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SOLUBLE MODEL CALCULATIONS OF THE CONTINUUM STRUCTURE
OF CLOSED-SHELL NUCLEI IN THE
EIGENCHANNEL REACTION THEORY

Ph. D. Thesis Submitted to Iowa State University, November 1971

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Soluble model calculations of the continuum structure
of closed-shell nuclei in the
eigenchannel reaction theory

by

Gerald Francis Gieraltowski

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Soluble model calculations of the continuum structure
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Gerald Francis Gieraltowski

ABSTRACT

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An analysis of the eigenchannel formalism as applied to the reaction theory of photonuclear absorption processes is discussed and analyzed within the one-particle-one-hole framework. An application is made of the eigenchannel theory to the photonuclear absorption processes for C^{12} in the energy range $16 \text{ MeV} \leq E_\gamma \leq 40 \text{ MeV}$ with a single-particle potential of the square well type plus $\vec{L} \cdot \vec{S}$ and $\vec{L}^2$ terms. The basic residual interaction between the particle and hole states is taken to be of the surface-delta form. Analytic expressions for both the neutron and proton wave functions are derived and the entire eigenchannel calculation is performed as exactly as possible with an absolute error in the photoabsorption cross section values of less than six per-cent. It was observed that spurious peaks occur in the cross section if the non-orthogonality of the single-particle basis states is not properly taken account of. A method for eliminating these spurious components is derived and an analysis of the resultant C^{12} photoabsorption cross sec-

tions shows relatively good agreement between the resonance peaks found by the eigenchannel analysis and those from experiment. The experimental interpretation of resonance structure above the giant resonance as being attributable to single-particle excitations from low-lying closed shells is supported by the eigenchannel analysis of the C^{12} photoabsorption reaction. The fact that the eigenchannel theory can and does produce nuclear reaction information in good accord with experiment tends to support its continued use. However, because of the excessive computer time involved in such a calculation and the preponderance of numerical difficulties associated with it, extensive applications of the eigenchannel theory as presently formulated must be questioned.

INTRODUCTION

The cross sections of photonuclear reactions show broad resonance peaks in different elements at an incident photon energy of 20 to 25 MeV. The most important contribution to these peaks comes from electric dipole transitions. Because of this, the states associated with these resonances are conventionally referred to as giant dipole states. The observed resonances point to the existence of long-lived intermediate states of the compound system which according to Niels Bohr (1) have this long lifetime due to their complexity. Accordingly, it was for a long time considered almost hopeless to approach nuclear reaction theory from a microscopic point of view. Thus the nucleons comprising the compound state were looked upon as an aggregate of particles exhibiting collective or group properties. Because the collective motion of the nucleus exhibited properties similar to that of an incompressible liquid, the classical liquid-drop model of the nucleus came into being. Similar investigations of the collective nature of the nucleus led to the statistical and collective models of the nucleus. The nuclear shell-model of Mayer and Jensen (2) was the first successful attempt made to describe the properties of the nucleus by examining the individual properties of its constituent nucleons. The success of this microscopic approach in describing the properties of bound nuclear levels stimulated the development of a microscopic approach to nuclear reactions.

Attempts have been made by various groups (3-10) to solve the nuclear reaction problem at least for that case where only one nucleon is in the

continuum, i.e., below the two-particle emission threshold. The case of more than one nucleon in the continuum must remain an unsolved problem at least until an adequate three-body theory has been formulated. Considering closed-shell nuclei, Brown and his collaborators (11, 12) have identified the compound states describing the giant dipole resonances as highly correlated superpositions of single-particle excitations out of the closed shell into an adjacent unfilled shell. The main mechanism giving rise to the properties of the giant dipole states is the interaction of the excited particles with the corresponding holes left in the lower shell. This mixes the possible $T = 1$, $J^\pi = 1^-$ shell-model configurations. One or two of the resulting states have energies appreciably larger than that of the basic shell-model excitations (11, p. 474) and it is exactly these states which describe the resonance peaks. The focal point of a successful nuclear reaction theory describing these excitations should thus be an accurate representation of these single-particle continuum states. The usual approach taken in nuclear reaction theory is to treat the entire continuum of positive energy states through the use of Green's functions. This invariably leads to integral equations incorporating integrals over the entire infinite range of possible energies. What one would like to do instead is to formulate a theory which involves only a countably infinite set of positive energy states or better yet a discrete spectrum of continuum states and still be able to describe the principal properties of the nuclear reaction process. To accomplish this aim, one must look at the properties of the single-particle potential describing the motion of these particles.

If one chooses an infinite range potential such as the harmonic oscillator potential only bound states can be described, i.e., those states with a negative energy. The nucleon emitted in the photonuclear reaction will, however, be unbound (possessing positive energy) so one must consider instead a finite-range potential. If in addition to the use of a finite-range potential one places some form of boundary condition on the wave function of the scattered particle, a discrete spectrum for the nuclear Hamiltonian is obtained. This is in complete analogy with the usual concept of "box normalization" employed in quantum theory. If the set of basis states comprising the scattered wave function is finite, the problem is reduced to a matrix diagonalization of the type encountered in conventional bound state configuration-mixing calculations.

What must the range of the potential be to describe adequately the properties of a continuum state in the truncated space? The guiding principle used in defining this truncated space is the idea that the nuclear interaction between target and projectile becomes negligibly small if their separation exceeds the value of several nuclear radii. Hence, nuclear interactions are relevant for the reaction process only when all nucleons are within a small volume which thus defines an internal region. The basis states of the Hamiltonian must be continuous and have a continuous derivative at the surface of the internal region. Thus some form of boundary condition is implied at the surface of the internal region. The form of this boundary condition has led to several different reaction theories, the most prevalent being the R-matrix theory of Wigner and Eisenbud (10) and the eigenchannel theory of Greiner and Danos (13).

The R-matrix theory has been widely applied with limited success but poses several drawbacks from a physical standpoint. The boundary condition chosen in the R-matrix theory is to have the logarithmic derivative of the basis states of the interior region equal a constant; the value of the constant being arbitrary. Thus the energies of the interior basis states have no physical connection with that of the scattering solution in the exterior region. Furthermore if one truncates the set of interior basis states according to an energy cutoff criterion, as is usually done, there seems to be no physical connection linking the energy cutoff employed with that of the scattering solution desired. The eigenchannel theory proposed by Greiner and Danos in 1965 makes use of a "natural" boundary condition dependent on energy which joins smoothly the basis functions of the interior region to the wave function of the scattered particle. This "natural" boundary condition merely matches the logarithmic derivative of the interior and exterior wave functions at the truncating radius. Thus the interior basis states are physically connected to the wave function of the scattered particle and an energy cutoff criterion on the interior states can easily be interpreted in terms of the energy of the scattered particle. Moreover, the eigenchannel theory leads to a diagonal representation of the S-matrix which makes the construction of the scattering matrix particularly easy. Since the nuclear cross sections are directly related to the matrix elements of the scattering matrix, the eigenchannel theory results in particularly simple forms for the various partial cross sections of interest.

The eigenchannel theory has been applied to various nuclei (14 - 19), and gives reasonably good agreement with experiment. However in the

recent years this theory has come under attack (20,21) because of its apparent ability to reproduce fine-structure resonances in the giant dipole region. Can the eigenchannel theory in the 1-particle-1-hole framework reproduce such narrow resonances or are the resonances merely spurious peaks due to an incomplete treatment of the basis functions of the model Hamiltonian? Questions such as this have led to heavy criticism being levied against this theory by Hans Weidenmüller and C. Mahaux (20). It is their opinion that the R-matrix method is at least as accurate as the eigenchannel method, the former being, however, both simpler and numerically much faster than the latter and that the cross sections obtained from the eigenchannel method may exhibit spurious wiggles or resonance peaks.

What was needed and had not been done was a calculation employing the eigenchannel theory but with an analytically solvable single-particle potential for which the exact wave functions are known. Working with known analytic solutions one is better able to estimate error accumulation, recognize numerical difficulties in the theory, and state with relative assurance whether calculated resonances are spurious or not. In Chapter I, the eigenchannel theory is reviewed and the heretofore neglected question of the non-orthogonality of the basis state wave functions is discussed and properly accounted for in the theory. Photonuclear cross sections and electric dipole absorption processes are discussed in the eigenchannel framework in Chapter II. In Chapter III, a calculation of the dipole absorption cross sections for C^{12} is presented with a single-particle potential of the spherically symmetric square well type. The analytic

solutions for both protons and neutrons is given along with a detailed outline of the method employed in the eigenchannel theory. It has been proposed (22.) that high energy structure in photonuclear cross sections may be attributable to essentially single particle excitations from deep lying nuclear shells. To test this hypothesis, the deep lying $1s_{1/2}$ states have been included in the calculation and photonuclear cross sections have been calculated to an energy of 40 MeV; greater than the binding energy of the $1s_{1/2}$ states of C^{12} and well beyond the two-nucleon threshold. Numerical means of calculating the proton wave functions and some new integral properties of the Coulomb functions are presented in Chapter IV. The neutron wave functions and their properties are treated in Chapter V along with a description of the many numerical pitfalls common to the eigenchannel calculation. In Chapter VI, the photonuclear cross sections of C^{12} as calculated in the eigenchannel formalism are discussed and analyzed. Included in this section is a discussion of some of the criticisms of this theory. The main conclusions reached in this thesis are summarized and reported in Chapter VII. The reader unfamiliar with basic angular momentum theory, particle-hole theory, and the channel notation of scattering theory might profit from first reading Appendix A before beginning this thesis.

CHAPTER 1. THE EIGENCHANNEL THEORY

1.1 Basic assumptions

In the normal reaction theory all considered channels are assumed to have only a single incoming or outgoing particle. Channels with two or more particles in the continuum must be excluded at least until an adequate three-body theory is formulated. Thus the more complicated reactions involving the emission of alpha particles, of deuterons, or of an unbound proton-neutron pair are omitted. As has been pointed out by Brown (11, p. 472), the observed peak in the giant resonance region should be adequately characterized by a one-particle-one-hole state formed by exciting a single particle out of the ground state of the target nucleus into the continuum. This premise has been well accepted and in analogy with other researchers, only one-particle-one-hole states are considered in this thesis. To account for the more complicated reactions it would be necessary to incorporate many-particle-many-hole states in the nuclear wave function. These components would also lead to fine structure in the cross section (23). Also without restricting the basis of single particle states to harmonic-oscillator functions, the center-of-mass motion can not be handled properly and it must be realized that uncertainties of the order $1/A$ will thus influence the results.

Restricting ourselves to the consideration of closed-shell nuclei suppose one were to remove a single particle from one of the filled shells of the ground state. From angular momentum considerations, the residual nucleus must have a total angular momentum equal to that of the missing

particle but with an opposite projection quantum number. Its energy must be minus that of the missing particle and its parity must be the same as that of the particle to conserve energy and parity. These are exactly the characteristics describing the hole state formed by the emitted particle. Thus, the residual nucleus of the A-particle system (target plus projectile) can be completely characterized by the single hole produced by the excitation of a particle into the continuum.

The nuclear Hamiltonian is assumed to have the form

$$H = H_0 + V_{ph} \quad (1.1)$$

where $H_0 = H_p + H_h$ is the shell-model Hamiltonian of the particles and holes and V_{ph} is a residual two-body interaction. The Hilbert space in which H is diagonalized consists only of a truncated set of eigenfunctions of H_0 . The scattering matrix, or S-matrix, defines the transformation of the initial state wave function to that of the final state wave function. It has the property (24, pp. 160-162) that

$$[H, S] = 0 \quad (1.2)$$

if one uses a complete set of scattering solutions to the total Hamiltonian H to construct the S-matrix. In Chapter II it will be shown that partial and total cross sections are easily related to the S-matrix. We seek therefore a complete set of scattering states, called the eigenchannel states, which simultaneously diagonalize the nuclear Hamiltonian H and the S-matrix. The S-matrix is a unitary and symmetric matrix (25, pp. 227-234)

and thus has the properties

$$S^\dagger S = I \quad (1.3a)$$

$$S_{ij} = S_{ji}^* \quad (1.3b)$$

Let V be an eigenvector of S and ϵ the eigenvalue satisfying

$$SV = \epsilon V \quad (1.4)$$

Then from the unitarity of S one obtains

$$(V, V) = (V, S^\dagger SV) = (SV, SV) = |\epsilon|^2 (V, V) \quad (1.5a)$$

$$\therefore |\epsilon|^2 = 1 \quad (1.5b)$$

Thus the eigenvalues of S have unit modulus and may be written in the form $\exp(2i\delta^v)$, ($v = 1, 2, \dots, \infty$); the "eigenphases" δ^v are real. Since the eigenvalues of the inverse of a matrix are the inverse eigenvalues of the original matrix

$$S^{-1}V = e^{-2i\delta^v} V = S^\dagger V \quad (1.6)$$

Equation 1.6 implies

$$S^\dagger V = (S^T)^* V = e^{-2i\delta^v} V \quad (1.7a)$$

$$= S^* V = e^{-2i\delta^v} V \quad (\text{since } S \text{ is symmetric}) \quad (1.7b)$$

Taking the complex conjugate of both sides of Equation 1.7b

$$SV^* = e^{2i\delta^v} V^* \quad (1.8)$$

But,

$$SV = e^{2i\delta^v} V \quad (1.9)$$

and thus if $e^{2i\delta^v}$ is non-degenerate, Equations 1.8 and 1.9 imply that V is proportional to V^* and so the eigenvectors of S may be chosen to be real.

If the eigenvalue is degenerate, a linear combination of V and V^* may still be formed so as to make the resultant eigenvector real. Therefore, the components of the eigenvectors of the S -matrix, labelled V_j^v may be chosen to be real. They satisfy the relations:

$$\sum_j S_{ij} V_j^v = e^{2i\delta^v} V_i^v = \sum_i S_{ij} V_j^v \quad (1.10)$$

$$\sum_j V_j^v V_j^{v'} = \delta_{vv'} \quad (1.11)$$

$$\sum_v V_j^v V_i^v = \delta_{ij} \quad (1.12)$$

1.2 The exterior wave function

As in all such theories, the configuration space of the A -particle system is separated into an exterior and interior region. One introduces an interaction radius a_c for each channel c , open or closed. Let $\mathfrak{S}_c$ designate the channel "surface" for the channel c . $\mathfrak{S}_c$ thus represents the equation

$$r_c = a_c \quad (1.13)$$

The totality of all channel surfaces we write as $\mathfrak{S} = \sum_c \mathfrak{S}_c$. Let E be an energy at which N channels, labelled $1, 2, \dots, N$ are open. To each channel corresponds a "surface" function $\tilde{\varphi}_c$ ($c = 1, 2, 3, \dots, N$) (26, pp. 267). The

surface functions are mutually orthogonal and normalized:

$$\int \tilde{\varphi}_{c'}^\dagger \tilde{\varphi}_c d\mathbf{g} = 4\pi a_c^2 \delta_{c,c'} \quad (1.14)$$

where the integral is taken over the totality of channel surfaces $\mathbf{g}$. As shown in Appendix A, Section A-4, the surface function $\tilde{\varphi}_c$ contains the hole state wave function and the explicit angular momentum coupling of the particle-hole pair. A channel threshold energy is defined to be the absolute value of the energy of the hole state characterizing that channel. At each channel threshold an infinity of angular momentum states is possible making N infinite. For practical calculations, N must be restricted so that one deals only with a finite number of angular momentum states. There exist N linearly independent scattering solutions with total angular momentum J of the Schrödinger equation

$$H\psi^J = (H_0 + V_{ph}) \psi^J = E\psi^J. \quad (1.15)$$

Such a set of linearly independent wave functions is for example, given by those N solutions $\psi^{J,i}$ ($i = 1, 2, \dots, N$) of Equation 1.15 which have an incoming wave in only one channel. The S -matrix is then defined, as usual, by the asymptotic form of these solutions. In the asymptotic region, the projection $\psi_j^{J,i}$ of $\psi^{J,i}$ onto channel j has the form (20, p. 847)

$$\psi_j^{J,i} \sim [\delta_{ij} I_j - S_{ij} O_j] \tilde{\varphi}_j. \quad (1.16)$$

The functions I_j and O_j are the familiar incoming and outgoing wave solutions, and (S_{ij}) is the scattering matrix. Multiplying Equation 1.16 by the S -matrix eigenvector component $V_i^{J,v}$, summing over i , and taking into

account Equation 1.10, one finds a new set of functions $\psi^{j,v}$ whose asymptotic behavior in channel j is,

$$\psi_j^{j,v} \sim v_j^{j,v} [I_j - e^{2i\delta_j^v} O_j] \tilde{\varphi}_j. \quad (1.17)$$

The functions $\psi^{j,v}$ are linearly independent since they are connected to the functions $\psi^{j,i}$ by an orthogonal transformation. Whether the set $\psi^{j,i}$ or the set $\psi^{j,v}$ is used is immaterial, since any set of N linearly independent scattering solutions of Equation 1.15 easily leads to the S -matrix. However, the choice of the $\psi^{j,v}$, called the "eigenchannels", will exhibit some particularly intrinsic characteristics which will become apparent from the following considerations. From Equation 1.17 we see that $\psi^{j,v}$ will be a linear superposition of all open channels. Thus it has the form

$$\psi^{j,v} \sim \sum_c v_c^{j,v} e^{i\delta_J^v} [e^{-i\delta_J^v} I_c - e^{i\delta_J^v} O_c] \tilde{\varphi}_c. \quad (1.18)$$

The incoming and outgoing radial functions I_c and O_c are defined by (26, p. 269)

$$\begin{aligned} I_c^* = O_c &= [G_L(k_c r) + iF_L(k_c r)] e^{-i\eta_c} \\ &\rightarrow \exp [i(k_c r - L\pi/2 - \eta_c \ln 2k_c r)]. \end{aligned} \quad (1.19)$$

Here F_L and G_L are respectively, the regular and irregular solutions of the radial differential equations. They are the Coulomb functions in the case of protons and the spherical Bessel and Neumann functions multiplied by $k_c r$

for neutrons. The Coulomb parameter η_c and the phase ω_c are given by

$$\eta_c = \frac{Z e^2}{\hbar v_c}, \quad \omega_c = \sum_{k=1}^L \arctan(\eta_c/k). \quad (1.20)$$

If we specialize Equation 1.18 to the case of uncharged particles and make use of Equation 1.19, $\psi^{J,v}$ takes on the following form

$$\psi^{J,v} \sim -2i e^{i\delta_J^v} \sum_c v_c^{J,v} \sin(k_c r + \delta_J^v - L\pi/2) \tilde{\varphi}_c. \quad (1.21)$$

A similar result holds for the case of charged particles. The eigenchannel states thus correspond to standing waves in all open experimental channels with a common phase shift, the eigenphase δ_J^v . Correctly normalized to unit incident flux, the $\psi^{J,v}$ becomes

$$\psi^{J,v} = \sum_c v_c^{-1/2} v_c^{J,v} [G_L(k_c r) \sin(\delta_J^v - \omega_c) + F_L(k_c r) \cos(\delta_J^v - \omega_c)] \tilde{\varphi}_c \quad (1.22)$$

where v_c is the relative velocity in channel c .

1.3 The interior region

As in section 1.2, the set a_c defines the separation of the configuration space. It is assumed that in each channel c , Equation 1.17 holds not only asymptotically, but for all values of the separation distance larger than or equal to a_c . This is the "channel orthogonality assumption" proposed by Lane and Thomas (26, p. 268). It implies that the surface functions $\tilde{\varphi}_c$ become negligibly small for values of r larger than a_c . From Equation A-4-10 of Appendix A one can see that this approximation is

quite valid in all channels since $\tilde{\varphi}_c$ contains the exponentially decreasing hole state wave function and thus for sufficiently large values of a_c

$$\tilde{\varphi}_c \approx 0 \text{ for } r > a_c. \quad (1.23)$$

To complete the theory, we need a set of properly antisymmetrized interior solutions for $r \leq a_c$ which will simultaneously diagonalize the nuclear Hamiltonian and be consistent with the asymptotic form, Equation 1.22. The interior solutions are expressed in terms of a set of unperturbed states $\chi_{\lambda_c, c}^J$ defined as follows. In each channel c , a "natural boundary condition", B_c , is imposed. One then determines a set of single particle radial wave functions $U_{\lambda_c, c}(r)$ ($\lambda_c = 1, 2, \dots, \infty$). These functions are regular eigenfunctions of H_0 , normalized in the internal region, and satisfying the boundary condition

$$[r(d/dr) U_{\lambda_c, c}(r)] \Big|_{r=a_c} = B_c U_{\lambda_c, c}(r) \Big|_{r=a_c}. \quad (1.24)$$

The single particle states define a set of normalized basis states $\chi_{\lambda_c, c}^J$ by

$$\chi_{\lambda_c, c}^J = G_A \{ U_{\lambda_c, c}(r_A) \tilde{\varphi}_c \} \quad (1.25)$$

where G_A antisymmetrizes between the A th and the other $A-1$ nucleons. The Hamiltonian H is then diagonalized in the truncated space of functions spanned by the set $\{\chi_{\lambda_c, c}^J\}$. The truncation is purely for numerical reasons and one hopes that the truncation of λ_c leads to an adequate representation

of $X_{\lambda_c, c}^J$. The eigenvalues and eigenvectors of the matrix

$$H = (X_{\lambda_c, c}^J | H | X_{m_{c'}, c'}^J) \quad (1.26)$$

are identified with the eigenvalues E_λ and the eigenstates X_λ of H , corresponding to the boundary condition parameters $\{B_c\}$. In Equation 1.26 as well as below, the round brackets indicate that the integration extends only over the internal region. The natural boundary condition B_c is chosen to insure that the interior solutions join smoothly to the asymptotic solution, Equation 1.22. Thus,

$$B_c = \left[\frac{r(d/dr) f_c(k_c r)}{f_c(k_c r)} \right]_{r=a_c} \quad (1.27)$$

$$f_c(k_c r) = G_L(k_c r) \sin(\delta_J - \omega_c) + F_L(k_c r) \cos(\delta_J - \omega_c). \quad (1.28)$$

Since the interior solutions are to be eigenchannel states, the same phase δ_J must be used in Equation 1.28 for each channel considered. However, any one choice of δ_J will not in general correspond to an eigenphase δ_J^v . The solution of this difficulty represents a self-consistency problem which must be solved by an iterative process.

