'e^2\mu}{\hbar^2 K} \qquad \text{C.6}$$

The $\pm$ sign in K^2 includes both positive and negative energy solutions, respectively.

We then obtain

$$\frac{d^2 F_{l\eta}(\rho)}{d\rho^2} + \left(\pm 1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2} \right) F_{l\eta}(\rho) = 0 \qquad \text{C.7}$$

The solutions of C.7 with the positive sign regular at the origin will be denoted by $F_{l\eta}$ and irregular ones by $G_{l\eta}$, while the solution of C.7 with the negative sign regular at infinity will be denoted by $W_{l\eta}$.

Now consider the Confluent Hypergeometric Series

$$M_{k m} = z^{m+\frac{1}{2}} e^{-\frac{1}{2}z} \, {}_1F_1 \left(\tfrac{1}{2}+m-k ; 2m+1 ; z \right) \qquad \text{C.8}$$

where $${}_1F_1(a b z) = 1 + \frac{a}{b \cdot 1} z + \frac{a(a+1)}{b(b+1)} z^2 + \cdots \qquad \text{C.9}$$

which is a solution of

$$z \frac{d^2 y}{dz^2} + (b - z) \frac{dy}{dz} - a y = 0 \qquad \text{C.10}$$

as can be verified by direct substitution.

To find an asymptotic expression we write the identity

$$\frac{1}{m!} = \frac{1}{2\pi i} \int_\gamma e^t \, t^{-m-1} \, dt \qquad \text{C.11}$$

and $$F(a b ; z) = (b-1)! \sum_{n=0}^{\infty} c_n \frac{z^n}{(b+n-1)!} \qquad \text{C.12}$$

where c_n is the coefficient of x^n in the expansion of $(1-x)^{-a}$

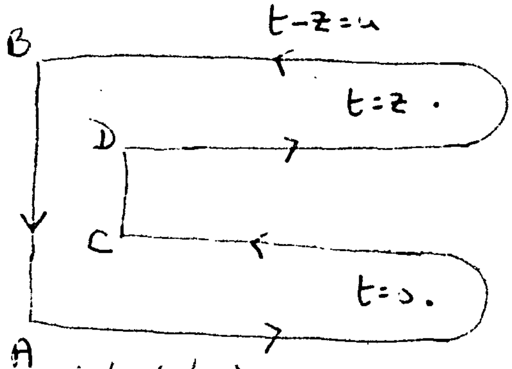
if $m = b+n-1$

$$F(a b ; z) = \frac{(b-1)!}{2\pi i} \sum_{n=0}^{\infty} c_n z^n \int_\gamma e^t \, t^{-b-n} \, dt \qquad \text{C.13}$$

Now choose the path γ s.t. $\frac{z}{t} < 1$.

Then $$F(ab;z) = \frac{(b-1)!}{2\pi i}\int_{\gamma}\left(1-\frac{z}{t}\right)^{-a} e^{t}\, t^{-b}\,dt \qquad \text{C.14}$$

To find asymptotic solution deform the path as shown, and let the portions of the path AB and CD tend to an infinite distance from the imaginary axis.



Then $$F(abz) = W_1(abz) + W_2(abz) \qquad \text{C.15}$$

where $$W_1(abz) = \frac{(b-1)!}{2\pi i}\int_{\gamma_1}\left(1-\frac{z}{t}\right)^{-a} e^{t}\, t^{-b}\,dt \qquad \text{C.16}$$

and putting $t - z = u$

$$W_2(abz) = \frac{(b-1)!}{2\pi i}\int_{\gamma_1} u^{-a}\, e^{u+z}\,\frac{du}{(u+z)^{-a+b}} \qquad \text{C.17}$$

$$W_1(abz) = \frac{(b-1)!}{2\pi i}\int_{\gamma_1}\left(1-\frac{t}{z}\right)^{-a} e^{t}\, t^{a-b}\,dt \qquad \text{C.18}$$

$$W_2(abz) = \frac{(b-1)!}{2\pi i}(z)^{a-b} e^{z}\int_{\gamma_1}\left(1+\frac{t}{z}\right)^{a-b} e^{t}\, t^{-a}\,dt \qquad \text{C.19}$$