1.4 The eigenphases and eigenvectors

The solution to the self-consistency problem can be formulated in the following manner:

- 1) Choose a phase δ_j and an excitation energy E_c .
- 2) For each open channel, find all the single-particle states which are solutions of H_0 for $r \leq a_c$ satisfying the natural boundary condition.
- 3) Diagonalize the full Hamiltonian H within the truncated basis of step 2) and check to see if any eigenvalue E_λ equals E .
- 4) If so, then δ_j is an eigenphase δ_j^ν . If not, choose a new phase value and repeat the process. The wave numbers k_c in the natural boundary conditions are related to the excitation energy E_c of the compound system by

$$E_c = \left(\frac{\hbar^2}{2\mu_c} \right) k_c^2 + Q_c \quad (1.29)$$

where μ_c is the reduced mass in channel c and Q_c is the threshold energy of channel c (i.e., Q_c equals the absolute value of the energy of the hole state characterizing the channel c). There are in general as many eigenphases as there are open channels. Once all the eigenphases have been found, it is relatively easy to construct the eigenvectors of the S -matrix from which all the necessary information regarding the reaction process can be extracted. In particular, the wave function, corresponding to a particular eigenphase δ_j^ν , obtained by the diagonalization of the nuclear Hamiltonian in the basis set defined by Equation 1.25 has the form

$$\Psi_{INT}^{J,\nu} = \sum_{c,\lambda_c} A_{c,\lambda_c}^{J,\nu} \chi_{\lambda_c}^{J,\nu} \quad (1.30)$$

The $A_{c,\lambda_c}^{J,\nu}$ are merely the eigenvectors of the resultant diagonalization

and the index ν on the particle-hole function indicates that the particle continuum state obeys the boundary condition of the ν th eigenchannel. Since $\Psi_{INT}^{J,\nu}$ and $\Psi^{J,\nu}$ (Equation 1.22) represent the same wave function, we can set Equations 1.22 and 1.30 equal to each other and solve for the eigenvectors $V_C^{J,\nu}$. However, the particle radial functions appearing in Equation 1.30 are normalized to unity over the internal region while the radial parts of Equation 1.22 are normalized to unit incident flux. To obtain continuity of the nuclear wave function at $r = a_c$ the V_C 's are replaced by unnormalized coefficients $C_C^{J,\nu}$. Equating the modified expression 1.22 and the expression 1.30 at $r = a_c$ and integrating over all coordinates except r , the following matching condition is obtained:

$$\begin{aligned}
 & V_C^{-1/2} C_C^{J,\nu} [G_L(k_c r) \sin(\delta_J^{\nu} - \omega_c) + F_L(k_c r) \cos(\delta_J^{\nu} - \omega_c)] \\
 & = \sum_{\lambda_c} A_{C,\lambda_c}^{J,\nu} U_{\lambda_c,\nu}^{(\nu)}(a_c).
 \end{aligned} \tag{1.31}$$

Finally, the amplitudes V_C of Equation 1.22 can be obtained by normalization.

$$V_C^{J,\nu} = C_C^{J,\nu} / N_{J,\nu} \tag{1.32}$$

$$N_{J,\nu}^2 = \sum_C (C_C^{J,\nu})^2. \tag{1.33}$$

One must not, however, be taken unaware by the apparent simplicity of the four step iterative procedure. It must be born in mind that the nuclear

Hamiltonian must be diagonalized many times over for each eigenphase δ_J^V . The iterative search procedure contains many pitfalls for the eager researcher and is the major drawback to a practical application of the eigenchannel theory.

1.5 Matrix elements of the Hamiltonian

When one speaks of a wave function as being a solution of the total nuclear Hamiltonian, it is implied that the wave function is defined over all space. The imposition of a radius 'a' which separates the configuration space into an external and internal region, poses some difficulty. If one were to normalize the wave function to unity over a sphere of radius 'a' as is implied in the eigenchannel theory then the wave function so formed is not equivalent to the true solution. In fact defining ψ_β as the true solution to the nuclear Hamiltonian, the modified wave function formed by truncating the space at 'a' is

$$\tilde{\psi}_\beta = \theta(a - r) \psi_\beta \quad (1.34)$$

with
$$\theta(a - r) = \begin{cases} 1 & \text{if } r \leq a \\ 0 & \text{if } r > a \end{cases} . \quad (1.35)$$

Why does one even need to utilize the tilde wave function? The true solution represents the motion of a free particle and as such is not a square-integrable function over all space. Thus if one were to construct matrix elements of the total Hamiltonian using the true solutions, many of these matrix elements would be infinite. The proper use of the tilde wave functions (Equation 1.34) circumvents this difficulty. Let us examine in

detail the matrix elements of the total Hamiltonian H given by Equation 1.1. Since in the eigenchannel theory the total Hamiltonian is diagonalized in the basis set of solutions of H_0 let us focus our attention on the matrix elements of H_0 . Let ψ_β be an eigenvector of H_0 :

$$H_0 \psi_\beta = \epsilon_\beta \psi_\beta. \quad (1.36)$$

If instead one were to use the tilde wave function $\tilde{\psi}_\beta$,

$$H_0 \tilde{\psi}_\beta = H_0 \theta(a-r) \psi_\beta = \theta(a-r) H_0 \psi_\beta + [H_0, \theta(a-r)] \psi_\beta \quad (1.37a)$$

$$= \epsilon_\beta \tilde{\psi}_\beta + [H_0, \theta(a-r)] \psi_\beta. \quad (1.37b)$$

Now, H_0 is a sum of kinetic and potential energy terms

$$H_0 = T + V \quad (1.38a)$$

where

$$T = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{d^2}{dr^2} r. \quad (1.38b)$$

The potential energy V commutes with $\theta(a-r)$ but the commutator of T and $\theta(a-r)$ is non-zero. In fact,

$$[T, \theta(a-r)] = -\frac{\hbar^2}{2\mu} \left[\frac{1}{r} \frac{d^2}{dr^2} r, \theta(a-r) \right] \quad (1.39a)$$

$$[T, \theta(a-r)] = -\frac{\hbar^2}{2\mu} \left[\theta'(a-r) + \frac{2}{r} \theta' + 2\theta' \frac{d}{dr} \right]. \quad (1.39b)$$

Using the fact that

$$\theta'(a-r) = -\delta(a-r) = -\delta(r-a) \quad (140)$$

and Equation 1.39 in Equation 1.37, one obtains

$$H_0 \tilde{\psi}_\beta = \epsilon_\beta \tilde{\psi}_\beta + \frac{\hbar^2}{2\mu} \delta'(r-a) \tilde{\psi}_\beta + \frac{\hbar^2}{\mu} \frac{1}{r} \delta(r-a) \tilde{\psi}_\beta + \frac{\hbar^2}{\mu} \delta(r-a) \tilde{\psi}'_\beta \quad (1.41)$$

Suppose one were to take a matrix element of H_0 between a tilde state, $\tilde{\psi}_\beta$ and an untilde state ψ_γ :

$$\begin{aligned} \langle \psi_\gamma | H_0 | \tilde{\psi}_\beta \rangle &= \epsilon_\beta \langle \psi_\gamma | \tilde{\psi}_\beta \rangle + \frac{\hbar^2}{2\mu} \int r^2 dr \psi_\gamma^* \delta'(r-a) \tilde{\psi}_\beta \\ &+ \frac{\hbar^2}{\mu} \int r dr \delta(r-a) \psi_\gamma^* \tilde{\psi}_\beta + \frac{\hbar^2}{\mu} \int r^2 dr \delta(r-a) \psi_\gamma^* \tilde{\psi}'_\beta. \end{aligned} \quad (1.42)$$

Using known properties of the delta function, and recognizing that

$$\langle \psi_\gamma | \tilde{\psi}_\beta \rangle = \langle \tilde{\psi}_\gamma | \tilde{\psi}_\beta \rangle \quad (1.43)$$

Equation 1.42 reduces to

$$\langle \psi_\gamma | H_0 | \tilde{\psi}_\beta \rangle = \epsilon_\beta \langle \tilde{\psi}_\gamma | \tilde{\psi}_\beta \rangle + \frac{\hbar^2}{2\mu} a^2 \psi_\gamma^*(a) \tilde{\psi}_\beta(a) \left[\frac{\tilde{\psi}'_\beta(a)}{\tilde{\psi}_\beta(a)} - \left(\frac{\psi'_\gamma(a)}{\psi_\gamma(a)} \right)^* \right]. \quad (1.44)$$

The term in brackets is not readily identifiable. However, consider the following:

$$\langle \tilde{\psi}_\beta | H_0 | \psi_\gamma \rangle = \epsilon_\gamma \langle \tilde{\psi}_\beta | \psi_\gamma \rangle. \quad (1.45)$$

Since H_0 is hermitian, ($H_0^\dagger = H_0$)

$$\langle \tilde{\psi}_\beta | H_0 | \psi_\gamma \rangle = \epsilon_\gamma \langle \tilde{\psi}_\beta | \psi_\gamma \rangle = \langle H_0 \tilde{\psi}_\beta | \psi_\gamma \rangle \quad (1.46a)$$

$$= \langle \psi_\gamma | H_0 | \tilde{\psi}_\beta \rangle^* = \langle \psi_\gamma | H_0 | \tilde{\psi}_\beta \rangle. \quad (1.46b)$$

Therefore,

$$\langle \psi_\gamma | H_0 | \tilde{\psi}_\beta \rangle = e_\gamma \langle \tilde{\psi}_\beta | \tilde{\psi}_\gamma \rangle = e_\gamma \langle \tilde{\psi}_\gamma | \tilde{\psi}_\beta \rangle. \quad (1.47)$$

Comparing Equation 1.47 with Equation 1.44 we see that the bracketed term times $-\frac{\hbar^2}{2\mu}$ is just the energy level shift from e_γ to e_β . Of more crucial importance, however, is the result of Equation 1.47. It implies that in constructing matrix elements of the Hamiltonian one must take matrix elements between tilde and untilde states because then and only then can the problem of infinite matrix elements be circumvented. Let us now make use of this fact to diagonalize the full Hamiltonian H . The solution vectors of the Hamiltonian H will be linear superpositions of the basis vectors satisfying

$$H_0 \psi_\beta = e_\beta \psi_\beta. \quad (1.48)$$

Let us write such a solution as

$$\varphi_\alpha = \sum_\beta A_{\beta\alpha} \psi_\beta. \quad (1.49)$$

Then,

$$H \varphi_\alpha = E_\alpha \varphi_\alpha = \sum_\beta A_{\beta\alpha} H \psi_\beta \quad (1.50a)$$

$$= \sum_{\beta'} E_\alpha A_{\beta'\alpha} \psi_{\beta'} = \sum_\beta A_{\beta\alpha} (H_0 + V) \psi_\beta \quad (1.50b)$$

$$= \sum_{\beta'} E_\alpha A_{\beta'\alpha} \psi_{\beta'} = \sum_\beta A_{\beta\alpha} (e_\beta + V) \psi_\beta. \quad (1.50c)$$

Now take the matrix element of H with the tilde state $\tilde{\psi}_\gamma$

$$\begin{aligned}
\langle \tilde{\psi}_\gamma | H | \varphi_\alpha \rangle &= \sum_{\beta'} E_\alpha A_{\beta'\alpha} \langle \tilde{\psi}_\gamma | \psi_{\beta'} \rangle \\
&= \sum_{\beta} A_{\beta\alpha} [\epsilon_\beta \langle \tilde{\psi}_\gamma | \psi_\beta \rangle + \langle \tilde{\psi}_\gamma | V | \psi_\beta \rangle] .
\end{aligned} \tag{1.51}$$

Making use of Equation 1.34, one obtains

$$\begin{aligned}
\langle \tilde{\psi}_\gamma | H | \varphi_\alpha \rangle &= \sum_{\beta'} E_\alpha A_{\beta'\alpha} \langle \tilde{\psi}_\gamma | \tilde{\psi}_{\beta'} \rangle \\
&= \sum_{\beta} A_{\beta\alpha} [\epsilon_\beta \langle \tilde{\psi}_\gamma | \tilde{\psi}_\beta \rangle + \langle \tilde{\psi}_\gamma | V | \tilde{\psi}_\beta \rangle] .
\end{aligned} \tag{1.52}$$

Denoting

$$O_{\gamma\beta} = \langle \tilde{\psi}_\gamma | \tilde{\psi}_\beta \rangle \tag{1.53a}$$

$$V_{\gamma\beta} = \langle \tilde{\psi}_\gamma | V | \tilde{\psi}_\beta \rangle . \tag{1.53b}$$

Equation 1.52 in matrix notation becomes

$$O A E = O \epsilon A + V A \tag{1.54a}$$

$$\text{which implies, } A E = (\epsilon + O^{-1} V) A . \tag{1.54b}$$

If the solutions $\tilde{\psi}_\beta$ of H_0 formed an orthogonal basis, the overlap matrix, O , would be identically the unit matrix and the resulting matrix $(\epsilon + V)$ would be trivial to diagonalize since it is hermitian. However, as we shall see in Chapter III, the overlap matrix is not in general the identity matrix and thus the solution of the eigenvectors A and the eigenvalues E of the total Hamiltonian H leads to the non-trivial problem of diagonalizing a non-hermitian matrix. Because the eigenvectors A are identical to the

$A_{c,\lambda_c}^{J,\nu}$ of Equation 1.30 one sees that to obtain the correct interior wave functions for the nuclear Hamiltonian, the question of whether the basis set of functions of H_0 is truly orthogonal or not can not be lightly overlooked. In the past, the usual approach taken was to form the matrix elements of the Hamiltonian H by constructing

$$\langle \tilde{\psi}_\gamma | H | \tilde{\psi}_\beta \rangle \quad (1.55)$$

with the assumed orthogonality condition that

$$\langle \tilde{\psi}_\gamma | \tilde{\psi}_\beta \rangle = \delta_{\gamma\beta} . \quad (1.56)$$

As pointed out above this treatment is incorrect. It will, in fact, lead to sharp discontinuities in the eigenvalues of the total Hamiltonian and may produce false peaks in the partial cross sections.

CHAPTER 11. PHOTONUCLEAR CROSS SECTIONS

In contrast to incoming particles, photons interact with the nuclear system only weakly and thus the photon channels may be treated, as usual, by perturbation methods (14, p. 894). Photon emission and absorption processes may then be described as transitions between, say, the ground state of a nucleus and a particular eigenchannel state. A transition involving a linear combination of eigenchannel states, for example the process $C^{12}(\gamma, n)C^{11*}$, is then described by a suitable superposition of the matrix elements for these eigenchannels (27, p. 897). The total absorption cross section has the form (14, p. 55).

$$\sigma_{\pm} = (2\pi/\hbar) \rho_E (2\pi \hbar \omega e^2/c) |M|^2. \quad (2.1)$$

The $\pm$ refers to the photon polarizations and $\hbar \omega$ equals the energy of the incident photon. Since the largest contribution to the strength of the interactions in the giant resonance region is due to electric dipole transitions, the matrix elements M can be written as

$$M = (4\pi/3)^{1/2} \langle f | r Y_{1\pm 1} | i \rangle \quad (2.2)$$

where the state $|f\rangle$ is an eigenchannel state of the form given by Equation 1.22, and $|i\rangle$ represents the initial state. Since the ground state of the nucleus is an even parity state of total angular momentum zero, the only final state wave functions which need to be considered are those having $J = 1$, negative parity, and total isospin $T = 1$. The normalization of the wave function appearing in Equation 2.2 and the energy density of the final

states ρ_E must be defined consistently. Since the radial parts of Equation 1.22 are not square-integrable functions the eigendifferential technique first introduced by Weyl (28, p. 220) is employed. According to that method a continuum state is made normalizable to unity by integration over a finite but small energy interval ΔE . Let us designate such a state as $|\tilde{f}\rangle$. Then the density of states is simply

$$\rho_E = 1/\Delta E . \quad (2.3)$$

Since the radial wave functions depend explicitly on the product $E^{1/2} \cdot r$, as long as ΔE is very small no modification of the wave function is apparent unless r is very large. Thus the modification of the wave function needed for convergence of the normalization integral is confined to extremely large r , say to $r > b$, so that all calculations for the matrix elements and the diverse matchings to be discussed can be performed with the non-modified form of the wave function. In the asymptotic region, but before any modifications of the wave function set in, the final-state wave function has the form

$$|f\rangle = \tilde{N}^{-1} \sum_c v_c^{-1/2} v_c \omega_c(r) \tilde{\varphi}_c \quad r < b \quad (2.4)$$

which except for the normalization constant $\tilde{N}$, is an abbreviated version of Equation 1.22. The Weyl function $\tilde{\omega}_c(r)$ is introduced as

$$\tilde{\omega}_c(r) = W_c \int_E^{E + \Delta E} \omega_c(r) dE . \quad (2.5)$$

The constant W_c is chosen so that in the non-modified region

$$\tilde{\omega}_c(r) = \omega_c(r) \quad \text{for } r < b . \quad (2.6)$$

Then $|f\rangle$ goes over to $|\tilde{f}\rangle$ upon replacing $w_c(r)$ by $\tilde{w}_c(r)$ in Equation 2.4. The normalization condition for $|\tilde{f}\rangle$ then becomes

$$1 = \langle \tilde{f} | \tilde{f} \rangle = \tilde{N}^{-2} \sum_c v_c^{-1} (v_c)^2 \langle \tilde{w}_c | \tilde{w}_c \rangle . \quad (2.7)$$

In the region $r \approx b$ the function $w_c(r)$ has already the completely asymptotic form $w_c(r) = \sin(k_c r + \delta - L\pi/2)/r$. The addition of the logarithmic Coulomb phase in the case of charged particles is unimportant in this context. If we solve Equation 2.5 and employ the matching condition, Equation 2.6, the value of w_c is found to be (Appendix D),

$$w_c = \frac{1}{\Delta E} . \quad (2.8)$$

Therefore the normalization of $\tilde{w}_c(r)$ leads to

$$\langle \tilde{w}_c | \tilde{w}_c \rangle = (\pi k_c \hbar^2 / \mu_c) (1/\Delta E) . \quad (2.9)$$

This gives an overall normalization constant of

$$\tilde{N}^2 = \frac{1}{2} \pi \hbar (1/\Delta E) . \quad (2.10)$$

Because of the matching condition, Equation 2.6 the dipole matrix elements computed with the function $|\tilde{f}\rangle$ are the same as those computed with the unmodified function $|f\rangle$ with the appropriate normalization constant $\tilde{N}$.

Instead of using Equation 1.22 for the final state wave function, one could just as easily use the equivalent function defined by Equation 1.30 if we insert the normalization constant $N_{j,v}$ defined by Equation 1.33 to account for the different normalizations of Equations 1.22 and 1.30. Therefore, we may write

$$|f\rangle^v = (\tilde{N} N_{J,v})^{-1} \Psi_{INT}^{1,v}; \quad (2.11)$$

the superscript "1" on Ψ_{INT} reflecting the fact that $J = 1$. Thus the total dipole absorption cross section is

$$\sigma_{\pm} = 4\pi^2 (e^2/\hbar c) (\hbar\omega) \sum_v |M_v|^2 \quad (2.12)$$

with

$$M_v = (4\pi/3)^{1/2} \left[\frac{1}{2} \pi \hbar \sum_c (c_c^{1,v})^2 \right]^{-1/2} \langle \Psi_{INT}^{1,v} | r Y_{1\pm 1} | i \rangle. \quad (2.13)$$

Keeping in mind that the basis functions $\chi_{\lambda c}^{J,v}$ are merely an antisymmetrized product of one-particle-one-hole functions and defining α to be the set of quantum numbers

$$\alpha = \{ n_h, \ell_h, j_h \} \quad (2.14)$$

n_h being the radial quantum number of the hole state, the channel index c can be completely characterized by the set

$$c = \{ \alpha, n_p, \ell_p, j_p \}. \quad (2.15)$$

The angular distributions as derived in Appendix E take the form

$$P(\theta, E) = \sum_L B_L P_L(\cos \theta) \quad (2.16)$$

$$B_L = \sum_{v, \ell_p, j_p} \sum_{v', \ell_p', j_p'} M_v M_{v'} V_{\alpha \ell_p j_p}^{1,v} V_{\alpha \ell_p' j_p'}^{1,v'} \cos(\delta_1^v - \delta_1^{v'})$$

$$\times \cos[(\ell_p' - \ell_p) \pi/2] (-)^{j_h + 1/2} (3)(2L+1) \frac{1}{2} [1 + (-)^L]$$

$$\begin{aligned}
& \times [(2j_p + 1)(2j'_p + 1)(2\ell_p + 1)(2\ell'_p + 1)]^{1/2} \begin{pmatrix} \ell_p & \ell'_p & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & L \\ 1 & -1 & 0 \end{pmatrix} \\
& \times \begin{Bmatrix} j'_p & j_p & L \\ \ell_p & \ell'_p & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} j'_p & j_p & L \\ 1 & 1 & j_h \end{Bmatrix} (4\pi)^{-1}. \quad (2.17)
\end{aligned}$$

With α characterizing a particular residual nucleus, the various partial cross sections have the form

$$\int \frac{d\sigma_\alpha}{d\Omega} d\Omega = 4\pi^2 \left(\frac{e^2}{\hbar c} \right) (\hbar \omega) \sum_{\ell, j} \left| \sum_{\nu} e^{i\delta_{\ell j}^{\nu}} V_{\alpha \ell j}^{1, \nu} M_{\nu} \right|^2. \quad (2.18)$$

This completes the basic framework of the eigenchannel theory as applied to photonuclear reactions in the giant dipole resonance region.

CHAPTER III, CONTINUUM STRUCTURE CALCULATION OF C^{12} 3.1 Single particle wave functions

One of the primary objectives of this thesis is to test the validity of the eigenchannel theory as accurately as possible. This does not mean that we necessarily use the best model to represent the actual physical process. Instead, we choose a model which can be solved analytically and which possesses properties similar to that of the actual physical process. For instance if one wished to approximate the physical process in the best possible way, one could choose a Saxon-Woods potential to represent the potential function of the single-particle states. However, the solution of the total nuclear Hamiltonian would then involve complete numerical differentiation and integration for which the accuracy obtainable is completely dependent on the expertise of the numerical analyst solving the problem. However, if instead, one were to use a cutoff oscillator or even a spherically symmetric square well to approximate the single-particle potential, then analytic solutions of the nuclear Hamiltonian are easily found and the accumulated error can be more readily analyzed. If one is only interested in testing the eigenchannel theory for validity, the choice of a potential for which analytic solutions are easily obtainable seems to be the most logical approach. This is the procedure I have employed. The best explanation of the eigenchannel procedure is found in the work of Greiner and Wahnseiler (14). In this work the value of the truncating radius 'a' was taken to be that point beyond which the effect of the nuclear interactions becomes negligible (14, p. 895). Thus originally I was under

the impression that a square well would be an excellent single-particle potential to employ since the value of 'a' could be chosen to be the edge of the well. However, the actual criterion for the value of 'a' is the validity of the channel-orthogonality assumption, Equation 1.14. In the actual physical process the two definitions of 'a' proposed above coincide because the physical potential approaches zero as r approaches infinity and thus if 'a' is chosen large enough the nuclear interactions do become negligible and the channel orthogonality assumption is fulfilled as well. However, in the case of a square well, the nuclear interactions become zero at the edge of the well while channel orthogonality is not achieved unless 'a' is chosen much larger than the radius of the well. The construction of single-particle wave functions is, however, relatively easy for the square well potential and because too much time had already been involved in constructing the computer program for this type of potential, it was decided to leave the single-particle potential as basically that of a square well type and extend the radius 'a' from the edge of the well to the value of

$$a = 12F. \quad (3.1)$$

This value of 'a' was employed by Greiner and Wahsweiler (14) and was seen to satisfy Equation 1.14 quite well. As outlined in Chapter I, one should really choose a different value of 'a' for each channel considered but since the value defined by Equation 3.1 works quite well for all channels, the same value of 'a' is chosen for each open channel. It should be noted that the only real criterion for choosing the value of 'a' is the

validity of the channel-orthogonality assumption. Thus one could equally as well have chosen 'a' to be 17F, 20F, etc., since the validity of the channel-orthogonality assumption improves with increasing 'a' value. However, a large value of 'a' results in increased computer time and this must be borne in mind. In order to improve the square well approximation, terms involving $\vec{L} \cdot \vec{S}$ coupling and L^2 were added. Thus, the single-particle potential chosen has the form

$$V(r) = \frac{2}{\hbar^2} d_L \vec{L} \cdot \vec{S} + b_L \frac{L^2}{\hbar^2} - V_{sw} \quad (r \leq r_w) \quad (3.2a)$$

$$= 0 \quad (r > r_w) \quad (3.2b)$$

where d_L and b_L are constants dependent on L determined from the experimentally observed energy level splittings, V_{sw} is the depth of the square well and r_w is the radius of the well. Since we wish to examine the partial cross sections for the (γ, n) and (γ, p) processes, we do not use the isospin formalism but treat neutrons and protons separately. This implies different values of d_L , b_L , V_{sw} , and r_w for neutrons and protons since the charged particles do not see the same type of well as the uncharged particles due to the Coulomb force. Let us first examine the structure of the single-particle solutions to the Hamiltonian H_0 of Equation 1.1.