But $$\frac{1}{\Gamma(x)} = \frac{1}{2\pi i}\int_{\gamma_1} e^{t}\, t^{-x}\,dt \qquad \text{C.20}$$

Hence $$W_1 = \frac{\Gamma(b)}{\Gamma(b-a)} (-z)^{-a} G(a, a-b+1, -z) \qquad \text{C.21}$$

$$W_2 = \frac{\Gamma(b)}{\Gamma(a)} e^{z} z^{a-b} G(1-a, b-a, z) \qquad \text{C.22}$$

where $$G(\alpha \beta z) = 1 + \frac{\alpha\beta}{z\,1!} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{z^2\,2!} + \cdots \qquad \text{C.23}$$

$\rightarrow 1$ for large z.

<u>Positive energy solutions</u>

Taking the $+$ sign in C.4

and substituting

$$\mathcal{F}_{l\eta} = C_l \rho^{l+1} e^{i\rho} \Phi_{l\eta} \quad \text{in C7} \qquad \text{C.24}$$

where C_l is a normalisation constant

we obtain

$$\rho \frac{d^2 \Phi_{l\eta}}{d\rho^2} + 2(l+1+i\rho)\frac{d\Phi_{l\eta}}{d\rho} + 2\{(l+1)i - \eta\}\Phi_{l\eta} = 0 \qquad \text{C.25}$$

Again substituting $\rho = \frac{1}{2i} z$ C.26

$$z \frac{d^2\Phi_{l\eta}}{dz^2} + (2l+2-z)\frac{d\Phi_{l\eta}}{dz} - (i\eta + l + 1)\Phi_{l\eta} = 0 \qquad \text{C.27}$$

which is of the form C.10

and has the two solutions

$$W_{1,2}(i\eta + l + 1, 2l+2, z)$$

The solution which is regular and has the value unity at the origin is

$$\Phi_{l\eta}^{reg}\left(i\eta+l+1,\, 2l+2,\, z\right) = W_1 + W_2 \qquad \text{C.28}$$

For large $\sqrt{\ }$
$$W_1 = \frac{\Gamma(2l+2)}{\Gamma(-i\eta+l+1)} (2i\rho)^{-i\eta-l-1}$$

$$W_2 = \frac{\Gamma(2l+2)}{\Gamma(i\eta+l+1)} (-2i\rho)^{-i\eta+l+1} e^{-2i\rho} \qquad \text{C.29}$$

If the normalisation constant C_l in C.24 is taken to give

$$F_{l\eta} = e^{-\frac{1}{2}\pi\eta} \frac{|\Gamma(l+1+i\eta)|}{(2l+1)!} e^{i\rho} (2\rho)^l \rho \,(W_1+W_2) \qquad \text{C.30}$$

if we use $\quad (\pm ix) = e^{\pm(\frac{\pi}{2}i + \ln x)} \qquad \text{C.31}$

and if we put $\quad \Gamma(i\eta+l+1) = |\Gamma(i\eta+l+1)|\, e^{i\delta_l} \qquad \text{C.32}$

$$F_{l\eta} \approx \frac{1}{2i}\left[e^{i\rho - i\frac{\pi}{2}l - i\eta\ln 2\rho + i\delta_l} - e^{-i\rho + i\frac{\pi}{2}l + i\eta\ln 2\rho - i\delta_l}\right]$$
$$\approx \sin\left(\rho - \frac{\pi}{2}l - \eta\ln 2\rho + \delta_l\right) \qquad \text{C.33}$$

for large ρ.

For the irregular solution it is convenient to choose

$$G_{l\eta} = i\, e^{-\frac{1}{2}\pi\eta} \frac{|\Gamma(l+1+i\eta)|}{\Gamma(2l+2)} (2\rho)^l \rho\, e^{i\rho}\left[W_1 - W_2\right] \qquad \text{C.34}$$

which has asymptotic form

$$\cos\left(\rho - \tfrac{1}{2}l\pi - \eta\ln 2\rho + \delta_l\right) \qquad \text{C.35}$$

These functions have been tabulated (Bloch et al 1951).