3.1.a. Neutron single-particle wave functions The single-particle radial wave functions are the solutions of

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{L(L+1)}{r^2} \right] R_{n,L}(r) + V(r) R_{n,L}(r) = E R_{n,L}(r) \quad (3.3)$$

with $V(r)$ defined as in Equation 3.2. The positive and negative energy radial solutions for the regions $r \leq r_w$ and $r \geq r_w$ are:

$$E > 0, \quad r \leq r_w : R_{n,L}(r) = j_L(kr) \quad (3.4a)$$

$$E > 0, \quad r \geq r_w : R_{n,L}(r) = \cos \delta_L j_L(\beta r) - \sin \delta_L n_L(\beta r) \quad (3.4b)$$

$$E < 0, \quad r \leq r_w : R_{n,L}(r) = j_L(k' r) \quad (3.4c)$$

$$E < 0, \quad r \geq r_w : R_{n,L}(r) = (-)^{L+1} \exp(3L\pi i/2) h_L^{(1)}(i\beta' r) \quad (3.4d)$$

with:

$$k^2 = \frac{2\mu}{\hbar^2} [E + V_{sw} - d_L \{J(J+1) - L(L+1) - S(S+1)\} - b_L L(L+1)] \quad (3.4e)$$

$$\beta^2 = \frac{2\mu}{\hbar^2} E \quad (3.4f)$$

$$k'^2 = \frac{2\mu}{\hbar^2} [V_{sw} - |E| - d_L \{J(J+1) - L(L+1) - S(S+1)\} - b_L L(L+1)] \quad (3.4g)$$

$$\beta'^2 = \frac{2\mu}{\hbar^2} |E| \quad (3.4h)$$

$$\delta_L = \text{real phase shift for angular momentum } L \quad (3.4j)$$

$$\mu = \text{reduced mass of the particle-residual nucleus system.} \quad (3.4k)$$

The functions j_L and n_L are the spherical Bessel and Neumann functions respectively and $h_L^{(1)}$ is the spherical Hankel function of the first kind. The phase factor multiplying $h_L^{(1)}$ ($i\beta'r$) insures that the function is real for all L -values and is the analogue of the charged particle solutions. The basic properties of these functions will be outlined in Chapter V. Suffice it to say that j_L , n_L , and $h_L^{(1)}$ are polynomials in their arguments and thus are easily calculable.

3.1.b. Proton single-particle wave functions To incorporate the dependence on charge we make the additional assumption that the charge distribution of the nucleus is also spherically symmetric. Therefore the potential function has the form

$$V(r) = \frac{Z_1 Z_2 e^2}{2r_w} \left[3 - \left(\frac{r}{r_w} \right)^2 \right] - V_{sw} + \frac{2d_L}{\hbar^2} \vec{L} \cdot \vec{S} + \frac{b_L \vec{L}^2}{\hbar^2} \quad (r \leq r_w) \quad (3.5a)$$

$$= Z_1 Z_2 e^2 / r \quad (r > r_w) \quad (3.5b)$$

The Hamiltonian H_0 for the charged particles is given by Equation 3.3 with the substitution of $V(r)$ as given by Equation 3.5. The positive and negative energy radial solutions for the charged particles in the regions $r \leq r_w$ and $r \geq r_w$ can be written in the following forms:

$$E > 0, \quad r \leq r_w : R_{n,L}(r) = S_L(\alpha, \gamma r) \quad (\text{see Appendix C}) \quad (3.6a)$$

$$E > 0, \quad r \geq r_w : R_{n,L}(r) = [\cos \delta_L F_L(\eta, \beta r) + \sin \delta_L G_L(\eta, \beta r)] / \beta r \quad (3.6b)$$

$$E < 0, r \leq r_w : R_{n,L}(r) = S_L(\alpha', \gamma r) \quad (3.6c)$$

$$E < 0, r \geq r_w : R_{n,L}(r) = W(-\eta', L + 1/2, 2\beta' r) \quad (3.6d)$$

with

$$\gamma^4 = Z_1 Z_2 e^2 \mu / (\hbar^2 r_w^3) \quad (3.6e)$$

$$\alpha = \frac{V_{sw} + E - 3 Z_1 Z_2 e^2 / 2r_w - d_L \{J(J+1) - L(L+1) - S(S+1)\} - b_L L(L+1)}{(2 \hbar^2 \gamma^2 / \mu)} \quad (3.6f)$$

$$\alpha' = \alpha \text{ with } E \text{ replaced by } -|E| \quad (3.6g)$$

$$\beta^2 = \frac{2\mu}{\hbar^2} E \quad (3.6h)$$

$$\beta'^2 = \frac{2\mu}{\hbar^2} |E| \quad (3.6j)$$

$$\eta = \mu Z_1 Z_2 e^2 / \beta \hbar^2 \quad (3.6k)$$

$$\eta' = \mu Z_1 Z_2 e^2 / \beta' \hbar^2 \quad (3.6l)$$

$$\delta_L = \text{real phase shift for angular momentum } L \quad (3.6m)$$

$$\mu = \text{reduced mass of the particle-residual nucleus system.} \quad (3.6n)$$

The functions F_L and G_L are the regular and irregular Coulomb functions respectively. The function W is a Whittaker function defined by

$$W(-\eta, L+1/2, 2\rho) = \frac{\exp(-\rho - \eta \ln 2\rho)}{\Gamma(1+L+\eta)} \int_0^\infty t^{L+\eta} e^{-t} \left(1 + \frac{t}{2\rho}\right)^{L-\eta} dt. \quad (3.7)$$

The function $S_L(\alpha, \gamma r)$ is essentially a confluent hypergeometric function most easily expressed as:

$$S_L(\alpha, \gamma r) = \left(\frac{\pi\alpha}{4}\right)^{1/2} (\gamma r)^L \sum_{k=0}^{\infty} a_k \frac{(\gamma r)^{2k}}{2^k k!} \quad (3.8a)$$

$$a_0 = 1; \quad a_1 = -2\alpha / (L + 3/2) \quad (3.8b)$$

$$(L + 3/2 + k) a_{k+1} = -2\alpha a_k - k a_{k-1} \quad (k = 1, 2, 3, \dots) \quad (3.8c)$$

The functions F_L , G_L , and W are discussed in Chapter IV and a full discussion of $S_L(\alpha, \gamma r)$ can be found in Appendix C.

3.2 Parameter values for the C^{12} nucleus

The experimental energy spectrum for the bound states of C^{12} can be easily obtained from binding energy considerations of the nuclei C^{11} , B^{11} , C^{13} , and N^{13} . Using the energy level schemes as reported by Lauritsen and Ajzenberg-Selove (29,30) for the neighboring nuclei of C^{12} , one obtains the positions of the bound proton and neutron states as given in Figure 1. The proton $1s_{1/2}$ state at -34 MeV was taken from (p, 2p) and (e, e'p) data (31,32,33). The position of the neutron $1s_{1/2}$ state at -37 MeV is deduced from the energy separation of the $1p$ - $1d$ states in the bound neutron spectrum. From the energy splittings of the $1p$ and $1d$ states the following parameter values for d_L and b_L were obtained:

Figure 1. Bound state spectrum for C^{12}

Neutrons

$$d_{L=1} = -4.593 \text{ MeV}; d_{L=2} = -0.766 \text{ MeV}; b_{L=1,2} = 0.382 \text{ MeV} \quad (3.9a)$$

Protons

$$d_{L=1} = -4.673 \text{ MeV}; d_{L=2} = -0.670 \text{ MeV}; b_{L=1,2} = 0.423 \text{ MeV}. \quad (3.9b)$$

The well depth, V_{sw} , and the radius of the square well, r_w , were obtained by correctly reproducing the energy dependence of the bound $1p_{3/2}$ and $1s_{1/2}$ states for both neutrons and protons. The following parameters for V_{sw} and r_w are obtained:

$$V_{sw}(\text{neutrons}) = 59.812 \text{ MeV}; r_w(\text{neutrons}) = 2.4654F \quad (3.10a)$$

$$V_{sw}(\text{protons}) = 56.165 \text{ MeV}; r_w(\text{protons}) = 2.4663F. \quad (3.10b)$$

In the calculation of the particle-hole wave functions, the energies of the hole states are taken directly from experiment as is customary in this type of calculation. This is essential in order to obtain the correct particle thresholds. Suppressing the radial quantum numbers, there are 10 1-particle -1-hole configurations contributing to the 1^- compound states of C^{12} which are taken into account:

(1) $(s_{1/2}, \bar{p}_{3/2})_n$	(6) $(s_{1/2}, \bar{p}_{3/2})_p$	
(2) $(d_{3/2}, \bar{p}_{3/2})_n$	(7) $(d_{3/2}, \bar{p}_{3/2})_p$	
(3) $(d_{5/2}, \bar{p}_{3/2})_n$	(8) $(d_{5/2}, \bar{p}_{3/2})_p$	
(4) $(p_{1/2}, \bar{s}_{1/2})_n$	(9) $(p_{1/2}, \bar{s}_{1/2})_p$	
(5) $(p_{3/2}, \bar{s}_{1/2})_n$	(10) $(p_{3/2}, \bar{s}_{1/2})_p$	(3.11)

The above numbering of the channels will be used throughout this thesis. So e.g., $c = 6$ will refer to the $(s_{1/2}, \bar{p}_{3/2})$ proton channel. The empirical thresholds for the various particle processes which have been used to fix the hole energies are listed in Table 1.

Table 1. Threshold energies

Name of the Residual Nucleus	Configuration of Residual Nucleus	Type of Particle	Q_c (MeV)
C^{11}	$\bar{p}_{3/2}$	n	18.72
B^{11}	$\bar{p}_{3/2}$	p	15.96
C^{11*}	$\bar{s}_{1/2}$	n	37.00
B^{11*}	$\bar{s}_{1/2}$	p	34.00

As stated previously, the value of the matching radius was set at

$$a = 12F. \quad (3.12)$$

The hole state for each channel is completely determined by the corresponding wave functions 3.4c, and 3.4d for the neutron channels and by 3.6c and 3.6d for the proton channels. The hole states are normalized to unity over all space.

3.3 Energies of the particle states

The reduced radial functions $U_{n,L}(r) = r \cdot R_{n,L}(r)$ of the positive energy particle states must obey the logarithmic derivative condition,

Equation 1.24 in each channel, c . The channel energy E_c and the wave number k_c are given by

$$E_c = E_\gamma - Q_c \quad (3.13a)$$

$$k_c^2 = 2\mu_c E_c / \hbar^2 \quad (3.13b)$$

with Q_c given by Table I. Choosing a phase δ_1 , one constructs the boundary condition value

$$B_c = \left[\frac{r (d/dr) f_c(k_c r)}{f_c(k_c r)} \right]_{r=a_c} \quad (3.14a)$$

where

$$f_c = G_L(\eta, k_c r) \sin(\delta_1 - \eta_c) + F_L(\eta, k_c r) \cos(\delta_1 - \eta_c) \quad (3.14b)$$

for a proton channel, and

$$f_c = r[j_L(k_c r) \cos \delta_1 - n_L(k_c r) \sin \delta_1] \quad (3.14c)$$

for a neutron channel. Once B_c is evaluated in a particular channel for a fixed energy E_c and phase δ_1 , it may be looked upon as a pure number. The single particle states in channel c must satisfy

$$r(d/dr) U_{n,L}(\beta r) \Big|_{r=a} = B_c U_{n,L}(\beta r) \Big|_{r=a} \quad (3.15)$$

where $U_{n,L}(\beta r)$ is given by Equation 3.6b for a proton channel and Equation 3.4b for a neutron channel. It is at this point that the choice of a cut-off potential becomes annoying because the real phase shift δ_L appearing in

Equations 3.4b and 3.6b is dependent on the matching of the wave functions for $r \leq r_w$ and $r \geq r_w$ at the well radius. Thus Equation 3.15 actually involves a double matching condition, one at $r = a$ and one at $r = r_w$. For the case of a neutron channel one finds that Equation 3.15 represents the equation

$$(\beta a) \frac{[j_L'(\beta a) - \tan \delta_L n_L'(\beta a)]}{[j_L(\beta a) - \tan \delta_L n_L(\beta a)]} = B_c - 1 \quad (3.16a)$$

where

$$\tan \delta_L = \frac{(kr_w) j_L' (kr_w) j_L (\beta r_w) - (\beta r_w) j_L (kr_w) j_L' (\beta r_w)}{(kr_w) j_L' (kr_w) n_L (\beta r_w) - (\beta r_w) j_L (kr_w) n_L' (\beta r_w)} \quad (3.16b)$$

$$\text{with } k^2 - \beta^2 = \frac{2\mu}{\hbar^2} [V_{sw} - d_L \{J(J+1) - L(L+1) - S(S+1)\} - b_L L(L+1)]. \quad (3.16c)$$

The derivatives of the functions in Equation 3.16 are taken with respect to their arguments. For the case of a proton channel one finds

$$B_c = \frac{(\beta a)[F_L'(\eta, \beta a) + \tan \delta_L G_L'(\eta, \beta a)]}{[F_L(\eta, \beta a) + \tan \delta_L G_L(\eta, \beta a)]} \quad (3.17a)$$

where

$$\tan \delta_L = \frac{\left[\frac{\gamma r_w s_L'(\alpha, \gamma r_w)}{s_L(\alpha, \gamma r_w)} + 1 \right] F_L(\eta, \beta r_w) - (\beta r_w) F_L'(\eta, \beta r_w)}{(\beta r_w) G_L'(\eta, \beta r_w) - \left[\frac{\gamma r_w s_L'(\alpha, \gamma r_w)}{s_L(\alpha, \gamma r_w)} + 1 \right] G_L(\eta, \beta r_w)} \quad (3.17b)$$

with the values of α and β related by Equations 3.6f and 3.6h. Neither Equation 3.16 nor Equation 3.17 is particularly easy to solve for β , the general result for a particular L-value being a highly complex transcendental equation. Because of the transcendental nature of these equations, the value β (and correspondingly the energy E) can take on an infinity of values and still satisfy the matching condition Equation 3.15 because B_c is merely a number independent of β . However if one were to plot the logarithmic derivative of the radial wave functions for a particular channel against the energy $E(\beta) \geq 0$ the following graph is obtained:

Figure 2. Boundary condition vs. E .

The fixed boundary condition B_c can then be represented by a horizontal line whose points of intersection with the cotangent-shaped curve determines the discrete particle energies for the states with different radial quantum

numbers. Obviously one can not handle numerically an infinity of positive energy states so the values of E_n ($n = 1, 2, \dots, \infty$) must be truncated at some value, say E_{MAX} . This truncation of the particle basis can only be justified on the ground that if one were to include particle states with an energy E greater than E_{MAX} , the higher lying states involved give a negligible contribution to the total wave function. The value of E_{MAX} chosen in this thesis was

$$E_{MAX} = 8 (E_\gamma - |E_{P_{3/2}}^-|_P). \quad (3.18)$$

Thus for an incident photon energy of 22 MeV, the cutoff value on the energy of the allowed particle states was 48.5 MeV. However, the energy cutoff value was converted to a value N specifying the number of states below E_{MAX} . In order to keep the dimension of the Hilbert space for the particle state energies as consistent as possible, the same value of N was chosen for each open channel even though the maximum energy determined by N in some of the open channels might be slightly larger than E_{MAX} . The relation of incident photon energy to the number of particle states kept within each open channel is given by Table 2. Thus, for example, if $E_\gamma = 22$ MeV, channels 1, 2, 3, 6, 7, and 8 are open and the number of particle states kept within each channel is four giving a total of twenty-four particle states used to construct the total wave function. This implies that the basis set of functions used to diagonalize the Hamiltonian consists of 24 wave functions and thus both the H-matrix and the S-matrix are 24×24 matrices. One can easily see that this type of calculation can

Table 2. Energy cutoff values

E_γ (MeV)	Number of particle states used
≤ 24	4
24 - 35	5
35 - 40	6
$\geq 40^*$	7

*Cross sections for $E_\gamma > 40$ MeV were not actually calculated because very little structure $^\gamma$ is seen experimentally for these energies and the amount of computer time involved is quite prohibitive.

be quite lengthy especially if one considers an incident photon energy of $E_\gamma > 40$ MeV for which the H and S matrices will be of order 70. The single particle energies $\beta_{c,\lambda}$ ($\lambda = 1, 2, \dots, N$) for each open channel c can be determined from Equations 3.12 - 3.14 by standard iterative methods which will be discussed in Chapter V. The particle states are then normalized to unity over a sphere of radius 'a.'

The single particle states thus formed in each open channel are then coupled to the corresponding hole state wave function for that channel to obtain a state of total angular momentum $J = 1$, parity = -1.

$$|n_{\beta,c}\rangle = \sum_{m_p m_h} (-)^{2j_h - j_p - m_p} \sqrt{3} \begin{pmatrix} j_p & j_h & 1 \\ m_p & -m_h & -m \end{pmatrix} U_{n_p, \ell_p}(\beta_{n_p} r_p) r_p^{-1} \times$$

$$U_{n_h, \ell_h}(\beta_{n_h} r_h) r_h^{-1} |(\ell_p s_p) j_p, m_p\rangle |(\ell_h s_h) j_h, m_h\rangle |\tau_h\rangle |\tau_p\rangle \quad (3.19)$$

(see Appendix A, Section A-4). This state must still be properly anti-symmetrized in particle-hole coordinates. The next step is to construct the energy matrix and diagonalize it.

3.4 Construction of the energy matrix

From Chapter 1, Section 1.5, we know how to construct the matrix elements of the total Hamiltonian H using the "tilde" wave functions which are analogous to the function defined by Equation 3.19. However, it is at this point that one must ask whether the overlap matrix is the identity matrix. Let us consider the overlap $\langle n'_{\beta} c' | n_{\beta} c \rangle$. Using Equation 3.19 one finds

$$\langle n'_{\beta} c' | n_{\beta} c \rangle = \int_0^a U_{n', l_p}^* (\beta' p r) U_{n, l_p} (\beta p r) dr \delta_{c, c'}$$

with

$$\delta_{c, c'} = \delta_{l_p l'_p} \delta_{m_{l_p} m'_{l_p}} \delta_{l_h l'_h} \delta_{m_{l_h} m'_{l_h}} \quad (3.20)$$

If $n'_{\beta} = n_{\beta}$, then

$$\langle n c' | n c \rangle = \delta_{c, c'} \quad (3.21)$$

since the particle functions are normalized over the sphere of radius 'a'. But if $n'_{\beta} \neq n_{\beta}$ then one is faced with the overlap integral given by Equation 3.20. If the upper limit of the integral were infinity then the value of the integral would be a delta-function in β, β' since

$$\int_0^{\infty} U_{n', \ell_p}^* (\beta' r) U_{n, \ell_p} (\beta r) dr = \frac{\pi}{2\beta} \delta(\beta - \beta') \quad (3.22)$$

for both the neutron and proton wave functions. But the delta function in Equation 3.22 is exactly what led us to consider the "tilde" wave functions normalized over the sphere $r = a$. One could lightly overlook the overlap integral and tacitly assume the overlap matrix to be the identity matrix but if one were to actually calculate the integral appearing in 3.20 for various β values, it soon becomes apparent that off-diagonal elements of the overlap matrix can be appreciably large. In this thesis, the maximum off-diagonal contribution was of the order 0.10 which means that if we assume the overlap matrix to be the identity matrix we incorporate an error as large as ten percent into the calculation. Therefore the overlap matrix must be constructed and utilized as outlined in Chapter I, Section 1.5. The end result of this utilization is a non-hermitian energy matrix to diagonalize. One could just as easily have turned this problem of the overlap matrix around and looked at it from the point of view of a non-orthonormal basis; the two concepts being equivalent. Why should one even consider using this non-orthonormal basis when procedures such as the Gram-Schmidt process are available to transform the non-orthonormal basis into an orthonormal one? If this could be done, the energy matrix would be hermitian and easily solvable by standard techniques such as the Givens-Householder or Jacobi methods. Look for a moment at the mechanics of the Gram-Schmidt orthogonalization procedure. Let $\{ \beta_1, \beta_2, \dots, \beta_N \}$ be the

non-orthogonal basis under consideration. One obtains the orthogonal basis $\{ \alpha_1, \alpha_2, \dots, \alpha_N \}$ by letting:

$$\alpha_1 = \beta_1 \quad (3.23a)$$

$$\alpha_2 = \beta_2 - \frac{(\beta_2, \alpha_1)}{|| \alpha_1 ||^2} \alpha_1 \quad (3.23b)$$

$$\alpha_{k+1} = \beta_{k+1} - \sum_{j=1}^k \frac{(\beta_{k+1}, \alpha_j)}{|| \alpha_j ||^2} \alpha_j \quad (3.23c)$$

If any value of β_k has an error ϵ the corresponding error in α_k is $k \cdot \epsilon$. Thus for a basis set of 24 functions with the first function off by .05%, the value of α_{24} will have accumulated an error of 12%. Obviously, on computational grounds, the use of any type of orthogonalizing procedure soon leads to unacceptable round-off error. With bases of order 24 to 70 as employed in this thesis, the use of the overlap matrix itself is crucial in order to control error build-up. Thus one must be content with diagonalizing a non-hermitian matrix. Whenever a truncating radius is imposed on the configuration space of the single-particle wave functions, the problem of the overlap matrix will arise and if and only if the off-diagonal elements of 0 are "sufficiently small" can one circumvent the diagonalization of a non-hermitian energy matrix.

Before we consider the explicit form of the elements of the energy matrix, let us consider the residual interaction V_{ph} of the total Hamiltonian, Equation 1.1. From the work of Brown and Bolsterli (11) and Eisenberg

and Letourneux (34) the residual interaction should have the following properties:

1) Since the nucleon-nucleon interaction is short-ranged, V_{ph} should reflect this near zero range behavior.

2) Due to the exclusion principle, nucleons will prefer to interact at the nuclear surface where more unoccupied states are available (34, p. 119).

3) The angular dependence of the particle and hole should be strongly correlated.

4) Since in dipole absorption the state of interest is a $J^\pi = 1^-$, $T = 1$ state, V_{ph} should have a term proportional to $\vec{\tau}_i \cdot \vec{\tau}_j$ which is repulsive for like particles and will push the $T = 1$ levels up (11, p. 475).