We note that if the quantity $C_0^2 \equiv |\Gamma(1+i\eta)|^2 e^{-\eta\pi}$

using $\Gamma(1+z) = z\,\Gamma(z)$

and $\Gamma(z)\,\Gamma(1-z) = \dfrac{\pi}{\sin \pi z}$

then $C_0 = \left(\dfrac{2\pi\eta}{e^{2\pi\eta}-1} \right)^{\frac{1}{2}}$ C.36

This will be recognised as the Gamov factor for large η .

Negative energy solutions

These must vanish at large distances.

The general expression for them is given for example by Thomas (1952).

$$W_{-\eta,\,l+\frac{1}{2}}(2\rho) = \frac{e^{-\rho-\eta \ln 2\rho}}{\Gamma(1+l+\eta)} \int_0^\infty t^{l+\eta}\, e^{-t} \left(1+\frac{t}{2\rho}\right)^{l-\eta} dt \qquad \text{C.37}$$

$$\rightarrow \text{const} \times e^{-\rho-\eta \ln 2\rho} \quad \text{for large } \rho \qquad \text{C.38}$$

They have not as yet been tabulated.

For the s state however, we can obtain solutions in terms of other tabulated functions for particular values of η (B. Davison 1959).

In this case **from C.7**

$$\frac{d^2W}{d\rho^2} = \left(1 + \frac{2\eta}{\rho}\right)W \qquad \text{C.39}$$

which has solution $W = \int_1^\infty \left(\frac{s-1}{s+1}\right)^\eta e^{-s\rho}\frac{ds}{(s^2-1)}$ C.40

This may be verified as follows

$$\frac{d^2W}{d\rho^2} - W = \int_1^\infty \left(\frac{s-1}{s+1}\right)^\eta e^{-s\rho}\,ds$$

$$= \frac{e^{-s\rho}}{-\rho}\left(\frac{s-1}{s+1}\right)^\eta\Big|_1^\infty - \int_1^\infty \frac{e^{-s\rho}}{-\rho}\left(\frac{s-1}{s+1}\right)^\eta \eta\left(\frac{1}{s-1} - \frac{1}{s+1}\right)ds$$

$$= \frac{2\eta}{\rho}W.$$

Case 1. η Integral:

Now substitute $s = 2t - 1$

$$W = \frac{e^\rho}{2}\int_1^\infty \frac{dt}{t^2}\left(1 - \frac{1}{t}\right)^{\eta-1} e^{-2t\rho} \qquad \text{C.41}$$

and expanding $\left(1 - \frac{1}{t}\right)^{\eta-1}$ in powers of $\frac{1}{t}$ and integrating term by term

$$W(\rho) = \frac{e^\rho}{2}\left\{E_2(2\rho) - \frac{(\eta-1)}{1!}E_3(2\rho) + \frac{(\eta-1)(\eta-2)}{2!}E_4(2\rho) - \cdots\right\} \qquad \text{C.42}$$

where $E_n(x) = \int_1^\infty \frac{dt}{t^n}e^{-xt}$ and have been tabulated. C.43
(G. Placzek 1946)

If η is an integer the series terminates.

Case 2. η half integral:

We have
$$W(\rho) = \frac{\rho}{2\eta}\left[\frac{d^2 W}{d\rho^2} - W\right] \tag{C.44}$$

$$= \frac{\rho}{2\eta}\int_1^{\infty}\left(\frac{s-1}{s+1}\right)^{\eta} e^{-\rho s}\,ds \tag{C.45}$$