5) V_{ph} should have mathematical simplicity if possible. The usual convention chosen for light nuclei is to take V_{ph} as the zero-range force.

$$V_{ph} = -V_0 \delta(\vec{r}_p - \vec{r}_h) [a_0 + a_1 \vec{\tau}(1) \cdot \vec{\tau}(2)] . \quad (3.24)$$

However, this potential results in an integration of the particle-hole functions which is very time-consuming on the computer. Instead, I chose to use the simple surface-delta function with a Meshkov-Soper exchange mixture (35)

$$V_{ph} = -V_0 \delta(\vec{r}_p - \vec{r}_h) \delta(r_p - r_w) r_w^{-2} [a_0 + a_\sigma \vec{\sigma}(1) \cdot \vec{\sigma}(2) + a_\tau \vec{\tau}(1) \cdot \vec{\tau}(2) + a_{\sigma\tau} \vec{\sigma}(1) \cdot \vec{\sigma}(2) \vec{\tau}(1) \cdot \vec{\tau}(2)] . \quad (3.25)$$

The parameters of the exchange mixture are:

$$a_o = 0.865 \quad (3.26a)$$

$$a_{\sigma} = 0.135 \quad (3.26b)$$

$$a_{\tau} = a_{\sigma\tau} = 0. \quad (3.26c)$$

As shown by Eisenberg and Letourneux (34) for O^{16} , this type of residual interaction produces reasonable results but is not superior to the zero-range force except for its extreme mathematical simplicity. The exchange parameters a_{τ} and $a_{\sigma\tau}$ are set equal to zero because as stated previously, the protons and neutrons are treated separately. The property that V_{ph} raise the $T=1$ levels can be simulated by raising the $S=1$ levels with the term $\vec{\sigma}(1) \cdot \vec{\sigma}(2)$. This follows from the Pauli principle which implies that

$$L + S + T = \text{odd number} . \quad (3.27)$$

The parity of the dipole state is odd so L is odd and since we seek $T=1$ levels, this implies S should be odd. Since neutrons and protons have spin $1/2$, a particle-hole state can only have a total spin S of 0 or 1. Thus, the states of interest are the $S=1$ states which can be raised by the $\vec{\sigma}(1) \cdot \vec{\sigma}(2)$ operator. To insure that strong mixing of the states is preserved the calculation of the matrix elements of V_{ph} is performed as though isotopic spin was a good quantum number and the terms a_{τ} and $a_{\sigma\tau}$ were not zero. In the final result, we set $a_{\tau} = a_{\sigma\tau} = 0$ and average over the charge. In Equation 3.20 the particle-hole state $|n_{\beta}, c\rangle$ must still be antisymmetrized before we take matrix elements of V_{ph} . One would like to be

able to use the second quantization formalism with the usual anti-commutation properties of the creation and annihilation operators $a, a^\dagger$ respectively. In terms of these operators, an uncoupled particle-hole state has the form

$$|j_1 j_2^{-1}\rangle = a_1^\dagger a_2 |core\rangle. \quad (3.28)$$

Throughout the rest of this thesis when we speak of the matrix elements of V_{ph} we mean those terms which are not part of the explicit definitions of the particle energy, the hole energy, or the ground state energy. Then in the usual manner the uncoupled matrix elements of V_{ph} derived from

$$(j_1 j_2^{-1} | V_{ph} | j_3 j_4^{-1}) = \frac{1}{2} \sum_{\alpha \beta \gamma \delta} (\alpha \beta | V | \gamma \delta)$$

$$\langle core | a_2^\dagger a_1 a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_3^\dagger a_4 | core \rangle \quad (3.29a)$$

become

$$(j_1 j_2^{-1} | V_{ph} | j_3 j_4^{-1}) = - (14 | V | 32) + (14 | V | 23) \quad (3.29b)$$

$$\text{with } (ij | V | km) = \iint d\vec{r}_1 d\vec{r}_2 \varphi_i^\dagger(1) \varphi_j^\dagger(2) V_{ph} \varphi_k(1) \varphi_m(2).$$

However, one is not entitled to use the second quantization formalism since different particle states in the same channel are not orthogonal (i.e., the overlap matrix is not the identity matrix). One could argue that since V_{ph} is a two-body operator of the delta function type that there will never be any overlap integrals in the matrix elements of V_{ph} .

It would seem unlikely that factors proportional to the overlap matrix would appear in the matrix elements of V_{ph} even if one could treat the problem correctly by employing the Slater determinant representations of the particle-hole states. For a non-orthogonal set of states the Slater determinant approach proves to be extremely unmanageable. What type of error do we incur if we use the matrix elements of V_{ph} as given by Equation 3.29? Instead of a particle state being represented by a single creation operator, one can think of the non-orthogonal particle states as being represented by the operator

$$b^\dagger = X a^\dagger + Y a \quad (3.30)$$

where X is almost one and Y is almost zero since the off-diagonal elements of the overlap matrix are small. The implied normalization of the particle state represented by Equation 3.30 is

$$X^2 + Y^2 = 1. \quad (3.31)$$

The uncoupled matrix elements of V_{ph} using the b -operator take the form

$$\langle j_1 j_2^{-1} | V_{ph} | j_3 j_4^{-1} \rangle = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta | V | \gamma\delta) \langle \text{core} | a_2^\dagger b_1 a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma b_3^\dagger a_4 | \text{core} \rangle \quad (3.32a)$$

with

$$b_1^\dagger = X a_1^\dagger + Y a_1 \quad (3.32b)$$

$$b_3^\dagger = X a_3^\dagger + Y a_3 \quad (3.32c)$$

Explicitly putting $b_1^\dagger$ and $b_3^\dagger$ into Equation 3.32 gives the result

$$\begin{aligned} \langle j_1 j_2^{-1} | V_{ph} | j_3 j_4^{-1} \rangle &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta | V | \gamma\delta) \{ \langle \text{core} | a_2^\dagger a_1 a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_3^\dagger a_4 | \text{core} \rangle \\ &+ Y^2 [\langle \text{core} | a_2^\dagger a_1 a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_3^\dagger a_4 | \text{core} \rangle + \\ &+ \langle \text{core} | a_2^\dagger a_1^\dagger a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_3 a_4 | \text{core} \rangle] \} . \end{aligned} \quad (3.33)$$

The first term is the usual second quantization result yielding Equation 3.29. The second term is a sum of matrix elements of a one-particle-one-hole state and a two-particle-two-hole state. Since Y is small, keeping this term would be the same as carrying out the calculation to second order in the overlap matrix. This is a very small contribution and we neglect it. So one could say that to first order in the overlap matrix, the matrix elements of V_{ph} are given by Equation 3.29. Explicitly, the coupled matrix elements of V_{ph} in this approximation are given by

$$\begin{aligned} V_{bB; aA} &= \left(\frac{V_0}{4\pi} \right) (-)^{l_A + l_B} \hat{l}_a \hat{l}_A \hat{l}_b \hat{l}_B \hat{j}_a \hat{j}_A \hat{j}_b \hat{j}_B \times \\ &\times \sum_{\lambda} \sum_{S=0,1} (2\lambda+1) (-)^{l_A - l_a + l_B - l_b} \begin{pmatrix} l_a & l_B & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_b & l_B & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times \\ &\times G_S^{m_T^A, m_T^B} (2S+1) \begin{Bmatrix} l_a & \frac{1}{2} j_a \\ l_A & \frac{1}{2} j_A \\ \lambda & S J \end{Bmatrix} \begin{Bmatrix} l_b & \frac{1}{2} j_b \\ l_B & \frac{1}{2} j_B \\ \lambda & S J \end{Bmatrix} R_b^*(r_w) R_A^*(r_w) R_a(r_w) R_B(r_w) \end{aligned} \quad (3.34a)$$

$$\text{where, } G_0^{m_\tau, m'_\tau} = (2 - \delta m_\tau, m'_\tau) a_o - (3\delta m_\tau, m'_\tau) a_\tau - (3\delta m_\tau, m'_\tau) a_\sigma - 3(2 - \delta m_\tau, m'_\tau) a_{\sigma\tau} \quad (3.34b)$$

$$G_1^{m_\tau, m'_\tau} = -(\delta m_\tau, m'_\tau) a_o - (2 - \delta m_\tau, m'_\tau) a_\tau + (2 + \delta m_\tau, m'_\tau) a_\sigma + (4 - 5 \delta m_\tau, m'_\tau) a_{\sigma\tau} \quad (3.34c)$$

with $\hat{x} = (2x + 1)^{1/2}$, and $R_c(r_w)$ is the radial particle (hole) function evaluated at the edge of the well (see Appendix B for a complete derivation); lower case subscripts indicate particles and upper case subscripts indicate holes.

Let us now recall the energy matrix Equation 1.54b;

$$AE = (\mathcal{E} + 0^{-1} V) A. \quad (3.35)$$

The matrix elements of V are given by Equation 3.34. The elements of the overlap matrix are constructed using Equation 3.18 and 3.19. The matrix $\mathcal{E}$ is a diagonal matrix with the difference of the particle and hole energies $(\mathcal{E}_p - \mathcal{E}_h)$ appearing on the diagonal. The matrix $(\mathcal{E} + 0^{-1} V)$ can be diagonalized by the double QR transformation of J. G. F. Francis (36,37). In general, a non-hermitian matrix will have both real and complex eigenvalues. Since the eigenvalues E_λ ($\lambda = 1, 2, 3, \dots, N$), N being the order of the matrix E , represent the energies of real physical states, we expect them to be real. In fact, since $\mathcal{E}$ and 0 are symmetric, positive-definite matrices and V is symmetric one can show that only real

eigenvalues will result from the diagonalization.

Let us stop and examine what we have done so far. First we chose an energy E_γ and phase δ_1 and constructed the boundary conditions B_c for each open channel c . Then we solved for the truncated set of single-particle functions which form the basis for the diagonalization of H . Constructing the subsidiary matrices $\mathcal{E}$, O , and V we diagonalized the energy matrix $E = \mathcal{E} + O^{-1} V$. Now we ask the following question. Does any one value of E_λ ($\lambda = 1, 2, 3, \dots, N$) equal E_γ ? If so, then from Section 1.4 we know that δ_1 is an eigenphase, $\delta_1^{1,\nu}$. If no value of E_λ ($\lambda = 1, 2, 3, \dots, N$) equals E_γ then δ_1 is not an eigenphase so we choose a new value of δ_1 and begin all over again. There are as many eigenphases in general as there are open channels so the iteration process involves solving for the particle states and diagonalizing the Hamiltonian many times over. This can be an extremely time consuming process even if one has a definite method of searching which proves successful. Before I describe the search procedure used for the eigenphases, I think it important to point out how one constructs the partial cross sections and angular distributions once the eigenphases are known. The eigenvectors $V_c^{1,\nu}$, Equation 1.32, are completely specified once the values of $A_{\lambda_c, c}^{1,\nu}$ are known. The values of A are the eigenvectors of the diagonalization process. In Equation 1.31, the $U_{\lambda_c, c}^{(\nu)}(a)$ are the reduced particle wave functions satisfying the ν th boundary condition (the values of B_c with δ_1 being the ν th eigenphase) evaluated at the radius "a." Once the values of $V_c^{1,\nu}$ are known for $\nu = 1, 2, 3, \dots, N$ the angular distributions and partial cross sections are easily evaluated from Equations 2.17 and 2.18. The dipole matrix elements

M_v (Equation 2.13) are easily calculated by assuming the initial state $|i\rangle$ to be the ground state of the nucleus which can be thought of as a particle and hole coupled to total angular momentum zero. Referring to Equation 2.14, the final state wave function $\Psi_{INT}^{l,v}$ is a linear superposition of the particle-hole states of the truncated basis; each state satisfying the v th boundary condition. Then the matrix element

$$\langle \Psi_{INT}^{l,v} | r Y_{l \pm 1} | i \rangle$$

will be a sum of terms of the following form:

$$\begin{aligned} \langle (j_p j_h) 1M | r Y_{l \pm 1} | (j_p' j_h') 00 \rangle = (-)^{j_h - 1/2} \frac{\hat{l}_p \hat{l}_h \hat{j}_p}{\sqrt{4\pi}} \times \\ \times \begin{pmatrix} l_p & 1 & l_h \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_h & j_h & \frac{1}{2} \\ j_p & l_p & 1 \end{Bmatrix} \delta_{j_p' j_p} \delta_{j_h' j_h} \int_0^a U_{n_p}^* (r) U_{n_h} (r) r^3 dr. \quad (3.36) \end{aligned}$$

Thus the prime objective is to find the eigenphases $\delta^{l,v}$ and the eigenvectors $V_c^{l,v}$ from which all the necessary information concerning the reaction can be obtained.

3.5 Search for the eigenphases

If one examines the form of the boundary condition B_c Equation 3.14, for a fixed energy E_c it is apparent that $B_c(\delta_1) = B_c(\delta_1 + \pi)$. Thus the boundary condition is periodic with period π . Therefore the eigenphases are restricted to an interval of length π and the conventional choice is

$$0 \leq \delta^{J,v} \leq \pi. \quad (3.37)$$

Let us now investigate Figure 2 in more detail. The boundary condition B_c is just a horizontal line on this graph, its intersection with the curve giving the particle state energies. Let us suppose B_c is negative. Then there will be a particle state in each of the regions I, II, III, etc. In fact, this will be the case whenever B_c is less than the value of the curve at zero energy (i.e., the point A in Figure 2). If B_c is greater than the function value at A then there will be a particle state in each of the energy regions II, III, IV, etc. Note that for this case, the state lying in region I is lost. This causes a rather sharp change in the Hilbert space of the particle states. Where does this discontinuity manifest itself? For a particular value of δ_1 ($0 \leq \delta_1 \leq \pi$) there will be an ϵ -neighborhood about δ_1 in which a particular value of B_c crosses the zero energy point, A. Within this ϵ -neighborhood of δ_1 there will be a correspondingly discontinuous jump in the eigenvalues of the energy matrix. If there are N open channels then B_c crosses the zero energy point N times; once in each open channel. Thus there are N ϵ -neighborhoods of δ_1 which produce a discontinuity in the eigenvalues of the energy matrix. If one were to plot the eigenvalues of the energy matrix versus the phase δ_1 ($0 \leq \delta_1 \leq \pi$), there would be exactly N points at which the graph would exhibit discontinuities. If X_1 and X_2 represent two such discontinuity points then the eigenvalues will be continuous in the interval $X_1 + \epsilon$ to $X_2 - \epsilon$. Are there any other values of B_c which could cause a similar discontinuity in the eigenphases of the energy matrix? The astute observer will point out the fact that when B_c goes

from $-\infty$ to $+\infty$ (the point separating regions I and II in Figure 2) the particle states seem to experience a similar discontinuity in that the state lying in region I is similarly lost. At first glance this would seem to indicate that instead of N discontinuity points we have $2N$ such values of δ_1 . However, since the truncation criterion is given by a fixed number of states we will always have the same total number of basis states and so the real determining factor as to whether a discontinuity appears is the progression of the energies of the states kept within a channel. From Figure 2 it is evident that if B_c starts out at a negative value and proceeds to become more negative eventually crossing the infinity point, the particle state energies follow an increasing energy pattern; that is, the energies of the states continuously increase. This is not the case when we consider B_c crossing the zero energy point, A . In this case a state of lower energy is introduced and the pattern of increasing energy is broken. This is the real reason for the discontinuity in the eigenvalues of the energy matrix. It is true that the eigenvalues of the energy matrix have a pattern all their own but a break in the pattern of the single-particle energies should and does manifest itself by breaking the pattern of the eigenvalues of the energy matrix. Because the infinity cross overs do not break this pattern they may be excluded as discontinuity points. Referring to Figure 3 let us examine the search procedure for the eigenphases.

Figure 3 is a representation of the search procedure in the case of five open channels. The five discontinuity points (X_1, X_2, X_3, X_4, X_5) are obtained by calculating in each open channel the value of δ_1

Figure 3. Search procedure for eigenphases

which will cause B_c to equal the boundary condition value of the particle states at zero energy. We first let $\delta_1 = 0$, solve for the eigenvalues of the energy matrix and keep count of the number of eigenvalues, say N_0 , less than the desired energy E_γ . We repeat the process at $\delta_1 = X_1 - \epsilon$ where

$$\epsilon = 0.001 \quad (3.38)$$

and obtain the number of eigenvalues less than E_γ at $X_1 - \epsilon$, say N_1 . The absolute value of the difference of N_1 and N_0 , ($|N_1| - |N_0|$), tells us the number of eigenphases lying within this interval. If no eigenphase exists within this interval we skip to the interval $(X_1 + \epsilon, X_2 - \epsilon)$ and repeat the testing process. If one or more eigenphases exist within the interval we successively bisect the interval saving the upper limit X_i and the value N_i of each i th subinterval. The subintervals are formed until only one eigenphase exists within the last interval formed.

The value of the eigenphase is then stored and the intervals are recursed in the forward direction until the original interval length is obtained. Then we skip to the next interval $(X_k + \epsilon, X_{k+1} - \epsilon)$ and repeat the process. Continuing in this manner, we find all the eigenphases. If all the regions between zero and π have not been explored after the last eigenphase has been found, the remaining regions are still checked to be sure that no extraneous phase values have been introduced because of error accumulation. A considerable amount of bookkeeping is necessary even for this simple approach to the searching problem and still take account of the discontinuities in the energy eigenvalues. The criterion for calling a particular phase δ_1 an eigenphase was the condition

$$|E_\lambda - E_\gamma| \leq 0.001$$

which implies that E_λ differ from the incident photon energy by 1 keV. The computational aspects of constructing the single-particle wave functions numerically and the many numerical pitfalls which had to be overcome will be discussed in the following two chapters. In Chapter V, we will see the results of this calculation and be better able to judge the effectiveness of the eigenchannel approach.

CHAPTER IV. COULOMB WAVE FUNCTIONS

4.1 Basic properties

In scattering problems involving charged particles, one encounters the special functions designated as Coulomb wave functions. The differential equation satisfied by these functions is

$$\frac{d^2 f_L(\eta, \rho)}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{L(L+1)}{\rho^2} \right] f_L(\eta, \rho) = 0 \quad (4.1)$$

The variables ρ and η are related to the charges Z_1, Z_2 of the scattering particles, the reduced mass μ and the excitation energy E by the following relations:

$$\rho = \alpha r \quad (4.2a)$$

$$\alpha^2 = 2\mu E / \hbar^2 \quad (4.2b)$$

$$\eta = \mu Z_1 Z_2 e^2 / (\hbar^2 \alpha). \quad (4.2c)$$

The values of ρ and η will be assumed positive and L a positive integer.

The Coulomb functions $F_L(\eta, \rho)$ and $G_L(\eta, \rho)$ are, for a particular value of L , two linearly independent solutions of Equation 4.1. The function $F_L(\eta, \rho)$ is regular at the origin and the function $G_L(\eta, \rho)$ is irregular.

They are constructed so that asymptotically they have the forms

$$F_L(\eta, \rho) \underset{\rho \rightarrow \infty}{\sim} \sin [\rho - \eta \ln 2\rho - L\pi/2 + \sigma_L] \quad (4.3a)$$

$$G_L(\eta, \rho) \underset{\rho \rightarrow \infty}{\sim} \cos [\rho - \eta \ln 2\rho - L\pi/2 + \sigma_L] \quad (4.3b)$$

$$\text{with} \quad \sigma_L = \arg \Gamma(L+1+i\eta). \quad (4.3c)$$

These functions have been studied in great depth from the earliest work by Breit, Wheeler and Yost (38) in 1963 up to the recent work of Gersten (39) in 1971. Quick and accurate algorithms for the numerical evaluation of these functions has yet to be reported although multitudinous schemes have been proposed and recorded (23, 40-77). Before describing the numerical techniques employed in this work to calculate these functions, it is imperative that we take a closer look at the basic properties of the Coulomb functions and the approximation schemes previously employed for their evaluation. The notation for the following sections is that employed in reference (44).

The regular function $F_L(\eta, \rho)$ can be expanded in a power series in ρ to obtain

$$F_L(\eta, \rho) = c_L(\eta) \rho^{L+1} \sum_{K=L+1}^{\infty} A_K^L(\eta) \rho^{K-L-1} \quad (4.4a)$$

$$A_{L+1}^L = 1, \quad A_{L+2}^L = \eta / L + 1$$

$$(K+L)(K-L-1) A_K^L = 2\eta A_{K-1}^L - A_{K-2}^L \quad (K > 2L+2)$$

$$c_L(\eta) = 2^L \exp(-\pi\eta/2) |\Gamma(L+1+i\eta)| / \Gamma(2L+2).$$

It is readily seen that this is equivalent to defining $F_L(\eta, \rho)$ as a confluent hypergeometric function. In fact, one finds

$$F_L(\eta, \rho) = c_L(\eta) \rho^{L+1} e^{-i\rho} {}_1F_1(L+1+i\eta, 2L+2, 2i\rho). \quad (4.4b)$$

The irregular solution $G_L(\eta, \rho)$ can similarly be expanded to obtain

$$G_L(\eta, \rho) = \frac{2\eta}{c_0^2(\eta)} F_L(\eta, \rho) [1 + 2\rho + q_L(\eta)/p_L(\eta)] + \theta_L(\eta, \rho)$$

$$\theta_L(\eta, \rho) = \frac{\rho^{-L}}{(2L+1)c_L(\eta)} \sum_{K=-L}^{\infty} b_K^L(\eta) \rho^{K+L} \quad (4.5)$$

$$b_{-L}^L = 1, \quad b_{L+1}^L = 0$$

$$(K-L-1)(K+L) b_K^L = 2\eta b_{K-1}^L - b_{K-2}^L - (2K-1) p_L(\eta) A_K^L(\eta) \quad (K > L+1)$$

$$(2L+1) [(2L)!]^2 p_L(\eta) = 2\eta (1+\eta^2)(4+\eta^2) \dots (L^2+\eta^2) 2^{2L}$$

$$\frac{q_L(\eta)}{p_L(\eta)} = \sum_{s=1}^L \frac{s}{s^2+\eta^2} - \sum_{s=1}^{2L+1} \frac{1}{s} + \operatorname{Re} \left\{ \frac{\Gamma'(1+i\eta)}{\Gamma(1+i\eta)} \right\} + 2\gamma + \frac{r_L(\eta)}{p_L(\eta)}$$

$$r_L(\eta) = \frac{(-1)^{L+1}}{(2L)!} \sum_{K=-L}^L \operatorname{Im} \left\{ \frac{2^{K+L} (i\eta-L)(i\eta-L+1) \dots (i\eta-K+1)}{(L+K)! (L-K+1)} \right\}$$

where Re and Im stand for the real and imaginary parts respectively, and γ is the Euler-Mascheroni constant. Most of the early work performed in tabulating these functions employed the use of Equations 4.4 and 4.5 and thus were limited to a rather select range of η and ρ for practical evaluation purposes. In fact, $F_L(\eta, \rho)$ and $G_L(\eta, \rho)$ were accurate to only two significant figures for $\rho > 1$ when the power series representations were used. From Equations 4.4 and 4.5 the behavior at the origin of F_L and G_L is easily deduced. As ρ approaches zero,

$$F_L(\eta, \rho) \underset{\rho \rightarrow 0}{\sim} c_L \rho^{L+1} [1 + \eta \rho / (L+1) + \dots] \quad (4.6a)$$

$$G_L(\eta, \rho) \underset{\rho \rightarrow 0}{\sim} \frac{1}{(2L+1)c_L(\eta)} \rho^{-L} \left[1 + \begin{cases} \theta(\eta \rho \ln \rho) & \text{if } L = 0 \\ \theta(\eta \rho / 2) & \text{if } L \neq 0 \end{cases} \right] \quad (4.6b)$$

where $\theta(x)$ means of the order x . The basic recurrence relations for these

functions were derived from their equivalent integral representations.

$$F_L(\eta, \rho) = \frac{e^{-\pi\eta} \rho^{L+1}}{C_L(\eta) (2L+1) (2L)!} \int_0^\infty (1 - \tanh^2 x)^{L+1} \cos(\rho \tanh x - 2\eta x) dx \quad (4.7)$$

$$G_L(\eta, \rho) = \frac{e^{-\pi\eta} \rho^{L+1}}{C_L(\eta) (2L+1) (2L)!} \left\{ \int_0^\infty (1+x^2)^L \exp(-\rho x + 2\eta \tan^{-1}(x)) dx - \int_0^\infty (1 - \tanh^2 x)^{L+1} \sin(\rho \tanh x - 2\eta x) dx \right\}. \quad (4.8)$$

From these representations, Powell (54) and Infeld (55) were able to deduce the following recurrence relations

$$L \, dU_L/d\rho = (L^2 + \eta^2)^{\frac{1}{2}} U_{L-1} - [L^2/\rho + \eta] U_L \quad (4.9)$$

$$(L+1) \, dU_L/d\rho = [(L+1)^2/\rho + \eta] U_L - [(L+1)^2 + \eta^2]^{\frac{1}{2}} U_{L+1} \quad (4.10)$$

$$L [(L+1)^2 + \eta^2]^{\frac{1}{2}} U_{L+1} = (2L+1) [\eta + L(L+1)/\rho] U_L - (L+1) [L^2 + \eta^2]^{\frac{1}{2}} U_{L-1} \quad (4.11)$$

where U_L is any linear combination of F_L and G_L independent of ρ . With the basic Equation 4.1 and the aid of the recurrence relations one can show that

$$F_L' G_L - F_L G_L' = 1 \quad (4.12)$$

$$F_{L-1} G_L - F_L G_{L-1} = L(L^2 + \eta^2)^{-\frac{1}{2}}. \quad (4.13)$$

The Wronskian relations, Equations 4.12 and 4.13, are the tools by which one verifies the accuracy of any set of tabulated values of F_L and G_L . It must be born in mind however that these relations will only indicate gross errors in the calculated values. But, nevertheless, they are an important

criterion for estimating the success of any numerical approach to evaluating F_L and G_L .

4.2 Integrals of Coulomb wave functions

Considering the differential Equation 4.1 first for an energy E and then for an energy E' (i.e. for the values $\rho = \alpha r$ and $\rho' = \alpha' r$), it is easily shown using the asymptotic properties of F_L and G_L that

$$\int_0^\infty F_L(\eta, \alpha r) F_L(\eta', \alpha' r) dr = \frac{\pi}{2} \delta(\alpha - \alpha') \quad (4.14a)$$

$$\int_0^\infty F_L(\eta, \alpha r) G_L(\eta', \alpha' r) dr = \frac{\pi}{2} \delta(\alpha - \alpha'). \quad (4.14b)$$

These are the usual orthogonality relations. Lowan and Horenstein (57) in 1942 provided us with the Laplace transform of F_L and its derivatives. Their results lead to the following set of relations valid for $\text{Re } \beta > 0$.

$$\int_0^\infty e^{-\beta \rho} \rho^L F_L(\eta, \rho) d\rho = \frac{C_L(\eta) (2L+1)!}{(\beta^2 + 1)^{L+1} \exp(2\eta \tan^{-1} \beta)} \quad (4.15)$$

$$\int_0^\infty e^{-\beta \rho} \frac{d}{d\rho} [\rho^L F_L(\eta, \rho)] d\rho = \frac{\beta C_L(\eta) (2L+1)!}{(\beta^2 + 1)^{L+1} \exp(2\eta \tan^{-1} \beta)} \quad (4.16)$$

$$\int_0^\infty e^{-\beta \rho} \rho^{L+1} F_L(\eta, \rho) d\rho = \frac{C_L(\eta) [(2L+1)! 2\eta + \beta (2L+2)!]}{(\beta^2 + 1)^{L+2} \exp(2\eta \tan^{-1} \beta)} \quad (4.17)$$

with $C_L(\eta)$ defined as in Equation 4.4.

The set of Equations 4.14 to 4.17 are of little use when one needs to evaluate integrals of F_L and G_L over a finite range. How then does one evaluate indefinite integrals of the Coulomb functions? Consider the

differential equation 4.1 for $\eta = 0$. The standard solutions are then the regular and irregular spherical Bessel functions $j_L(\rho)$ and $n_L(\rho)$ multiplied by ρ . In fact, in the limit $\eta \rightarrow 0$,

$$F_L(0, \rho) = \rho j_L(\rho) \quad (4.18)$$

$$G_L(0, \rho) = -\rho n_L(\rho). \quad (4.19)$$

Since the indefinite integrals of j_L and n_L are well known, a logical starting point would be to consider the functions $F_L(\eta, \rho)/\rho$ and $G_L(\eta, \rho)/\rho$.

Define the constant

$$c = \mu Z_1 Z_2 e^2 / \hbar^2. \quad (4.20)$$

Then the differential Equation 4.1 takes the following form

$$f_L'' + \left[1 - \frac{2c}{\alpha^2 r} - \frac{L(L+1)}{\alpha^2 r^2} \right] f_L = 0 \quad (4.21)$$

where f_L'' indicates the second derivative of f_L with respect to αr .

Let $f_L = (\alpha r) U_L(\alpha r)$. Then,

$$U_L'' + \frac{2U_L'}{\alpha r} + \left[1 - \frac{2c}{\alpha^2 r} - \frac{L(L+1)}{\alpha^2 r^2} \right] U_L = 0. \quad (4.22)$$

Consider Equation 4.21 with solution $g_L = (\beta r) V_L(\beta r)$, ($\beta \neq \alpha$).

$$V_L'' + \frac{2V_L'}{\beta r} + \left[1 - \frac{2c}{\beta^2 r} - \frac{L(L+1)}{\beta^2 r^2} \right] V_L = 0. \quad (4.23)$$

Multiply Equation 4.22 by $\alpha^2 V_L$, Equation 4.23 by $\beta^2 U_L$ and subtract to obtain

$$(\alpha^2 - \beta^2) U_L V_L + \frac{2}{r} [\alpha U_L' V_L - \beta V_L' U_L] + [\alpha^2 V_L U_L'' - \beta^2 U_L V_L''] = 0. \quad (4.24a)$$

The derivatives are taken with respect to the arguments. Rewriting $U_L(\alpha r)$ and $V_L(\beta r)$ in terms of f_L and g_L and integrating over r one obtains

$$(\alpha^2 - \beta^2) \int f_L(\eta_\alpha, \alpha r) g_L(\eta_\beta, \beta r) dr = [\beta f_L(\eta_\alpha, \alpha r) g_L'(\eta_\beta, \beta r) - \alpha g_L(\eta_\beta, \beta r) f_L'(\eta_\alpha, \alpha r)] \quad (4.24b)$$

where η_α, η_β are defined by Equation 4.2c.

Using the recurrence relations, Equations 4.9, 4.10 and 4.11, we get the result

$$(L+1)(\alpha^2 - \beta^2) \int f_L(\eta_\alpha, \alpha r) g_L(\eta_\beta, \beta r) dr = \alpha [(L+1)^2 + \eta_\alpha^2]^{\frac{1}{2}} f_{L+1}(\eta_\alpha, \alpha r) \times \\ \times g_L(\eta_\beta, \beta r) - \beta [(L+1)^2 + \eta_\beta^2]^{\frac{1}{2}} f_L(\eta_\alpha, \alpha r) g_{L+1}(\eta_\beta, \beta r). \quad (4.25)$$

Since f_L and g_L may be any linear combination of solutions to the Coulomb differential equation with coefficients independent of r , Equation 4.25 is a completely general result. To be able to calculate the integral when $\alpha = \beta$ we set $\beta = \alpha + \delta_\alpha$ and expand all terms dependent on β in a Taylor's series of $(\beta - \alpha)$ to terms of order δ_α . Then we take the limit as β goes to α . Performing this expansion on the β dependent terms of Equation 4.25 and letting

$$\sqrt{} = [(L+1)^2 + \eta^2]^{\frac{1}{2}} \quad (4.26)$$

Equation 4.25 becomes

$$(L+1) (-2\alpha) \delta_\alpha \int f_L g_L dr = \alpha \sqrt{[f_{L+1} g_L - f_L g_{L+1}]} + \\ + \left\{ \alpha \sqrt{f_{L+1}} \frac{dg_L}{d\alpha} + \frac{(L+1)^2}{\sqrt{}} f_L g_{L+1} - \alpha \sqrt{f_L} \frac{dg_{L+1}}{d\alpha} \right\} \delta_\alpha. \quad (4.27)$$

The αr and η_α dependence is understood to be present in the functions f_L and g_L . If $f_L = g_L$, the term independent of δ_α in Equation 4.27 is zero automatically and if $f_L \neq g_L$ then from Equation 4.13

$$f_{L+1} g_L - f_L g_{L+1} = -(L+1)/\sqrt{}$$

Therefore, $\alpha \sqrt{[f_{L+1} g_L - f_L g_{L+1}]} = -\alpha (L+1)$.

Since the indefinite integral is evaluated over a finite range, the contribution of this constant term vanishes. So, to terms of order δ_α

$$2\alpha(L+1) \int f_L(\eta, \alpha r) g_L(\eta, \alpha r) dr = \frac{(L+1)^2}{\sqrt{}} f_L(\eta, \alpha r) g_{L+1}(\eta, \alpha r) + \\ + \alpha \sqrt{[f_L(\eta, \alpha r) \frac{d}{d\alpha} (g_{L+1}(\eta, \alpha r)) - f_{L+1}(\eta, \alpha r) \frac{d}{d\alpha} (g_L(\eta, \alpha r))]} \quad (4.28)$$

Since $\eta = c/\alpha$ and $\rho = \alpha r$, the derivative with respect to α can be related to those with respect to η and ρ . Equation 4.28 can then be written with the help of the recurrence relations as

$$4(L+1)^2 \int f_L(\eta, \rho) g_L(\eta, \rho) d\rho = 2\rho [(L+1)^2 + \eta^2] \{ f_L(\eta, \rho) g_L(\eta, \rho) + \\ + f_{L+1}(\eta, \rho) g_{L+1}(\eta, \rho) \} + \left\{ (L+1)/\sqrt{ } - \frac{2\sqrt{ }\rho}{(L+1)^2} \left[\frac{(L+1)^2}{\rho} + \eta \right] \right\} \times \\ \times [f_L(\eta, \rho) g_{L+1}(\eta, \rho) + f_{L+1}(\eta, \rho) g_L(\eta, \rho)] - 2\eta(L+1)\sqrt{ } [f_L(\eta, \rho) \times \\ \times \frac{dg_{L+1}(\eta, \rho)}{d\eta} - f_{L+1}(\eta, \rho) \frac{dg_L(\eta, \rho)}{d\eta}] \quad (4.29)$$

with $\sqrt{}$ defined by Equation 4.26. It is rather disconcerting to be faced with derivatives with respect to η because the values of these derivatives cannot be rewritten in terms of the original functions and their ρ -derivatives. However, Equation 4.23 is exact and is useful in estimating the accuracy of any numerical technique employed to evaluate this integral.

If one employs the same techniques that were used to obtain Equation 4.25 for the case of two different L values, the resulting integral is obtained:

$$\begin{aligned} (L-m)(L+m+1) \int f_L(\eta, \rho) g_m(\eta, \rho) \rho^{-2} d\rho &= \frac{[(m+1)^2 + \eta^2]^{\frac{1}{2}}}{(m+1)} f_L(\eta, \rho) g_{m+1}(\eta, \rho) \times \\ &\times \frac{-[(L+1)^2 + \eta^2]^{\frac{1}{2}}}{(L+1)} f_{L+1}(\eta, \rho) g_m(\eta, \rho) + (L-m) f_L(\eta, \rho) g_m(\eta, \rho) \times \\ &\times \left[1/\rho - \frac{\eta}{(L+1)(m+1)} \right]. \end{aligned} \quad (4.30)$$

We specialize Equation 4.30 so that f_L and g_L are the regular solutions F_L and F_m respectively and integrate over all ρ .

$$\begin{aligned} \int_0^\infty F_L(\eta, \rho) F_m(\eta, \rho) \rho^{-2} d\rho &= \left(\frac{1}{\rho} - \frac{\eta}{(L+1)(m+1)} \right) \frac{F_L(\eta, \rho) F_m(\eta, \rho)}{(L+m+1)} \Big|_0^\infty + \\ &+ \frac{[(m+1)^2 + \eta^2]^{\frac{1}{2}}}{(L+m)(m+1)(L+m+1)} F_L(\eta, \rho) G_{m+1}(\eta, \rho) \Big|_0^\infty - \\ &- \frac{[(L+1)^2 + \eta^2]^{\frac{1}{2}}}{(L-m)(L+1)(L+m+1)} F_{L+1}(\eta, \rho) G_m(\eta, \rho) \Big|_0^\infty. \end{aligned}$$

Using Equations 4.3a and 4.6a and the relation

$$\sigma_{L+1} = \sigma_L + \arctan (\eta/L+1) \quad (4.31)$$

one finds that the integral reduces to

$$\int_0^\infty F_L(\eta, \rho) F_m(\eta, \rho) \rho^{-2} d\rho = \frac{\sin \{ (L-m) \pi/2 - (\sigma_L - \sigma_m) \}}{(L-m)(L+m+1)} \quad (4.32)$$

where

$$\sigma_L = \arg \Gamma(L+1+i\eta)$$

$$\sigma_m = \arg \Gamma(m+1+i\eta).$$

In particular, for $L = m$ one obtains the interesting result

$$\int_0^\infty F_L^2(\eta, \rho) \rho^{-2} d\rho = \frac{\pi}{2(2L+1)}. \quad (4.33)$$

It is also of interest to note that from the differential properties of the Coulomb functions, the following integrals are easily obtained

$$\begin{aligned} & [(L+1)^2 + \eta^2]^{\frac{1}{2}} \int \rho^{L+1} \exp(\eta \rho/(L+1)) f_L(\eta, \rho) d\rho = (L+1) \rho^{L+1} \times \\ & \times \exp(\eta \rho/(L+1)) f_{L+1}(\eta, \rho) \end{aligned} \quad (4.34)$$

$$[L^2 + \eta^2]^{\frac{1}{2}} \int \rho^{-L} \exp(-\eta \rho/L) f_L(\eta, \rho) d\rho = -L \rho^{-L} \exp(-\eta \rho/L) f_{L-1}(\eta, \rho). \quad (4.35)$$

4.3 Negative energy Coulomb wave function

For negative energies the bound state wave functions are exponentially decaying Whittaker functions. Let us take the defining Equation 4.26 for α'^2 when E is negative and define

$$\alpha'^2 = -\alpha^2 = -2\mu E / \hbar^2. \quad (4.36a)$$

Then if we define

$$\eta = \mu Z_1 Z_2 e^2 / (\hbar^2 \alpha') \quad (4.36b)$$

$$\rho = \alpha' r \quad (4.36c)$$

the differential Equation 4.1 becomes

$$\frac{d^2 f_L(\eta, \rho)}{d\rho^2} - \left[1 + \frac{2\eta}{\rho} + \frac{L(L+1)}{\rho^2} \right] f_L(\eta, \rho) = 0. \quad (4.37)$$

Letting $Z = 2\rho$ Equation 4.37 becomes

$$\frac{d^2 f_L(\eta, Z)}{dZ^2} + \left[-1/4 - \frac{L(L+1)}{Z} - \frac{\eta}{Z^2} \right] f_L(\eta, Z) = 0. \quad (4.38)$$

Equation 4.38 is known as Whittaker's equation. The solution of interest is written as (26, p. 349)

$$W(-\eta, L + \frac{1}{2}, 2\rho) = \frac{\exp(-\rho - \eta \ln 2\rho)}{\Gamma(L + 1 + \eta)} \int_0^\infty t^{L+\eta} e^{-t} \left(1 + \frac{t}{2\rho}\right)^{L-\eta} dt. \quad (4.39)$$

Asymptotically $W(-\eta, L + \frac{1}{2}, 2\rho)$ is an exponentially decaying solution

$$W(-\eta, L + \frac{1}{2}, 2\rho) \underset{\rho \rightarrow \infty}{\sim} \exp(-\rho - \eta \ln 2\rho). \quad (4.40)$$

Comparing the integral representations for $F_L(i\eta, -i\rho)$ and $G_L(i\eta, -i\rho)$ one sees that the W-function satisfies the relation

$$W(-\eta, L + \frac{1}{2}, 2\rho) = (-1)^{L+1} \exp[i\pi(L+1-\eta)/2] \Gamma(L+1-\eta) / \Gamma(L+1+\eta) \times \\ \times \{F_L(i\eta, -i\rho) + i G_L(i\eta, -i\rho)\}. \quad (4.41)$$

Using the integral representation, Equation 4.39, we find that the derivative of the W-function with respect to ρ satisfies the relation

$$\frac{dW(-\eta, L + \frac{1}{2}, 2\rho)}{d\rho} = -(1 + \frac{\eta}{\rho}) W(-\eta, L + \frac{1}{2}, 2\rho) - \frac{(L-\eta)(L+\eta+1)}{\rho} \\ \times W(-[\eta+1], L + \frac{1}{2}, 2\rho). \quad (4.42)$$

If we take the limit as $\eta \rightarrow 0$ of Equation 4.41 we obtain

$$W(0, L + \frac{1}{2}, 2\rho) = (-1)^{L+1} \exp(i 3L\pi/2) h_L^{(1)}(2i\rho) \quad (4.43)$$

where

$$h_L^{(1)}(i\rho) = j_L(i\rho) + in_L(i\rho)$$

and thus apart from the phase factor, the W-function with $\eta = 0$ is equal to the normal bound state solution for uncharged particles, i.e. a hankel function of the first kind.

4.4 Numerical evaluation of Coulomb functions

The success and failure of various methods to evaluate $F_L(\eta, \rho)$ and $G_L(\eta, \rho)$ would in itself form an encyclopedia of numerical analysis. One learns however from the attempts of previous authors whether a particular method has any real computational merit. In the case of the Coulomb functions, any closed form analytic solution proposes countless

difficulties and as proposed by Fröberg (50) perhaps the best approach is to subsection the $\rho - \eta$ plane and use a different method in each subsection, the method to be employed depending explicitly on the properties of the functions F_L and G_L in each subsection. This is the method of approach utilized in this work. I will not attempt to outline the pitfalls of all the approximations proposed to date. I will instead give a brief description of those procedures explicitly employed in this research and recommendations for those who would wish to achieve a higher accuracy than is reported in this work. The methods employed in each subsection labelled I through V in Figure 4 can be described by the following:

a. Subsection I The numerical evaluation of special functions normally employs the use of a recurrence relation satisfied by the particular solutions of interest. In the case of the Coulomb functions, the linear difference equation of interest is Equation 4.11. If two values of the functions F_L or G_L for successive L-values can be found, it would seem apparent that functions of higher L-values could easily be obtained by forward recursion of Equation 4.11. This however is not the case. The stability of the recurrence relations is highly dependent on the L-value desired. It may prove beneficial to use backward recurrence instead. The reason for this conclusion is best expressed in reference 44 page 697 and I quote,

"In cases where straightforward use of the L-wise recurrence relation results in loss of accuracy by cancellation of leading digits, it may be worthwhile to remark that greater accuracy is usually attainable by use of the recurrence relation in the reverse direction from arbitrary starting values for two values of L somewhat beyond the last value desired. This is because the

Figure 4. Regions in which various numerical techniques are employed for the evaluation of the Coulomb wave functions

recurrence relation is a second order homogeneous linear difference equation, and has two independent solutions. Loss of accuracy by cancellation occurs when the solution desired is diminishing as L varies, while the companion solution is increasing. By reversing the direction of progress in L , the roles of the two solutions are interchanged, and the contribution of the unwanted solution diminishes to the point of negligibility. By starting sufficiently beyond the last value of L for which the function is desired, we can ensure that the unwanted solution is negligible but, because the starting values were arbitrary, we have an unknown multiple of the solution desired. The computation is then carried back until a value of L is reached, when the precise multiple that we have of the desired solution may be determined and hence removed throughout."

For $L \rightarrow \infty$, F_L is a decreasing function of L while G_L is an increasing function of L (41, pg. 1851). Thus, forward recurrence is stable for G_L while backward recurrence is stable for F_L . Since the Coulomb functions degenerate into spherical Bessel functions when $\eta \rightarrow 0$, the same remark holds true for the functions $j_L(\rho)$ and $n_L(\rho)$, n_L being stable for increasing L and j_L being stable for decreasing L .

1) The regular solution $F_L(\eta, \rho)$ The method employed for the regular function $F_L(\eta, \rho)$ is an adaptation of the technique proposed by Abramowitz and Stegun (41). In particular, define $L_{MAX} = \max(\lfloor p+1 \rfloor, 6) + 11$ where $\lfloor x \rfloor$ denotes the greatest integer n such that $n \leq x$. Set $\bar{F}_{L_{MAX}}(\eta, \rho) = 0.0$ and $\bar{F}_{L_{MAX}-1}(\eta, \rho) = 0.1$. The successive values of $\bar{F}_L$ for $L = L_{MAX}-2, L_{MAX}-3, \dots, 0$ are generated by backward recursion of Equation 4.11. Every value of $\bar{F}_L$ is directly proportional to the true value F_L by the same proportionality constant, say α . The constant α is determined from the equation

$$\alpha \rho \cos \rho = \left(\frac{e^{2\pi\eta} - 1}{2\pi\eta} \right)^{\frac{1}{2}} \sum_{L=0}^{\infty} (2L+1) \cos \delta_L(\eta) \bar{F}_L(\eta, \rho) \quad (4.44)$$

$$\delta_0 = 0 : \delta_L(\eta) = L\pi/2 + \sum_{K=1}^L \tan^{-1}(\eta/K). \quad (4.45)$$

Having determined α , the value of $F_L(\eta, \rho)$ desired is obtained from

$$F_L(\eta, \rho) = \bar{F}_L(\eta, \rho) / \alpha. \quad (4.46)$$

2) The irregular solution $G_L(\eta, \rho)$ Since forward recursion is stable for $G_L(\eta, \rho)$ one needs only to determine $G_0(\eta, \rho)$ and $G_1(\eta, \rho)$. Then, forward recursion of Equation 4.11 will produce all successive L -values desired. The value of $G_0(\eta, \rho)$ is obtained by Gaussian quadrature applied to the integral representation, Equation 4.8. The cutoff values of x were chosen so that

$$\rho x(\text{cutoff}) - \pi \eta = 37 \quad (4.47)$$

for the integral containing the exponential term, and

$$x(\text{cutoff}) = 12 \quad (4.48)$$

for the integral containing the sine term. The region between $x = 0$ and $x = x(\text{cutoff})$ for each integral was divided into five sections and the 16-point Gauss formula was applied to each of them. This is equivalent to approximating the integrands of the integrals in each section by a polynomial of degree 31. The value of $G_1(\eta, \rho)$ is obtained using the previously calculated values of $F_0(\eta, \rho)$, $F_1(\eta, \rho)$ and the relation

$$F_0 G_1 - F_1 G_0 = (1 + \eta^2)^{-\frac{1}{2}}, \quad (4.49)$$

The values of $G_L(\eta, \rho)$ for $L > 1$ were then generated by forward recursion.

b. Subsection II Considering the integral representation for $F_0(\eta, \rho)$, Abramowitz(40) deduced an asymptotic expansion for large values of ρ in 1949. In the introduction of reference(42) this method was extended to all L -values and the following results were obtained:

$$\begin{aligned} F_L &= g \cos \theta_L + f \sin \theta_L \\ G_L &= f \cos \theta_L - f^* \sin \theta_L \\ F_L' &= g^* \cos \theta_L + f^* \sin \theta_L \\ G_L' &= f^* \cos \theta_L - g^* \sin \theta_L \end{aligned} \quad (4.50)$$

$$\begin{aligned} \theta_L &= \rho - \eta \ln 2\rho - L\pi/2 + \sigma_L \\ \sigma_L &= \arg \Gamma(L+1+i\eta) \\ \sigma_{L+1} &= \sigma_L + \arctan(\eta/L+1) \end{aligned} \quad (4.51)$$

$$f \sim \sum_{K=0}^{\infty} f_K, \quad g \sim \sum_{K=0}^{\infty} g_K, \quad f^* \sim \sum_{K=0}^{\infty} f_K^*, \quad g^* \sim \sum_{K=0}^{\infty} g_K^* \quad (4.52)$$

where

$$f_0 = 1, g_0 = 0, f_0^* = 0, g_0^* = 1 - \eta/\rho$$

$$f_{K+1} = a_K f_K - b_K g_K$$

$$g_{K+1} = a_K g_K + b_K f_K \quad (4.53)$$

$$f_{K+1}^* = a_K f_K^* - b_K g_K^* - f_{K+1}/\rho$$

$$g_{K+1}^* = a_K g_K^* + b_K f_K^* - g_{K+1}/\rho$$

$$a_K = \frac{(2K+1)\eta}{(2K+2)\rho}, \quad b_K = \frac{L(L+1) - K(K+1) + \eta^2}{(2K+2)\rho}.$$