If $W(\rho;\eta)$ is the value of $W(\rho)$ for a particular value of η we obtain the recurrence relation:

$$W(\rho;\eta+1) = \frac{\rho}{2(\eta+1)}\int_1^{\infty}\left(\frac{s-1}{s+1}\right)^{\eta+1} e^{-\rho s}\,ds$$

$$= \frac{\rho}{2(\eta+1)}\int_1^{\infty}\left(\frac{s-1}{s+1}\right)^{\eta}\frac{s^2-2s+1}{s^2-1}\,e^{-\rho s}\,ds.$$

$$= \frac{\rho}{2(\eta+1)}\left[\frac{d^2}{d\rho^2} + 2\frac{d}{d\rho} + 1\right] W(\rho;\eta)$$

$$\therefore W(\rho;\eta+1) = \frac{\rho}{\eta+1}\left[\frac{d}{d\rho} + 1 + \frac{\eta}{\rho}\right] W(\rho;\eta) \tag{C.46}$$

Thus any $W(\rho; n+\tfrac{1}{2})$ can be readily expressed in terms of $W(\rho;\tfrac{1}{2})$ On the other hand

$$W(\rho;\tfrac{1}{2}) = \rho\int_1^{\infty}\left(\frac{s-1}{s+1}\right)^{\frac{1}{2}} e^{-\rho s}\,ds$$

$$= \rho\int_1^{\infty}\frac{(s-1)}{(s^2-1)^{\frac{1}{2}}}\,e^{-\rho s}\,ds$$

$$= -\rho\left[\frac{d}{d\rho} + 1\right] K_0(\rho)$$

$$= \rho\left[K_1(\rho) - K_0(\rho)\right] \tag{C.47}$$

where $K_n(\rho)$ are the modified Bessel functions of the second kind, using the Macdonald definition. (G.N. Watson 1944).

C.48

We have, using the relations

$$\rho K_n'(\rho) - n K_n(\rho) = -\rho K_{n+1}(\rho)$$

$$K_{\nu-1}(\rho) - K_{\nu+1}(\rho) = -\frac{2\nu}{\rho} K_\nu(\rho)$$

$$W(\rho;\tfrac{3}{2}) = \frac{2}{3}\rho\left\{K_1(2\rho+\tfrac{3}{2}) - K_0(2\rho+\tfrac{1}{2})\right\}$$

however for higher values of η the expression proves cumbersome.

APPENDIX D

<u>The Method of Steepest Descents</u>. (See D. Ter Haar 1954).

This method may be used for computing integrals of the form.

$$I = \int_{-\infty}^{\infty} e^{\psi(x)} dx \qquad \text{D.1}$$

Let $x = x_m$ be a saddle point of $\psi(x)$

Expand $\psi(x)$ about this point.

$$\psi(x) = \psi(x_m) + \tfrac{1}{2}(x - x_m)^2 \psi''(x_m) + O(x - x_m)^3 \quad \text{since } \psi'(x_m) \text{ vanishes} \qquad \text{D.2}$$

Define $\psi(x) - \psi(x_m) = -\tfrac{1}{2} \xi^2$ D.3

i.e. $(x - x_m)^2 \psi''(x_m) \approx -\xi^2$ D.4

Then $\dfrac{dx}{d\xi} = |\psi''(x_m)|^{-\frac{1}{2}}$ D.5

and $$I = \int_{-\infty}^{\infty} e^{\psi_m} e^{-\frac{1}{2}\xi^2} \frac{dx}{d\xi} d\xi \qquad \text{D.6}$$

$$= \int_{-\infty}^{\infty} \frac{e^{\psi_m}}{|\psi''(x_m)|^{\frac{1}{2}}} e^{-\frac{1}{2}\xi^2} d\xi \qquad \text{D.7}$$

$$= 2\int_{0}^{\infty} \frac{e^{\psi_m}}{|\psi''(x_m)|^{\frac{1}{2}}} e^{-\frac{1}{2}\xi^2} d\xi \qquad \text{D.8}$$

But $$\int_0^{\infty} e^{-\frac{1}{2}\xi^2} d\xi = \sqrt{\frac{\pi}{2}} \qquad \text{D.9}$$

$$\therefore \quad I = \sqrt{\frac{2\pi}{\gamma_m}}\, e^{\psi_m} \qquad \text{D.10}$$

where $\gamma_m = |\psi''(x_m)|$ D.11

APPENDIX E

Evaluation of the W.K.B. expression for the Whittacker function.