Since the series' for f , g , f^* , and g^* are asymptotic series', the summations on K in Equation 4.52 can only be carried out for the first N terms beyond which point the individual series begin to diverge. If we let x_K represent the K th term in the series expansions for f , g , f^* , and g^* , then each series was terminated according to the following criterion

$$\left| \frac{x_N}{\sum_{K=0}^N x_K} \right| \leq 0.5 \times 10^{-5}, \text{ or } N = 40. \quad (4.54)$$

This criterion proved successful for the evaluation of $F_0(\eta, \rho)$, $G_0(\eta, \rho)$, $F'_0(\eta, \rho)$, and $G'_0(\eta, \rho)$. The values of $F_1(\eta, \rho)$ and $G_1(\eta, \rho)$ were then obtained from Equation 4.10 and forward recursion of Equation 4.11 was employed to obtain higher L -values.

c. Subsection III The accuracy obtainable in this region is based on the condition $\rho < 2\eta$. The method was first devised by Abramowitz(40) in 1949 and extended by Fröberg (50) in 1955. Consider the differential Equation 4.1 for $L = 0$. We let $\rho = 2\eta t$ in the resulting equation to obtain

$$f''_0 + 4\eta^2 (1 - t^{-1}) f_0 = 0. \quad (4.55)$$

If we now let $f_0 = \exp \varphi$ the differential equation for the function φ is

$$\varphi'^2 + \varphi' + 4\eta^2 (1 - t^{-1}) = 0. \quad (4.56)$$

The derivatives in Equation 4.55 and 4.56 are taken with respect to t . Equation 4.56 can be solved if we take for $\varphi(t, \eta)$ an expression of the form

$$\varphi(t, \eta) = \sum_{K=0}^{\infty} (2\eta)^{-(K-1)} g_K(t). \quad (4.57)$$

Equating coefficients of successive powers of 2η to zero the functions $g_K(t)$ can be determined successively. This process results in the regular solution $F_0(\eta, \rho)$. If instead we make the substitution $f_0 = \exp \psi(t, \eta)$ with

$$\psi(t, \eta) = \sum_{K=0}^{\infty} (-)^{K+1} (2\eta)^{-(K+1)} g_K(t) \quad (4.58)$$

we obtain the irregular solution $G_0(\eta, \rho)$. Carrying through this procedure, Fröberg obtained the following results:

$$F_0 = \left(\frac{1}{2}\right) \exp(\varphi(t, \eta)) ; F'_0 = (2\eta)^{-1} \cdot F_0 \cdot d\varphi/dt \quad (4.59)$$

$$G_0 = \exp(\psi(t, \eta)) ; G'_0 = (2\eta)^{-1} \cdot G_0 \cdot d\psi/dt.$$

Here $t = \rho/2\eta$ and

$$\varphi(t, \eta) = 2\eta \cdot g_0 + g_1 + (2\eta)^{-1} g_2 + (2\eta)^{-2} g_3 + \dots \quad (4.60)$$

$$\psi(t, \eta) = -2\eta \cdot g_0 + g_1 - (2\eta)^{-1} g_2 + (2\eta)^{-2} g_3 - \dots$$

$$g_0 = (t(1-t))^{\frac{1}{2}} + \arcsin(t^{\frac{1}{2}}) - \pi/2$$

$$g_1 = (1/4) \ln(t/(1-t))$$

$$g_2 = -(8t^2 - 12t + 9)/48t^{\frac{1}{2}}(1-t)^{3/2}$$

$$g_3 = (8t - 3)/64t(1-t)^3 \quad (4.61)$$

$$g_4 = \frac{2048t^6 - 9216t^5 + 16128t^4 - 13440t^3 - 12240t^2 + 7560t - 1890}{92160t^{3/2}(1-t)^{9/2}}$$

$$g_5 = 3(1024t^3 - 448t^2 + 208t - 39)/8192t^2(1-t)^6$$

$$g_6 = -(262144t^{10} - 1966080t^9 + 6389760t^8 - 11714560t^7 + 13178880t^6 - 9225216t^5 + 13520640t^4 - 3588480t^3 + 2487240t^2 - 873180t + 130977)/10321920t^{5/2}(1-t)^{15/2}$$

$$g_7 = \frac{1105920t^5 - 55296t^4 + 314624t^3 - 159552t^2 + 45576t - 5697}{323216t^3(1-t)^9}$$

$$g'_0 = t^{-1/2}(1-t)^{1/2}$$

$$g'_1 = 1/4t(1-t)$$

$$g'_2 = -(8t - 3)/32t^{3/2}(1-t)^{5/2}$$

$$g'_3 = 3(8t^2 - 4t + 1)/64t^2(1-t)^4$$

$$g'_4 = -(1536t^3 - 704t^2 + 366t - 63)/2048t^{5/2}(1-t)^{11/2} \quad (4.62)$$

$$g_5' = 3(2560t^4 - 832t^3 + 728t^2 - 260t + 39) / 4096t^3 (1-t)^7$$

$$g_6' = \frac{-368640t^5 - 30720t^4 + 114944t^3 - 57792t^2 + 16632t - 2079}{65536t^{7/2} (1-t)^{17/2}}$$

$$g_7' = 3(860160t^6 + 196608t^5 + 308480t^4 - 177280t^3 + 73432t^2 - 17724t + 1899) / (131072t^4 (1-t)^{10}).$$

The values of F_0 , F_0' , G_0 , and G_0' were obtained from Equations 4.55 - 5.62.

The values of F_1 and G_1 were then obtained from Equation 4.10 and forward recursion of Equation 4.11 was employed to obtain higher L-values.

d. Subsection IV The method employed in this region was first proposed by Abramowitz and Rabinowitz (44) in 1954 and used most effectively by Lutz and Karvelis (58) in 1963. In essence, it involves a Taylor's series expansion of F_0 , G_0 , F_0' and G_0' about the transition line $\rho = 2\eta$. The same formulas apply to both the F_0 and G_0 Taylor series development

$$\sigma_0 = F_0(\eta, \rho), \text{ or } G_0(\eta, \rho) \quad (4.63)$$

$$\sigma_1 = \Delta \rho F_0'(\eta, \rho), \text{ or } \Delta \rho G_0'(\eta, \rho) \quad (4.64)$$

$$\sigma_2 = -\frac{1}{2} (\Delta \rho)^2 (1 - 2\eta/\rho) \sigma_0, \quad (4.65)$$

$$\rho n(n+1) \sigma_{n+1} + \Delta \rho (n^2 - n) \sigma_n + (\rho - 2\eta) (\Delta \rho)^2 \sigma_{n-1} + (\Delta \rho)^3 \sigma_{n-2} = 0, \\ n = 2, 3, 4, \dots \quad (4.66)$$

$$F_0(\eta, \rho + \Delta \rho) \\ \text{or} \quad = \sum_{n=0}^{\infty} \sigma_n, \quad (4.67) \\ G_0(\eta, \rho + \Delta \rho)$$

$$\begin{aligned}
 &F'_0(\eta, \rho + \Delta \rho) \\
 &\quad \text{or} \quad = \frac{1}{\Delta \rho} \sum_{n=1}^{\infty} n \sigma_n \quad (4.68) \\
 &G'_0(\eta, \rho + \Delta \rho)
 \end{aligned}$$

The Taylor series' being terminated according to

$$\left| \frac{\sigma_M}{\sum_{n=0}^M \sigma_n} \right|, \left| \frac{M \sigma_M}{\sum_{n=1}^M n \sigma_n} \right| < 10^{-8} \quad (4.69)$$

Following Lutz and Karvelis (58, pp. 33-34), if $\bar{\rho}$ is the starting point and ρ_{MAX} the desired point, we determine the interval $\Delta \rho$ and the number of times the above expansion must be applied by the following method:

$$\text{Is } |\rho_{MAX} - \bar{\rho}| < 0.20 ?$$

If the answer is NO, divide by 5 and test the result.

If N is the number of times we apply this test, then

$$\Delta \rho = \frac{\rho_{MAX} - \bar{\rho}}{5^{(N-1)}} \quad (4.70)$$

where

$$\text{number of times} = 5^{(N-1)}. \quad (4.71)$$

The starting point is $\bar{\rho} = 2\eta$ and the starting values are taken from Tore Isacson's results (66),

$$\begin{aligned}
\left\{ \begin{array}{l} F_o(2\eta) \\ G_o(2\eta) \end{array} \right\} &= \left\{ \begin{array}{l} 0.7063326373 \\ 1.223404016 \end{array} \right\} \eta^{1/6} \left\{ 1 \mp \frac{0.04959570165}{\eta^{4/3}} - \right. \\
&\quad - \frac{0.00888888889}{\eta^2} \mp \frac{0.002455199181}{\eta^{10/3}} - \frac{0.0009108958061}{\eta^4} \\
&\quad \mp \frac{0.0008453619999}{\eta^{16/3}} - \frac{0.0004096926351}{\eta^6} \mp \frac{0.0007116506205}{\eta^{22/3}} \\
&\quad \left. - \frac{0.00002439615603}{\eta^8} \mp \dots \dots \dots \right\}. \tag{4.72}
\end{aligned}$$

$$\begin{aligned}
\left\{ \begin{array}{l} F_o'(2\eta) \\ G_o'(2\eta) \end{array} \right\} &= \left\{ \begin{array}{l} 0.4086957323 \\ -0.7078817734 \end{array} \right\} \eta^{-1/6} \left\{ 1 \pm \frac{0.1728260369}{\eta^{2/3}} + \right. \\
&\quad + \frac{0.0003174603174}{\eta^2} \pm \frac{0.003581214850}{\eta^{8/3}} + \frac{0.0003117824680}{\eta^4} \\
&\quad \pm \frac{0.009073066427}{\eta^{14/3}} + \frac{0.0002128570749}{\eta^6} \pm \frac{0.0006215584171}{\eta^{20/3}} \\
&\quad \left. + \frac{0.00003685244766}{\eta^8} \pm \dots \dots \dots \right\}. \tag{4.73}
\end{aligned}$$

The values of $F_1(\eta, \rho)$ and $G_1(\eta, \rho)$ were obtained from Equation 4.10, and forward recursion of Equation 4.11 was then employed to obtain higher L-values.

e. Subsection V In this region, the functions F_L and G_L vary extremely rapidly and if one attempts to use the Taylor series method of Subsection IV, round-off errors soon destroy the accuracy of the function

$F_L(\eta, \rho)$. The reason for this is exactly the same one as outlined for Subsection I. Thus one needs to employ a different procedure to evaluate $F_L(\eta, \rho)$ in this region. The function $G_L(\eta, \rho)$ is calculated exactly as in Subsection IV, i.e. a Taylor's series expansion. The next logical step would be to employ the procedure used in Subsection I to evaluate $F_L(\eta, \rho)$. However, as pointed out by Gautschi (62), the three-term recurrence relation is also dependent on the value of η and since the proportionality constant α , Equation 4.41, depends primarily on η , one must be careful as to how α is evaluated. The simple procedure of Equation 4.44 does not work in this region. Gautschi (63,64) has developed a method that will evaluate α for all regions. However, his approach is both slow and requires excessive storage (12K bytes on the model IBM 360/65 computer). It was found however that the evaluation of $F_0(\eta, \rho)$ by Gaussian quadrature gives satisfactory results in this region. The integral representation, Equation 4.7 was used and the same method employed as for $G_0(\eta, \rho)$ in Subsection I with

$$x(\text{cutoff}) = 12. \quad (4.74)$$

The values of G_0 and G_1 being determined by the Taylor's series expansion, the value of F_1 was then obtained from Equation 4.49. The values of F_L and G_L for $L > 1$ were then generated by forward recursion.

f. The negative energy solution For negative energies, the function $W(-\eta, L + \frac{1}{2}, 2\rho)$ was computed to seven significant figures accuracy by means of a 16-point Gaussian-Laguerre quadrature formula. Since the Gaussian-Laguerre quadrature formulae apply to integrals of the form

$$y = \int_0^{\infty} e^{-x} f(x) dx$$

one sees from Equation 4.39 that no subdivision of the range is necessary. Thus, the evaluation of this function is particularly straightforward once the order of the polynomial approximating the integrand is deduced; the term integrand excludes the decreasing exponential term. The use of the 16-point formula implies that the integrand is well approximated by a polynomial of degree 31 over the entire range from zero to infinity.

4.5 Accuracy of the numerical evaluations

The computer algorithm I wrote to evaluate the Coulomb functions was constructed so as to return values of F_L , G_L , F_{L+1} and G_{L+1} simultaneously because all derivative relations employed in this thesis were written in terms of the function values for L and $L+1$. All calculations for the function values were performed in double-precision arithmetic (15 significant figures) on the model IBM 360/65 computer at the Iowa State Computation Center. The complex gamma function appearing in Equation 4.51 was computed in complex double-precision arithmetic with 15 significant figure accuracy by a separate algorithm I wrote based on the asymptotic properties of the gamma function. As a computational check, the tables of Abramowitz, Tubis, Lutz and Karvelis, and Luk'yanov et al. (42, 68, 58, 75) were reproduced for wide ranges of L , η , and ρ . A thorough analysis of the results of this computation produced the various boundary lines separating the subsections I-V in Figure 4. The corresponding function values for the range $\eta, \rho \leq 40$, $L \leq 6$ were accurate to

± 3 units in the fifth significant figure. The Wronskian relation, Equation 4.13, was found to be satisfied to within an absolute error of 0.2% in all cases. The maximum relative error for any L value from 0 to 6 was less than or equal to 0.1% thus justifying the use of forward recursion for $F_L(\eta, \rho)$ in Regions II-V of Figure 4. It may be noted (68) that most nuclear reaction calculations would require values of $F_L(\eta, \rho)$ and $G_L(\eta, \rho)$ in the ranges

$$0.1 \leq \eta \leq 30 \quad (4.75a)$$

$$1 \leq \rho \leq 30. \quad (4.75b)$$

The length of time necessary to calculate any one function value in a particular ρ - η region is difficult to estimate since the algorithm returns F_L , G_L , F_{L+1} and G_{L+1} simultaneously. Average run times (in milliseconds) on the IBM 360/65 to calculate the set $\{F_L, G_L, F_{L+1}, G_{L+1}\}$ are reported below for each region:

Subsection I : 138.50

Subsection II : 12.21

Subsection III : 4.24

Subsection IV : 71.60

Subsection V : 160.96 .

Increased accuracy for the regular solution $F_L(\eta, \rho)$ can be achieved by using Gautschi's excellent algorithm (63) which will reproduce the exact value of F_L up to 14 significant figures. Recent work (78) at the Argonne National Laboratory by W. J. Cody and Kathleen A. Paciorek has resulted in

an adaption of Gautschi's algorithm for the evaluation of $F_L(\eta, \rho)$ tested for the ranges:

$$0 \leq L \leq L_{\text{MAX}}$$

$$0 \leq \eta, \rho \leq 30$$

with 14 significant figure accuracy. The execution time for any particular value of F_L ranges from 10 to 70 milliseconds. An algorithm for the evaluation of $G_L(\eta, \rho)$ with the same accuracy is currently being tested by the aforementioned researchers. These algorithms, although resulting in much improved numerical accuracy, were not used because of their increased execution time and larger core storage requirement. It may be noted that one does not often need 14 significant figures since most experimental reaction data is good to only ten percent accuracy. One must however be careful in using function values good only to five significant figures, as has been done here, so that the accumulated round off at the end of the calculation does not result in less accuracy than experimentally achieved. The Coulomb functions although possessing various closed form analytic representations are numerically extremely difficult to calculate but I feel that the five significant figure accuracy obtained from my investigations is sufficient for most single precision nuclear physics calculations.

CHAPTER V. NEUTRON WAVE FUNCTIONS AND NUMERICAL ANALYSIS

5.1 Basic properties of neutron wave functions

The neutron wave functions referred to in this thesis are solutions of the equation

$$x^2 u_L'' + 2x u_L' + [x^2 - L(L+1)] u_L = 0$$

$$(L = 0, \pm 1, \pm 2, \pm 3, \dots). \quad (5.1)$$

The particular solutions of interest are the spherical Bessel functions of the first, second, and third kind; j_L , n_L and $h_L^{(1)}$ respectively. They are related to the Bessel functions of half-odd integer order by

$$j_L(x) = (\pi/2x)^{1/2} J_{L+1/2}(x) \quad (5.2a)$$

$$n_L(x) = (-)^L (\pi/2x)^{1/2} J_{-L-1/2}(x) \quad (5.2b)$$

$$h_L^{(1)}(x) = j_L(x) + in_L(x) = (\pi/2x)^{1/2} H_{L+1/2}^{(1)}(x). \quad (5.2c)$$

The function $j_L(x)$ is regular at the origin and $n_L(x)$ is irregular having a pole of order $L+1$ at the origin:

$$j_L(x) \underset{x \rightarrow 0}{\sim} x^L / (2L+1)!! \quad (5.3a)$$

$$n_L(x) \underset{x \rightarrow 0}{\sim} \frac{-(2L+1)!!}{(2L+1)} x^{-L-1} \quad (5.3b)$$

The functions j_L , n_L and $h_L^{(1)}$ have the following power series

representations

$$j_L(x) = \frac{\sqrt{\pi}}{2} \sum_{k=0}^{\infty} \frac{(-)^k}{k!} \frac{(x/2)^{L+2k}}{\Gamma(k+L+3/2)} \quad (5.4a)$$

$$n_L(x) = (-)^{L+1} \frac{\sqrt{\pi}}{2} \sum_{k=0}^{\infty} \frac{(-)^k}{k!} \frac{(x/2)^{2k-L-1}}{\Gamma(k-L+1/2)} \quad (5.4b)$$

$$h_L^{(1)}(x) = i^{-L-1} x^{-1} e^{ix} \sum_{k=0}^L \frac{\Gamma(L+k+1)}{k! \Gamma(L-k+1)} (-2ix)^{-k}. \quad (5.4c)$$

Asymptotically, j_L and n_L have the form

$$j_L \underset{x \rightarrow \infty}{\sim} x^{-1} \sin(x-L\pi/2) \quad (5.5a)$$

$$n_L \underset{x \rightarrow \infty}{\sim} -x^{-1} \cos(x-L\pi/2). \quad (5.5b)$$

From the power series representations, the following recurrence formulae may be derived:

$$f_L(x) : j_L(x), n_L(x), h_L^{(1)}(x) \quad (L = 0, \pm 1, \pm 2, \dots)$$

$$L f_{L-1}(x) - (L+1) f_{L+1}(x) = (2L+1) \frac{d}{dx} f_L(x) \quad (5.6a)$$

$$\frac{L+1}{x} f_L(x) + \frac{d}{dx} f_L(x) = f_{L-1}(x) \quad (5.6b)$$

$$\frac{L}{x} f_L(x) - \frac{d}{dx} f_L(x) = f_{L+1}(x) \quad (5.6c)$$

$$f_{L-1}(x) + f_{L+1}(x) = (2L+1) x^{-1} f_L(x). \quad (5.6d)$$

The Wronskian of j_L and n_L is most easily obtained from their asymptotic forms giving

$$j_L(x) n_{L-1}'(x) - j_{L-1}'(x) n_L(x) = x^{-2}. \quad (5.7)$$

Using the Wronskian relation and the recurrence formulae the following cross products are obtained:

$$j_L(x) n_{L-1}(x) - j_{L-1}(x) n_L(x) = x^{-2} \quad (5.8a)$$

$$j_{L+1}(x) n_{L-1}(x) - j_{L+1}(x) n_{L+1}(x) = (2L+1) x^{-3}. \quad (5.8b)$$

The spherical Bessel functions j_L and n_L are merely polynomials in x^{-1} times $\sin x$ or $\cos x$ as shown by Rayleigh's formulas (42, p. 439)

$$j_L(x) = x^L \left(-\frac{1}{x} \frac{d}{dx}\right)^L \frac{\sin x}{x} \quad (5.9a)$$

$$n_L(x) = -x^L \left(-\frac{1}{x} \frac{d}{dx}\right)^L \frac{\cos x}{x} \quad (L = 0, 1, 2, \dots). \quad (5.9b)$$

Thus, they should be easily calculable. As pointed out in Chapter IV, the irregular solution n_L is stable with respect to forward recursion and in fact using the relations

$$n_0(x) = -\frac{\cos x}{x}, \quad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x} \quad (5.10a)$$

$$n_{L+1}(x) = (2L+1) x^{-1} n_L(x) - n_{L-1}(x) \quad (5.10b)$$

the function $n_L(x)$ is readily calculated for all positive L -values. For

negative L -values, $n_L(x)$ is related to the regular solution by

$$n_L(x) = (-)^{L+1} j_{-L-1}(x) \quad (L = 0, \pm 1, \pm 2, \dots). \quad (5.11)$$

The function $j_L(x)$ is however stable with respect to backward recurrence. However, the forward stability of $j_L(x)$ is not as prone to error accumulation as its counterpart, the regular Coulomb function. The function $j_L(x)$ may also be written conveniently as

$$j_L(x) = f_L(x) \sin x + (-)^{L+1} f_{-L-1}(x) \cos x \quad (5.12a)$$

$$f_0(x) = x^{-1}, \quad f_1(x) = x^{-2} \quad (5.12b)$$

$$f_{L-1}(x) + f_{L+1}(x) = (2L+1) x^{-1} f_L(x) \quad (L = 0, \pm 1, \pm 2, \dots). \quad (5.12c)$$

Equation 5.12 amounts to using forward recurrence on the polynomial in x^{-1} and thus reduces round-off error. The use of Equation 5.12 gives 14 significant figures in double precision arithmetic for the range

$$2 \leq x \leq 100 \quad (5.13a)$$

$$-10 \leq L \leq 10. \quad (5.13b)$$

For the region $0 \leq x < 2$, the value of $j_L(x)$ is correctly given by the series expansion, Equation 5.4a, with the cutoff criterion

$$\left| \frac{a_n (x/2)^{2n-L-1}}{\sum_{k=0}^n a_k (x/2)^{2k-L-1}} \right| \leq 10^{-8} \quad (5.14)$$

where a_k is given by Equation 5.4a. One could use the same backward recurrence technique as outlined in Chapter IV for the regular Coulomb function but for the range of values of interest in nuclear physics this is not necessary. The use of Equation 5.12 and the power series expansion give accurate (≥ 7 significant digits) results in the order of one millisecond on the IBM-360/65 computer. The function $h_L^{(1)}(x)$ was calculated using the power series representation, Equation 5.4c. Note that the sum occurring in Equation 5.4c is finite making $h_L^{(1)}(x)$ easily calculable. The wave function of interest in the neutron calculations is $h_L^{(1)}(ix)$ which is either pure real or pure imaginary depending on whether L is even or odd. The function actually calculated by the computer was

$$(-)^{L+1} \exp(i3L\pi/2) h_L^{(1)}(ix) \quad (5.15)$$

which is seen to agree with the proton limiting case, Equation 4.43 and which leaves the normalization constant for this function independent of L .

5.2 Integrals of spherical Bessel functions

Definite and indefinite integrals of the spherical Bessel functions have been scattered throughout the literature of nuclear physics. Most of these integrals can easily be derived using the basic differential Equation 5.1 and the recurrence formulae, Equation 5.6. Some of the most important of these integrals are presented below as an aid to future researchers:

$$\int x^{L+2} f_L(x) dx = x^{L+2} f_{L+1}(x) \quad (5.16)$$

$$\int x^{1-L} f_L(x) dx = -x^{1-L} f_{L-1}(x) \quad (5.17)$$

$$\int x^2 f_L^2(x) dx = \frac{x^3}{2} [f_L^2(x) - f_{L-1}(x) f_{L+1}(x)] \quad (5.18)$$

$$\int f_L(x) g_m(x) dx = \frac{x^2 [f_{L-1}(x) g_m(x) - g_{m-1}(x) f_L(x)]}{(L-m)(L+m+1)} - \frac{x f_L(x) g_m(x)}{(L+m+1)} \quad (5.19)$$

$$\int f_L(\alpha x) g_L(\beta x) x^2 dx = \frac{x^2}{(\alpha^2 - \beta^2)} [\beta f_L(\alpha x) g_{L-1}(\beta x) - \alpha f_{L-1}(\alpha x) g_L(\beta x)] \quad (5.20)$$

$$\int_{-\infty}^{\infty} j_m(x) j_n(x) dx = \frac{\pi}{2n+1} \delta_{nm} \quad (5.21)$$

$$\int_0^{\infty} j_m(x) j_n(x) dx = \sin[(n-m)\pi/2] / [n(n+1) - m(m+1)] \quad (5.22)$$

$$\int_0^{\infty} \{j_n(x)\}^2 dx = \pi/2(2n+1) \quad (5.23)$$

If one employs the trick of expanding $\beta = \alpha + \delta_\alpha$ in Equation 5.20 and follows the same procedure used to obtain Equation 4.29 in Chapter IV, the following important normalization integral results

$$\int f_L(\alpha x) g_L(\alpha x) x^2 dx = \frac{x^3}{2} [f_L(\alpha x) g_L(\alpha x) - f_{L-1}(\alpha x) g_{L+1}(\alpha x)] \quad (5.24)$$

As is easily seen from the limit Equations 4.18 and 4.19, many of the properties of the Coulomb and spherical Bessel functions are quite similar and in fact this similarity was employed to obtain many of the results given in Chapter IV. It seems reasonable to assume that by properly choosing the wave number k in $j_L(kr)$ and $n_L(kr)$ that one could simulate the Coulomb functions $F_L(\eta, k'r)$ and $G_L(\eta, k'r)$; the relationship of k to k' however is not obvious. This has not been tested since there was no explicit need to search for such an interrelationship. In the past, researchers have attempted such a simulation to circumvent the actual computation of the Coulomb functions. It is my opinion that one should not try to make a spherical Bessel function "look" like a Coulomb function when perfectly adequate algorithms exist for the computation of both.

5.3 Numerical analysis

In constructing the computer program for the eigenchannel procedure applied to C^{12} it was found that having explicit forms for the wave functions was a good way to estimate error build-up but was a poor way of getting fast execution time. Various numerical techniques had to be employed to reduce the execution time to a reasonable value. If one were to solve the transcendental boundary conditions for the particle state energies by standard techniques the amount of time consumed is appreciable. Referring to the boundary condition versus E graph, Figure 2 of Chapter III, we see that a fixed boundary condition value B_c intersects the curve in only one point in each region; a region being defined by the values of E for which the boundary condition becomes infinite. Thus the first method

employed was to define the range of each region and then by using successive bisection and inverse interpolation (Muëller's method) find the value of βa which satisfied Equations 3.14 or 3.15 in each region. If six channels were open and five states kept within each channel, this means that Muëller's method had to be employed thirty times. A strict use of Equations 3.14 or 3.15 for the boundary condition value would easily lead to a total time of 62 seconds for the preceding example. One must keep in mind that this is 62 seconds for each guess of the phase δ_1 and that calculating the particle state energies is only the first step in the eigenchannel process. It proved more practical to tabulate the inverse graph of (E) vs. (βa) . These are essentially arc-cotangent curves and in every region except the first the function

$$E = c_1 + c_2 [\pi/2 - \cot^{-1} (c_3 \cdot B_c)] \quad (5.25)$$

was fitted to the data by a non-linear least squares technique (79, p. 382). In the region between $E \geq 0$ and the point where B_c first goes to minus infinity it was necessary to join the two curves

$$E_{<} = c_4^2 [c_5^2 - (B_c - c_6)^2]^{1/2} \quad (\text{an ellipse}) \quad (5.26a)$$

and

$$E_{<} = c_1 + c_2 [\pi/2 - \cot^{-1} (c_3 \cdot B_c)] \quad (5.26b)$$

to obtain the necessary curvature for low energy. Again a non-linear least squares technique was employed and the parameters of Equation 5.26 were further constrained so that $E_{<}$ and $E_{>}$ matched at some point x_0 , x_0 being an additional parameter. These methods were employed for all of the

possible allowed energy regions and a table of parameter values was then stored in the program. The relative error in any one energy value found by this curve-fitting technique was found to be $\leq 1\%$. For the case of six open channels referred to earlier the total execution time was found to be less than 10 milli-seconds, roughly 1/2000 of the previous time.

When constructing matrix elements and performing normalization integrals, exact values for the integrals were used when possible. Those integrals involving the function $S_L(\alpha, \gamma r)$, Equation 3.8, were performed by dividing the range from zero to r_w into twelve subregions and using Weddle's rule (80, pp. 133-134) in each subregion. The use of Weddle's rule implies that

$$\int_{x_0}^{x_0+nh} f(x) dx = \frac{3h}{10} \sum_{m=0}^n k_m f(x_m) \quad (5.27a)$$

where n is a multiple of six and

$$k = 1, 5, 1, 6, 1, 5, 2, 5, 1, 6, 1, 5, \dots \quad (5.27b)$$

The value of n chosen was $n=12$ and thus in each subregion by using Weddle's rule we approximate the graph of the function by two arcs of sixth-degree polynomials. Equation 5.27 is more accurate, in general, than the corresponding Simpson's rule, but it requires at least seven consecutive values of the function. In constructing the matrix elements of the dipole operator, integrals involving the products of Coulomb functions were performed over the entire range $r_w \leq r \leq a$ by a single application of a 10-point Gaussian quadrature formula. This approximation of the integrand by a

polynomial of order 19 over the entire range gave correct values for the integrals in the least amount of time. The method employed to test whether this integration method would yield the correct answer was to compare that value against the answer given by dividing the total range into twenty intervals and applying Weddle's rule to each interval. The use of such numerical integration techniques such as the Gauss and Weddle formulas is an important means by which one can evaluate integrals for which closed form expressions are not known or involve more computation time than doing the integral numerically. What does one do however when even numerical integration techniques prove too time consuming? This problem arises from the normalization of the proton single-particle states. The integral in question is

$$\int_{r_w}^a [F_L(\eta, \beta r) \cos \delta_L + \sin \delta_L G_L(\eta, \beta r)]^2 dr. \quad (5.28)$$

The range of the integral is large and the integrand must be approximated by a large order polynomial. It is more expedient in such cases to tabulate the values of the integral at fixed points and use numerical interpolation. The integral, Equation 5.28, was split into the nine integrals

$$\int_{r_w}^a F_L^2(\eta, \beta r) dr ; \quad \int_{r_w}^a G_L^2(\eta, \beta r) dr ; \quad \int_{r_w}^a F_L(\eta, \beta r) G_L(\eta, \beta r) dr$$

$$(L = 0, 1, 2) . \quad (5.29)$$

Each integral was then computed as a function of energy E in 1 MeV steps from $0 \leq E \leq 252$ MeV and stored as nine linear arrays. In Figure 5 we see

Figure 5. Normalization integrals for the $L = 0$ Coulomb wave functions

a plot of these integrals. Interpolation within any 1 MeV interval was performed according to Table 3.

Table 3. Interpolation scheme for the normalization integrals of the proton states

Range	Method	Function Interpolated	Technique	Relative Error
$0 \leq E \leq 1$	Aitken's	$\int F_L^2, \int F_L G_L,$ $e^{-2\pi\eta} \int G_L^2$	First 8 succeeding values used	1 %
$1 < E \leq 7$	Aitken's	$\int F_L^2, \int F_L G_L,$ $\int G_L^2$	First 5 succeeding values used	≤ 1 %
$7 < E \leq 245$	Bessel's	$\int F_L^2, \int F_L G_L,$ $\int G_L^2$	Differences up to fifth order	$\leq .05$ %
$E > 245$	Aitken's	$\int F_L^2, \int F_L G_L,$ $\int G_L^2$	First 5 preceding values used	≤ 1 %

In the range $0 \leq E \leq 1$, the integral of the square of G_L goes to infinity as E goes to zero so interpolation of $\int G_L^2$ proved disastrous. However the first term in an expansion of this integral is $e^{2\pi\eta}$ so interpolation of the function $e^{-2\pi\eta} \int G_L^2$ gives far better results.

The eigenvalues of the energy matrix were found by using the fortran routine, "Rilmat" appearing in the excellent compendium, "The Programmer's Handbook" (81). This routine was adapted to make the most efficient use of the QR transformation which it employs by first scaling the energy matrix to be diagonalized. The true eigenvalues and eigenvectors were then obtained by reversing the scaling transformation. The real eigenvectors were constructed using Wielandt's deflation technique (82, p. 483) which after each eigenvector calculated effectively reduces the order of the matrix by one; the next eigenvector being calculated from this reduced matrix.

It should be pointed out that the search procedure as outlined in Chapter III can run into difficulty. If an eigenphase falls within an ϵ - neighborhood of a discontinuity point, one eigenphase will be lost. If the curve representing $E_\lambda - E_\gamma$ should cross the axis more than once in the interval being searched, merely subtracting the number of eigenvalues less than E_γ at either end of the interval will not give the correct number of eigenphases. Since all intervals between zero and π are searched, any loss of eigenphases due to either of the above difficulties is easily noted and by changing E_γ slightly the problem can be corrected. In earlier works on the eigenchannel theory a search procedure was utilized which started at zero phase and successively searched succeeding intervals until the correct number of eigenphases were obtained. The entire range from zero to π was not however checked if the correct number of eigenphases was found before reaching π . In addition, the basis states were assumed orthogonal. Making a similar assumption, it was found that extraneous eigenphases are

generated which are undetectable unless the entire range of $\delta^{J,v}$ is searched. As stated in Chapter I, these false eigenphases lead to spurious peaks in the cross sections and thus it is imperative that one properly take into account the non-orthonormality of the basis states and sweep the entire range of $\delta^{J,v}$ to be sure that no extra eigenphases have been introduced and that none of the true eigenphases are lost. The numerical techniques pointed out in this chapter were only a small fraction of the various techniques employed in constructing the computer program for C¹². They indicate, however, the approximations used and the relative accuracy obtainable. In analyzing all of the techniques employed in this calculation, I believe it is safe to say that the final cross section values were in error by less than 6 % due to round-off and error accumulation. This is well within the bounds of experimental error. Let us now examine in the following chapter the results of this calculation.

CHAPTER VI. EIGENCHANNEL CROSS SECTIONS FOR C^{12} 6.1 Calculation of the photoabsorption cross sections

The theory as outlined in Chapters III - V contains only one adjustable parameter; the strength of the residual interaction, V_0 . Using the experimental photoneutron cross section data of Cook et al. (83) as a guide, many preliminary runs were made of the photoabsorption cross sections in the giant resonance region for various values of V_0 . Not only did we wish to reproduce structure similar to that seen by Cook but simultaneously we wanted the photoproton cross section to agree with experimental data. The shape and amplitude of the cross sections are highly dependent on the value of V_0 . The best agreement with experimental data was obtained with

$$V_0 = 2200 \text{ MeV } F^6. \quad (6.1)$$

A change of only 200 units in the value of V_0 was sufficient to change the amplitude by several orders of magnitude while a change in V_0 of 500 units was sufficient to completely alter the structure of the photoproton curve. The value of V_0 at 2200 MeV F^6 produced resonances in approximate accord with experimental findings although the amplitudes of the giant resonance peaks were much too large. However an overestimate of the amplitudes of the resonances is common to all one-particle-one-hole shell model calculations.

The reaction in which the emitted particle leaves the product nucleus in its ground state is denoted by the symbols (γ, p_0) and (γ, n_0) corresponding respectively to the reactions $C^{12}(\gamma, p_0)B^{11}$ and $C^{12}(\gamma, n_0)C^{11}$.

The threshold energies for these reactions are 15.96 and 18.72 MeV respectively. The reactions in which the product nucleus is in an excited state are denoted by (γ, p') and (γ, n') for the respective reactions $C^{12}(\gamma, p')B^{11*}$ and $C^{12}(\gamma, n')C^{11*}$. In our one-particle-one-hole framework, the threshold energies for these channels are 34 and 37 MeV respectively. The giant resonance region for the (γ, p_0) and (γ, n_0) reactions is approximately between 21 - 24 MeV excitation energy. Some structure has been seen below the giant resonance for both photoneutron and photoproton total absorption reactions (83, 84, 85). Thus, the (γ, n_0) and (γ, p_0) cross sections were calculated in 250 keV intervals from 16 to 20 MeV. The giant resonance region itself has been a mystery to experimental researchers for many years because of the conflicting evidence of fine structure in this region. A step width of 125 keV was used for the region from 20 to 24 MeV to insure that possible resonances were not overlooked. Again using experimental evidence as a guide, the region from 24 to 35 MeV was searched in 250 keV steps and steps of 500 keV were used for the region from 35 to 40 MeV. Some structure attributable to photoabsorption by the $1s_{1/2}$ state of C^{12} has been reported by Fultz et al. (86), Fossa et al. (87), and Cook et al. (22) for the total photoneutron absorption reaction $C^{12}(\gamma, n)C^{11}$ in the region of 35 MeV excitation energy. This resonance should be of the order of 1 or 2 MeV wide so that a step width of 500 keV in this region is not inappropriate. Previous research (14, 88, 15, 16, 17) employing the eigenchannel formalism failed to explicitly state the amount of time involved in this type of

calculation. The amount of time necessary to calculate adequate cross sections is, however, very important. After all, if similar results can be obtained by other means in a shorter amount of time, why should the researcher limit himself solely to the eigenchannel theory. The amount of time involved in this calculation is a function of the excitation energy and greatly increases for higher energies where the number of open channels increases. The average amount of time necessary to compute one set of (γ, n_0) , (γ, p_0) , (γ, n') and (γ, p') cross section values was 8 minutes for the 16 to 18.72 MeV interval, 12 minutes in the range 18.72 to 34 MeV, 60 minutes in the interval 34 to 37 MeV and 120 minutes from 37 to 40 MeV. These estimates are based on the IBM Model 360/65 computer at the Iowa State Computation Center. The reader should bear in mind that these time estimates are in minutes whereas usual nuclear shell-model calculations are of the order of seconds or milliseconds. As one can see, the amount of time needed to calculate a particular set of cross section points at a fixed value of the excitation energy becomes quite large above the giant resonance region. The total amount of time necessary to adequately construct the photoabsorption cross sections for C^{12} was 46 hours. In the high energy region an incorrect number of eigenphases for a fixed excitation energy was often encountered for the reasons outlined in Chapter V, Section 5.3 and thus approximately one-third of the total time involved was spent in correctly analyzing these regions. The resultant photoabsorption cross sections are shown in Figures 6 and 7.

Figure 6. Photoneutron cross section of C^{12} in the eigenchannel reaction theory

Figure 7. Photoproton cross section of C^{12} in the eigenchannel reaction theory

6.2 The reaction $^{12}\text{C}(\gamma, n_0)^{11}\text{C}$

The structure of the photoneutron cross section (Figure 6) resulting from the eigenchannel theory is seen to be in good accord with the experimental data although the absolute value of the cross section is overestimated in the giant resonance region. The giant resonance itself is split into two narrow peaks at 22.25 MeV and 23.00 MeV. The ratio of the heights of these peaks is approximately 1.30 as compared to the value of 1.09 by Cook et al. (83) and 1.30 by Fultz et al. (86). Thus the relative strengths of these peaks seems to be in good agreement with experiment. A comparison of the photoneutron resonances found in this thesis and the experimentally observed peaks is shown in Table 4. The four experimental works used for comparison employed different techniques in obtaining the photoneutron cross section. Lochstet and Stephens (89) produced the (γ, n) reaction by means of the monochromatic gamma rays from the $T(p, \gamma)\text{He}$ reaction. Their cross section values were determined absolutely to a claimed accuracy of 10% although the heights of their peaks at the giant resonance peaks 22.20 and 23.00 MeV were approximately equal within experimental accuracy. The work of Fultz et al. (86) was performed with nearly monochromatic photons obtained from the annihilation of positrons in flight with an energy resolution for the positrons and photons of 1%. By carefully subtracting out the (γ, n_0) component of their total photoneutron absorption cross section they arrived at the conclusion that 83% of the neutrons were being emitted in transitions to the ground state of ^{12}C for excitation energies up to 28 MeV. Thus the prominent structure in the

Table 4. Photoneutron resonances in C^{12}

Experimental Papers $C^{12}(\gamma, n)C^{11}$				
This work	Cook et al. (83)	Lochstedt (89)	Fultz et al. (86)	Fossa et al. (87)
19.25	19.80 20.10 20.35			
20.50	20.60 20.90 21.30			
21.50	21.65			
22.00		21.75	22.00	
	22.10			
22.25		22.20		
	22.75			
23.00		23.00	23.20	
23.50	23.60	23.70		
			24.00	
		24.90		
	25.35			
		25.60	25.50	
26.25	26.10	26.00		
		26.50		
	27.55		27.10	
	29.50		28.30	
	32.70		20.50	
33.50				
			35.20	35.00
	36.40			
38.00				53.00

giant resonance region is due primarily to the $C^{12}(\gamma, n_0)C^{11}$ reaction. The resonance seen at 35 MeV by Fossa et al. (87) was obtained by a Penfold and Leiss analysis of the yield curve obtained by exposing a liquid scintillator to the γ -ray beam of a 100 MeV Synchrotron. Although their results are somewhat uncertain because of the experimental technique involved they do agree with similar findings by Reay et al. (85) in the $B^{11}(p, \gamma_0)C^{12}$ reaction. The strength of this resonance is thought to come from the process of knocking a particle out of the $1s_{1/2}$ shell; the resulting particle-hole state being the $(1p_{1/2}, 1\bar{s}_{1/2})$ state. Greater precision was obtained in the work of Cook et al. (83) with the source of photons being bremsstrahlung radiation having endpoint energies up to 65 MeV. The method of 'least structure' analysis was employed to the yield curves of the (γ, n) reaction with reported resolution of (100 - 300 keV) in the giant resonance region. Although the number of dipole absorption peaks found in this thesis falls short of the total resonances found by Cook the general agreement of resonance positions is good. It must be noted that the data of Cook represents the total (γ, n) reaction and thus some of the observed resonances must be associated with multipoles other than the $T=1$ dipole absorption transitions. Although the results of Cook do not support the idea of large dipole oscillator strength near 35 MeV the existence of a $(1p_{1/2}, 1\bar{s}_{1/2})$ excitation at 29.50 MeV was suggested where a resonance of about 1 MeV in width was seen. A later analysis by Frederick (90) in collaboration with Cook's group suggests that the hole in the $1s$

shell is probably found at 31 or 36 MeV or split between the 31 and 36 MeV resonances by interactions of higher order than the one-particle-one-hole residual interaction. The resonance found in this thesis at 33.50 MeV is a $(1d_{5/2}, 1\bar{p}_{3/2})$ excitation since the $1\bar{s}_{1/2}$ channel is not open in our model until an excitation energy of 37 MeV is reached. The question of whether resonances seen in this energy region may be reasonably interpreted as excitations from the $1s_{1/2}$ state will be discussed in Section 6.6. From Table 4 we can see that the one-particle-one-hole dipole absorption peaks found by the eigenchannel theory show remarkable similarity to corresponding experimental peaks. One must bear in mind that the model used in this thesis is overly simplified and thus only the general shape of the photoabsorption curve was expected. The relatively low amplitude of the theoretical cross section in the high energy regions is in part a reflection of the fact that only one-particle-one-hole states were employed. The experimental (γ, n_1) cross section data adds appreciable strength in these regions and since higher particle-hole configurations would be necessary to adequately describe this reaction it is not surprising that the theoretical amplitude for the cross section above the giant resonance is too small. The (γ, np) and $(\gamma, 2n)$ channels are open at excitation energies of 27.7 and 31.9 MeV respectively so that the theoretical cross section also omits the contributions of these reactions.

If one were to expand the angular distribution in a series of Legendre polynomials as

$$P(\theta, E) = \sum_{L=0}^{\infty} B_L P_L(\cos \theta) \quad (6.2)$$

and normalize the distribution so that $B_0 = 1$, the value of the coefficient B_2 is a direct measure of the dipole absorption strength.

A plot of B_2 versus excitation energy was not calculated for the neutron distribution (although this could easily have been done) since there is only one experimental data point available for comparison.

However, we can say something about the character of the states comprising the resonance peaks by looking at a graph of the strength of a particle state as a function of energy. In Figure 8 we see a graph of the strengths of the $2s_{1/2}$ and $1d_{5/2}$ particle states as a function of excitation energy for both the neutron and proton channels. The percentage strength of a state is defined as that fraction of the partial cross section at a fixed excitation energy directly attributable to that particular state. This is easily found from the partial cross section expression given in Chapter II, Equation 2.18.

A rather immediate observation is that the strength curves for the $2s_{1/2}$ and $1d_{5/2}$ states are nearly mirror images of one another. Thus the $1d_{3/2}$ state has negligible strength over the giant resonance region and in fact never exceeds fifteen per-cent over the entire range to 40 MeV. One would have to conclude that this state contributes to $T = 0$ states which are not highly excited by the residual interaction or that the $1d_{3/2}$ state must lend its strength to other multipole transitions. The resonance peak at 19.25 MeV is found to have 84% $2s_{1/2}$ state and 13% $1d_{5/2}$ state. Beyond this resonance the strength of the

Figure 8. Strength curves for the neutron and proton $2s_{1/2}$ and $1d_{5/2}$ states from the $C^{12}(\gamma, n)C^{11}$ and $C^{12}(\gamma, p)B^{11}$ reactions (a. Strength curve for neutron states. b. Strength curve for proton states. The positions of the resonance peaks are indicated by arrows in both graphs.)

$2s_{1/2}$ state decreases while that of the $1d_{5/2}$ state increases. At the giant resonance energy of 22.250 MeV we find a state which is 34% $2s_{1/2}$ state and 65% $1d_{5/2}$ state. The $1d_{5/2}$ state dominates in the resonances beyond the giant resonance except for the anomaly observed at 26.125 MeV seen as a sharp dip in the neutron strength curve. The fact however that the $1d_{5/2}$ and $2s_{1/2}$ states have nearly equal strength in the giant resonance region is totally unexpected and will be discussed in connection with the proton angular distribution for the (γ, p_0) reaction.