$$W(\rho) = \left[\frac{Q(\beta a)}{Q(\rho)}\right]^{\frac{1}{2}} e^{-\int_a^r Q(\rho)\,d\rho} \qquad \text{E.1}$$

$$= \left[Q(\beta a)\right]^{\frac{1}{2}} e^{-\int_a^r Q(\rho)\,d\rho - \frac{1}{2}\ln Q(\rho)} \qquad \text{E.2}$$

$$= \left[Q(\rho a)\right]^{\frac{1}{2}} e^{-\phi(\rho)} \qquad \text{E.3}$$

where $$\phi(\rho) = \int_a^r \frac{\left(\rho^2 + 2\eta_1\rho + n(n+1)\right)^{\frac{1}{2}}}{\rho}\,d\rho + \frac{1}{2}\ln\left\{\frac{\left(\rho^2+2\eta_1\rho+n(n+1)\right)^{\frac{1}{2}}}{\rho}\right\} \qquad \text{E.4}$$

The integral is of the form

$$\int \frac{(a+bx+cx^2)^{\frac{1}{2}}}{x}\,dx = \int \frac{X^{\frac{1}{2}}}{x}\,dx \qquad \text{E.5}$$

$$= X^{\frac{1}{2}} + \frac{b}{2}\int \frac{dx}{X^{\frac{1}{2}}} + a\int \frac{dx}{xX^{\frac{1}{2}}} \qquad \text{E.6}$$

while $$\int \frac{dx}{xX^{\frac{1}{2}}} = -\frac{1}{\sqrt{a}}\ln\left(\frac{X^{\frac{1}{2}}+a^{\frac{1}{2}}}{x} + \frac{b}{2a^{\frac{1}{2}}}\right) \qquad a>0 \qquad \text{E.7}$$

and $$= \frac{2X^{\frac{1}{2}}}{bx} \qquad a=0 \qquad \text{E.8}$$

also $$\int \frac{dx}{X^{\frac{1}{2}}} = \frac{1}{c^{\frac{1}{2}}}\ln\left(X^{\frac{1}{2}} + xc^{\frac{1}{2}} + \frac{b}{2c^{\frac{1}{2}}}\right) \qquad \text{E.9}$$

Thus $$\phi(r) = \Bigg[\left(\rho^2+2\eta_1\rho+n(n+1)\right)^{\frac{1}{2}} + \eta_1\ln\left(\left(\rho^2+2\eta_1\rho+n(n+1)\right)^{\frac{1}{2}}+\rho+\eta_1\right)$$

$$-\left(n(n+1)\right)^{\frac{1}{2}}\ln\left(\frac{\left(\rho^2+2\eta_1\rho+n(n+1)\right)^{\frac{1}{2}}}{\rho} + \frac{\eta_1}{\left(n(n+1)\right)^{\frac{1}{2}}}\right)\Bigg]_a^r$$

$$+\frac{1}{2}\ln\left(\frac{\left(\rho^2+2\eta_1\rho+n(n+1)\right)^{\frac{1}{2}}}{\rho}\right) \qquad \text{E.10}$$

Thus
$$W(\rho) = \left\{ \frac{1 + \frac{2\eta_1}{\rho_0} + \frac{n(n+1)}{\rho_0^2}}{1 + \frac{2\eta_1}{\rho} + \frac{n(n+1)}{\rho^2}} \right\}^{\frac{1}{4}} \left\{ \frac{\rho_0\left(\left(1 + \frac{2\eta_1}{\rho_0} + \frac{n(n+1)}{\rho_0^2}\right) + 1\right) + \eta_1}{\rho\left(\left(1 + \frac{2\eta_1}{\rho} + \frac{n(n+1)}{\rho^2}\right) + 1\right) + \eta_1} \right\}^{\eta_1}$$

$$\times \left\{ \frac{\left(1 + \frac{2\eta_1}{\rho} + \frac{n(n+1)}{\rho^2}\right)^{\frac{1}{2}} + \frac{(n(n+1))^{\frac{1}{2}}}{\rho} + \frac{\eta_1}{(n(n+1))^{\frac{1}{2}}}}{\left(1 + \frac{2\eta_1}{\rho_0} + \frac{n(n+1)}{\rho_0^2}\right)^{\frac{1}{2}} + \frac{(n(n+1))^{\frac{1}{2}}}{\rho_0} + \frac{\eta_1}{(n(n+1))^{\frac{1}{2}}}} \right\}^{\sqrt{n(n+1)}} \qquad \text{E.11}$$

$$\times \exp - \left\{ \rho\left(1 + \frac{2\eta_1}{\rho} + \frac{n(n+1)}{\rho^2}\right) - \rho_0\left(1 + \frac{2\eta_1}{\rho_0} + \frac{n(n+1)}{\rho_0^2}\right) \right\}$$

where here $\rho_0 = \beta a$

$\rho = \beta r$

A better solution is obtained if $(n+\frac{1}{2})^2$ is substituted for $n(n+1)$ (see Schiff 1955).

APPENDIX F

The expressions $\frac{d\psi}{dx}$ and $\frac{d^2\psi}{dx^2}$

$$\psi(x) = \int^{x} Q\beta e^{x}\,dx + \tfrac{1}{2}\ln Q + \tfrac{1}{2}\ln P - \int^{x} P\alpha e^{x}\,dx - 2x \qquad \text{F.1}$$

where P and Q are given by 2.1 + 2.2 .

$$\frac{d\psi}{dx} = \left(\beta^2 e^{2x} + 2\eta_1\beta e^{x} + n(n+1)\right)^{\frac{1}{2}} - \left(-\alpha^2 e^{2x} + 2\eta_2\alpha e^{x} + l(l+1)\right)^{\frac{1}{2}}$$
$$- \left(\frac{\eta_1\beta e^{x} + n(n+1)}{2\left(\beta^2 e^{2x} + 2\eta_1 e^{x} + n(n+1)\right)}\right) - \left(\frac{\eta_2\alpha e^{x} + l(l+1)}{2\left(-\alpha^2 e^{2x} + 2\eta_2\alpha e^{x} + l(l+1)\right)}\right) - 2 \qquad \text{F.2}$$

or in terms of

ρ + ρ'

$$\frac{d\psi(x)}{dx} = \left(\rho^2 + 2\eta_1\rho + n(n+1)\right)^{\frac{1}{2}} - \left(-\rho'^2 + 2\eta_2\rho' + l(l+1)\right)^{\frac{1}{2}}$$
$$- \frac{\left(\eta_1\rho + n(n+1)\right)}{2\left(\rho^2 + 2\eta_1\rho + n(n+1)\right)} - \frac{\left(\eta_2\rho' + l(l+1)\right)}{2\left(-\rho'^2 + 2\eta_2\rho' + l(l+1)\right)} \qquad \text{F.3}$$

Also

$$\frac{d^2\psi(x)}{dx^2} = \frac{\left(\rho^2 + \eta_1\rho\right)}{\left(\rho^2 + 2\eta_1\rho + n(n+1)\right)^{\frac{1}{2}}} - \frac{\left(-\rho'^2 + \eta_2\rho'\right)}{\left(-\rho'^2 + 2\eta_2\rho' + l(l+1)\right)^{\frac{1}{2}}} .$$

$$- \frac{\eta_1\rho^3 + 2n(n+1)\rho^2 + \eta_1 n(n+1)\rho}{2\left(\rho^2 + 2\eta_1\rho + n(n+1)\right)^2} - \frac{\eta_2\rho'^3 + 2l(l+1)\rho'^2 - l(l+1)\eta_2\rho'}{2\left(\rho'^2 + 2\eta_2\rho' + l(l+1)\right)^2} \qquad \text{F.4}$$

In all these W.K.B. expressions a better solution is obtained if $\left(l+\frac{1}{2}\right)^2$ is substituted for $l(l+1)$ (see Schiff 1955).

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