6.3 The reaction $C^{12}(\gamma, p_0)B^{11}$

In Figure 7 we see the (γ, p_0) cross section compared with the experimental data of Frederick (90) and Gemmell et al. (91). The giant resonance centered at 23.00 MeV is predominantly a single peak with narrow resonances calculated at 21.50 MeV and 22.00 MeV. Most of the experimental data derived from the (γ, p) reaction and the inverse reaction (p, γ) show only a single peak in the giant resonance region centered at approximately 22.50 MeV. The experimental data is, however, not inconsistent with the possibility of fine structure resonances appearing in the giant resonance region. A comparison of the main resonances found in this thesis and those from various experimental groups is shown in Table 5. Again we see comparable agreement between theory and experiment although the position of the theoretical peak at 23.00 MeV seems to be about a half MeV too high. A comparison with the work of Gemmell et al. (91) shows surprising agreement with the results

Table 5. Photoproton resonances in C^{12}

This work	Experimental Papers $C^{12} (\gamma, p) B^{11a}$					
	Allas et al. (84)	Shin and Stephens (92)	Frederick (90)	Vanhuyse (93)	Barber and Dodge (94)	Gemmell et al. (91)
18.75			19.2			
19.50						
20.40		20.57 20.95				
			21.3			
	21.4	21.40				21.90
21.50						
22.00				(22.00)	(22.00)	
	22.1		(22.36)			
		(22.40)				
					22.70 22.90	
						22.50
(23.00)						(23.15)
	23.70				24.2 24.8	
24.62						
25.00			25.10			
25.50				25.50		
	25.60					
			26.00		26.2	
26.25			27.25			
	28.60				26.9	
			29.60			
				30.00		
33.50						

^aThe numbers enclosed in parentheses indicate the giant resonance peak.

of this group in regards to the two resonances immediately below the 23.00 MeV peak. Because the results of Gemmell's group at the time were in conflict with other researchers, Gemmell questioned the actual existence of these resonances. Shin and Stephens (92) studied the (γ, p) reaction through the use of monochromatic photons produced by the $T^3(p, \gamma)He^4$ reaction and also suggested the appearance of several smaller resonances just below the giant resonance. As in the photoneutron cross section the amplitude of the (γ, p_0) cross section is overestimated; the height of the 23.00 MeV resonance is about four times that of experiment. The resonance structure found in the (γ, p_0) cross section by the eigenchannel formalism is not in contradiction with experimental data. The experimental data itself is still not firmly established. Although the energy and angular distributions agree (93), the absolute experimental cross sections for the $Cl^{12}(\gamma, p)B^{11}$ reaction and that of the inverse reaction $B^{11}(p, \gamma)Cl^{12}$ are not always in total accord. Vanhuyse and Barber (93) examined the (γ, p) reaction by the virtual photon technique claiming greater statistical accuracy and improved precision measurements as compared to previous (γ, p) experiments and still found some anomalies between their data and that of other researchers. All of the experimental evidence since 1958 supports the existence of an abnormally sharp peak in the (γ, p_0) curve in the vicinity of 22.50 MeV excitation energy. None of the existing data is in sharp conflict with the existence of fine structure resonances below 22.50 MeV. Above ≈ 25.4 MeV, all of the data exhibit a broad maximum at ≈ 26.4 MeV and

then a slow decline to 30 MeV (84). All of the above characteristics of the (γ, p) cross section are certainly confirmed by our theoretical results using the eigenchannel theory. Thus as far as the positions of the dipole resonances and the relative strengths of these peaks is concerned, the eigenchannel theory as employed in this thesis is in good accord with experiment. A comparison of the total γ -ray absorption data of Dolbilkin (95) with the sum of the (γ, n_0) and (γ, p_0) cross sections up to 24 MeV excitation energy is shown in Figure 9 and except for the amplitude of the theoretical curve we see good agreement with the hypothesis that dipole transitions account for most of the total γ -ray absorption cross section.

6.4 Comparison with other theories

A number of theoretical calculations have been performed to predict the strengths and energy positions of particle-hole excitations in ^{12}C . Vinh Mau and Brown (96) used the model of Brown (11) with zero-range particle-hole residual interactions both with and without ground state correlations. Gillet and Vinh Mau (6) computed in the same framework the states of ^{12}C and ^{16}O but used instead a finite-range residual interaction. A similar analysis was performed by Boeker (97) while Nilsson et al. (98) used a deformed potential to take account of the unclosed shell. Mikeska (99) employed a time-dependent Hartree-Fock approximation using a finite square well with $\vec{L} \cdot \vec{S}$ coupling. Mihailovic and Rosina (100) investigated the influence of two or more particle-hole pair configurations on the structure of the giant resonance. A comparison of the

Figure 9. A comparison of the total γ -ray absorption cross section of C^{12} and the dipole absorption cross section found from the eigenchannel theory (The experimental cross section has been scaled upwards by a factor of three.)

Figure 10. A plot of the eigenphases found in the C^{12} photo-absorption reaction

results of these works with data from the eigenchannel calculation is presented in Table 6. The giant resonance near 23.00 MeV is seen to be in accord with the work of Nilsson and Mihailovic whereas the resonances near 18.75 and 22.00 MeV are similarly reflected in the works of Vinh Mau and Brown and that of Mikeska. In general the theoretical papers predict that the resonances below and at the giant resonance should be principally $(2s_{1/2}, 1\bar{p}_{3/2})$ and $(1d_{5/2}, 1\bar{p}_{3/2})$ states; the resonance near 18.70 MeV being almost entirely a $(2s_{1/2}, 1\bar{p}_{3/2})$ state while the giant resonance should be approximately 78% or more of the $(1d_{5/2}, 1\bar{p}_{3/2})$. The resonance in the 33 MeV region is believed to be a 98% $(1p_{1/2}, 1\bar{s}_{1/2})$ state. The eigenchannel state listed in Table 6 at 33.50 MeV is a $(1d_{5/2}, 1\bar{p}_{3/2})$ state. Do the strengths of the states in the giant resonance region found by the eigenchannel theory agree with other theoretical approaches? From the strength curves (Figure 8) one can see that although the $(2s_{1/2}, 1\bar{p}_{3/2})$ state dominates below the giant resonance, the strengths of the $(2s_{1/2}, 1\bar{p}_{3/2})$ state and the $(1d_{5/2}, 1\bar{p}_{3/2})$ state are approximately equal in the giant resonance region. In fact a graph of the B_2 coefficient for the photoproton angular distribution compares very poorly with the experimental data of Allas et al. (84), Barber and Dodge (94) and Gove et al. (101). The difficulty, as we shall see in the next section, can be traced back to the form of the residual interaction employed in this calculation.

Table 6. A comparison of the eigenchannel results with other theoretical works

This work	Theoretical papers					Boeker (97)
	Vinh Mau and Brown (96)	Gillet and Vinh Mau (6)	Mikeska (99)	Nilsson et al. (98)	Mihailovic and Rosina (100)	
18.75	18.7	17.7	18.3		19.7	17.7
19.50						
21.50						
22.00	22.2	21.9	21.7	22.2		21.5
22.25						
23.00						
23.50	23.9			23.0	23.6	
24.62		24.2	25.0		24.6	24.2
25.00						
26.25						
				26.3	25.4	
				29.5	27.4	
				31.9	28.0	
33.50	34.3	33.8	34.3		29.2	33.6
38.00					30.7	
					31.7	
					40.7	

6.5 Accuracy of the calculation

The angular distribution is highly model dependent and as one can see from Equation 2.17 of Chapter II, the model dependence is concentrated in the values of the eigenvectors of the S-matrix, the $V_C^{J,\nu}$. For a fixed ν value, $V_C^{J,\nu}$ is proportional to the relative strength of the state in channel c . Thus if one were to follow the strength curves for the states assumed dominant in a particular reaction a rather quick estimate of the angular distribution coefficients can be drawn. Performing such a comparison with experimental data conclusively indicates that the strengths of the $2s_{1/2}$ and $1d_{5/2}$ states are incorrect near and above the giant resonance region. This implies that the corresponding values of $V_C^{J,\nu}$ are in error. The size of the error can be estimated by calculating the orthogonality relations Equations 1.11 and 1.12 of Chapter I for various values of the excitation energy. The results of such a calculation are given in Table 7.

Table 7. Orthogonality of the $V_C^{J,\nu}$

$E_{exc.} \text{ (MeV)}$	$\Delta_{\nu,\nu'} = \sum_j V_j^{\nu} V_j^{\nu'} \quad (\nu \neq \nu')$	$\Delta_{i,j} = \sum_{\nu} V_i^{\nu} V_j^{\nu} \quad (i \neq j)$
16.75	0.0	0.0
19.00	.00001 $\leq \Delta \leq$.055	.00001 $\leq \Delta \leq$.055
22.25	.004 $\leq \Delta \leq$.382	.002 $\leq \Delta \leq$.245
27.50	.002 $\leq \Delta \leq$.217	.006 $\leq \Delta \leq$.117
41.12	.0003 $\leq \Delta \leq$.202	.00001 $\leq \Delta \leq$.087

It is apparent that the $V_c^{J,\nu}$ are poor in the giant resonance region. Since the values of these functions are inherently dependent on the number of single-particle states kept within each channel, we must conclude that more states should have been kept within each open channel particularly in the giant resonance region. This of course would imply an increase in the total amount of computer time needed. Since the position of the resonance is solely determined by the excitation energy, the positions of the resonances as reported are correct. If one keeps a larger number of single-particle states in each open channel, the deviation from unitarity of the S-matrix will diminish. However, merely keeping more single-particle states in each open channel will not improve the angular distributions or the amplitudes of the resonance peaks. The relative strengths of the $V_c^{J,\nu}$ directly affect the angular distributions and the amplitudes of the resonance peaks. The $V_c^{J,\nu}$ are a reflection of the relative strengths of the various open channels. If the strength of a state is incorrect, the angular distribution involving that state will similarly be incorrect. The use of a surface-delta type residual interaction is the cause of the incorrect distribution of strength among the various channels. If one considers the two types of residual interactions usually employed (i.e., the zero-range and surface-delta interactions) the essential difference between the two is that the zero-range force results in an integration of the particle-hole states up to the radius 'a' whereas the surface-delta function merely evaluates the particle-hole wave functions at the radius of the square well. Therefore, an integration of the $(1d_{3/2}, 1\bar{p}_{3/2})$ states will carry

more strength than merely evaluating the state wave functions at the edge of the square well. In fact, the surface-delta interaction is more democratic in its relative strength assignments than the zero-range interaction. Thus, we would expect that if one were to employ the zero-range residual interaction instead of the surface-delta type, the strengths of the various single-particle states would be more nearly in accord with the results of experimental angular distributions. The amplitudes of the resonance peaks should also tend to agree more favorably with experiment. Again, however, the use of a zero-range force would increase the amount of computer time involved. One could also question the validity of the eigenphases which would be in doubt if the curves of the phases versus excitation energy should cross each other. According to the results of Wahsweiler and Greiner (14) this should never happen. Indeed from Figure 10 one can see that the curves for each eigenphase remain separate and never cross so there is no reason to doubt the values of the eigenphases found in this calculation. The eigenchannel theory as employed in this thesis is still somewhat incorrect. In the calculation of the single-particle states, only those states with positive energy were kept; the negative energy bound state solutions being discarded. On physical grounds the wave function of the scattered particle must reflect the fact the scattered particle has positive energy and thus the coefficient of any negative energy state in an expansion of the scattered wave function must be near zero. However it is possible for a state to be quasi-bound in the sense that the strength of the residual interaction could force the bound state

up into the continuum. Such effects have not been included. Weidenmüller and Mahaux (20) have also pointed out that in addition to keeping the true bound state solutions to the nuclear Hamiltonian one should also include the complete set of negative energy single-particle states which satisfy the "natural boundary condition". However, these states would have an exponentially increasing character outside the range of the finite potential used in the model and thus also represent highly unphysical states. In an investigation of this criticism, Wahsweiler et al. (19) came to the conclusion that only a finite number of these states give any appreciable contribution to the residual interaction and furthermore that the number of such states that should be included is not sizable. One cannot escape the fact that such states should be included for completeness but the question of exactly how many of these states (if any) are relevant to a particular calculation is still an open question. Weidenmüller and Mahaux (20) suggest that the exclusion of such states leads to spurious peaks in the cross section. We do not find this to be the case.

6.6 Low lying shells from photonuclear cross sections

It would be interesting from the standpoint of experimental photonuclear research to ascertain whether resonance peaks in the energy region above the giant resonance can be ascribed to single-particle excitations out of the low-lying closed shells. To examine this possibility in detail would have involved an intensive search of the region between 30 and 40 MeV excitation energy. Because of the excessive com-

puter time necessary for this region, a step width of 500 keV was originally proposed to search this region. However, numerical difficulties in the region beyond 34 MeV soon proved this to be an impractical undertaking. Instead, cross section curves were determined exactly at the excitation energies of 34.50, 35.25, 36.30, 37.30, 38.00 and 40.00 MeV and then a plot of the eigenphases versus excitation energy was employed to interpolate the eigenphases for intermediate energies. At the excitation energy of 38.00 MeV, the (γ, n') cross section exhibited a strong but narrow resonance corresponding almost entirely (98%) to a $(1p_{1/2}, 1\bar{s}_{1/2})$ transition. The amplitude of this resonance was 13.3 mb with the width of the resonance being less than 1 MeV. From our previous considerations, the amplitude of this resonance is probably in error and because higher order configurations than one-particle-one-hole have been excluded, one can not reasonably estimate the width of this resonance. However, the fact that this $(1p_{1/2}, 1\bar{s}_{1/2})$ resonance does appear with a much more pronounced amplitude than any other structure in this region is a good indication that perhaps the experimental interpretation of Cook (22) is correct. It may indeed be possible to ascribe these high energy resonances to essentially single-particle excitations out of low-lying closed shells. A similarly strong resonance was not however observed in the (γ, p') cross section data but it may be that we have merely overlooked this resonance. It may have the same width as the neutron resonance or be much smaller in width so that our search procedure in this range failed to detect it. It may be noted that the theoretical work of Mikeska (99) employing a similar square well po-

tential also predicted a sharp narrow (< 1 MeV) resonance in the same region but with an amplitude far exceeding expectation. This suggests the possibility that perhaps the amplitude of this resonance may be peculiar to the square-well potential. Nevertheless, definite structure is observed in the region 30 - 40 MeV which is attributable to a $(1p_{1/2}, 1\bar{s}_{1/2})$ transition.

CHAPTER VII. CONCLUSIONS

The eigenchannel theory, in principle, is a very appealing approach to the study of nuclear reaction theory. Since it results in the derivation of the complete S-matrix (in the one-particle-one-hole approximation) the eigenchannel theory readily yields all the relevant information concerning a particular reaction. However, as shown in this thesis the orthonormality of the single-particle wave functions must properly be taken into account to eliminate the appearance of spurious peaks in the cross sections. When the orthogonality of the basis states is properly accounted for, the various partial cross sections obtained from the eigenchannel theory are seen to be in good accord with experimental data. Nevertheless, the major drawback to a continued use of this formalism is the amount of computer time involved in such a calculation and the preponderance of numerical difficulties which appear. Even in an exact calculation, as has been employed in this thesis, the numerical difficulties encountered are excessive. If one could analytically relate the eigenphases of the S-matrix to the real phase shifts of the nuclear reaction, the time consuming search procedure of the eigenchannel theory could be avoided and the use of this theory as a powerful means of exploring both photonuclear and direct reactions would be greatly enhanced.

The resonance peaks found in the analysis of the C^{12} photo-absorption cross sections are in relatively good agreement with experiment although a larger number of single-particle basis states should

be kept within each open channel to insure the unitarity of the S-matrix. The relatively large amplitudes of the resonance peaks in the obtained cross sections indicate the need for a more realistic residual interaction than that of the surface-delta type.

The experimental interpretation of resonance structure above the giant resonance as being attributable to single-particle excitations from low-lying closed shells is supported by the eigenchannel analysis of the C^{12} photoabsorption reaction. The fact that the eigenchannel theory can and does produce nuclear reaction information in good accord with experiment tends to support its continued use. But, until all of the conceptual and numerical difficulties of the eigenphase search procedure have been eliminated, extensive applications of the eigenchannel theory must be questioned.

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APPENDIX A

A-1. Angular momentum

The angular momentum labels j, J are used to represent half-integral and integral values respectively. States of good total angular momentum $\vec{J} = \vec{j}_1 + \vec{j}_2$ and projection quantum number $\vec{M} = \vec{m}_1 + \vec{m}_2$ are obtained through the unitary transformation

$$|j_1 j_2 JM\rangle = \sum_{m_1 m_2} (-)^{j_2 - j_1 - M} \hat{J} \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix} |j_1 m_1\rangle |j_2 m_2\rangle \quad (\text{A-1-1})$$

where $\hat{J} = \sqrt{2J+1}$. The 3-j symbol $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ vanishes unless the following "triangle" relations are satisfied.

$$|j_1 - j_2| \leq j_3 \leq |j_1 + j_2| \quad (\text{A-1-2})$$

$$m_1 + m_2 + m_3 = 0$$

$$j_1 + j_2 + j_3 = \text{integer.}$$

They satisfy the following orthogonality relations

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j'_3 \\ m_1 & m_2 & m'_3 \end{pmatrix} = \frac{1}{2j_3 + 1} \delta_{j_3 j'_3} \delta_{m_3 m'_3} \quad (\text{A-1-3})$$

$$\sum_{JM} (2J+1) \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} j_1 & j_2 & J \\ m'_1 & m'_2 & M \end{pmatrix} = \delta_{m_1 m'_1} \delta_{m_2 m'_2} \quad (\text{A-1-4})$$

In calculating matrix elements of one and two-body operators, use is made of the well known 'recoupling' formula

$$\sum_{m_3} \begin{pmatrix} j_1 j_2 j_3 \\ m_1 m_2 m_3 \end{pmatrix} \begin{pmatrix} j'_1 j'_2 j_3 \\ m'_1 m'_2 -m_3 \end{pmatrix} = \sum_{j'_3} (2j'_3 + 1) \begin{Bmatrix} j_1 & j_2 & j_3 \\ j'_1 & j'_2 & j'_3 \end{Bmatrix} \times$$

$$\times \sum_{m'_3} (-)^{j'_3 + j_3 + m_1 + m'_1} \begin{pmatrix} j'_1 j'_2 j'_3 \\ m'_1 m'_2 m'_3 \end{pmatrix} \begin{pmatrix} j_1 j'_2 j'_3 \\ m_1 m'_2 -m'_3 \end{pmatrix}. \quad (\text{A-1-5})$$

The equation A-1-5 may be taken as the definition of the 6-j symbol

$$\begin{pmatrix} j_1 j_2 j_3 \\ j_4 j_5 j_6 \end{pmatrix}. \quad \text{The symmetry properties of the 3-j and 6-j symbols are}$$

well known and an excellent discussion of their properties may be found

in Edmonds(102). It may be noted that the 3-j symbol characterizes

the coupling $\vec{J} = \vec{j}_1 + \vec{j}_2$ and the 6-j symbol the coupling

$\vec{J} = \vec{j}_1 + \vec{j}_2 + \vec{j}_3$. A natural extension to the case $\vec{J} = \vec{j}_1 + \vec{j}_2 + \vec{j}_3 + \vec{j}_4$

leads to the transformation coefficients termed 9-j symbols. The 9-j

symbols are directly related to the 6-j symbols by the relation

$$\sum_J (-)^{K+K'+2J} (2J+1) \begin{pmatrix} j_1 j'_1 J \\ j_2 j'_2 J_1 \end{pmatrix} \begin{pmatrix} j'_2 j_2 J \\ K' K J_2 \end{pmatrix} \begin{pmatrix} K' K J \\ j_1 j'_1 J_3 \end{pmatrix} =$$

$$= (-)^{j_1 + j_2 + j'_1 + j'_2 + J_1 + J_2 + J_3} \begin{Bmatrix} j_1 & j_2 & j_1 \\ j'_2 & J_2 & K \\ j'_1 & K' & J_3 \end{Bmatrix}. \quad (\text{A-1-6})$$

Transformation coefficients representing the coupling of more than four

angular momentum vectors are not necessary for the purposes of this

thesis. A useful appendix of relations governing the basic properties

of the 3-j, 6-j, and 9-j symbols may be found in the work of de-Shalit

and Talmi(103). These symbols are tabulated by Rotenberg et al. (104)

in prime number notation, and their decimal counterparts may be found in

volume 3 of the Landolt-Börnstein series(105). For the actual computation involved in this work, algorithms were constructed for the evaluation of the 3-j, 6-j, and 9-j symbols from the work of J. H. Gunn (71,72).

A-2. Hole States

The excitation of a single particle from an occupied level produces a "hole" in that level. The hole state may be thought of as a time-reversed particle state. The time reversal operator K when operating in coordinate and momentum space produces the results

$$K \vec{r} K^\dagger = \vec{r}; \quad K \vec{p} K^\dagger = -\vec{p}. \quad (\text{A-2-1})$$

The time-reversal operator is thus antiunitary. If we designate the eigenstate of the $\vec{J}^2$ and J_3 operators as ψ_{jm} then the time reversed state ($K \psi_{jm}$) will satisfy

$$\vec{J}^2 (K \psi_{jm}) = j(j+1) (K \psi_{jm}) \quad (\text{A-2-2})$$

$$J_3 (K \psi_{jm}) = -K J_3 \psi_{jm} = -m (K \psi_{jm}). \quad (\text{A-2-3})$$

These equations indicate that $K \psi_{jm}$ transforms contragradiently to ψ_{jm} . If we take

$$\tilde{\psi}_{jm} = (-)^{j+m} K \psi_{j, -m} \quad (\text{A-2-4})$$

then this function transforms in the conventional way with the rotation matrix $D_{m',m}^j(\theta_1, \theta_2, \theta_3)$. The phase factor $(-)^{j+m}$, being the usual

convention, does not play any privileged role. Any phase factor dependent on m would produce the same result (106, pp. 335-337). Equivalently, one could write,

$$\psi_{jm}(\text{hole}) = (-)^{j+m} \psi_{j-m}(\text{particle}). \quad (\text{A-2-5})$$

An alternative derivation using Slater determinants may be found in the work of Brown (107, pp. 38-40). Thus the wave function of total angular momentum $\vec{J}$ found by coupling a single particle and hole state takes on the representation.

$$|j_p j_h JM\rangle = \sum_{m_p m_h} (-)^{j_m - j_p - M} \hat{J} \begin{pmatrix} j_p & j_h & J \\ m_p & m_h & -M \end{pmatrix} |j_p m_p\rangle (-)^{j_h + m_h} |j_h - m_h\rangle. \quad (\text{A-2-6})$$

A-3. Channel notation

A channel is defined as a possible pair of product nucleus and outgoing particle, each in a definite quantum state. The product nucleus is assumed to be totally represented by the single hole state produced by knocking a particle up into the continuum. The set of quantum numbers $n_h, \ell_h, j_h, n_p, \ell_p, j_p$ where n_h and n_p are the radial quantum numbers, completely characterize a channel. Thus a particular channel is represented by the set

$$c = \{\alpha, n_p, \ell_p, j_p\} \quad (\text{A-3-1})$$

$$\text{where } \alpha = \{n_h, \ell_h, j_h\}. \quad (\text{A-3-2})$$

The total angular momentum of the system is $\vec{J} = \vec{j}_p + \vec{j}_h$. Another representation of the channel particularly useful in particle-particle reactions is found by the coupling

$$\vec{S} = \vec{S}_p + \vec{j}_h \quad (\text{A-3-3})$$

$$\vec{J} = \vec{\ell}_p + \vec{S} \quad (\text{A-3-4})$$

where $\vec{S}$ denotes the channel spin and $\vec{S}_p$ is the spin of the outgoing particle. Denoting the Z- components of $\vec{\ell}_p$ and $\vec{S}$ as m_{ℓ_p} and μ respectively, an equivalent representation for the channel is

$$c = \{\alpha, S, \ell_p, m_{\ell_p}, \mu\} . \quad (\text{A-3-5})$$

Denoting the outgoing particle by the subscript 'p' and the residual nucleus by the subscript 'h', the following channel quantities are of importance in this work.

$$\mu_c = \frac{M_p \cdot M_h}{M_p + M_h} , \quad \text{the reduced mass}$$

$$\vec{r}_c = \vec{r}_p - \vec{r}_h , \quad \text{the relative coordinate vector}$$

E_c = energy of relative motion of the particle and residual nucleus.

$$K_c = [2\mu_c E_c / \hbar^2]^{1/2} , \quad \text{the wave number}$$

$$\theta_c = \vartheta_c = \text{polar angles of } \vec{r}_c$$

$$v_c = \hbar k_c / \mu_c , \quad \text{the relative velocity at infinite separation}$$

E_c is positive for those channels energetically allowed. These

are denoted as 'open' channels. If E_c is negative the channel is called 'virtual'. Closed channels are those which are not energetically allowed. Considering the photon interactions studied in this work,

$$E_\gamma = E_{\text{Res. Nucl.}} + E_{\text{C. M.}} + E_c \quad (\text{A-3-6a})$$

$$E_c = \frac{1}{2} \mu_c v_c^2 \quad (\text{A-3-6b})$$

$$E_{\text{Res. Nucl.}} = E_{\text{Hole}} \quad (\text{A-3-6c})$$

$$E_{\text{C. M.}} = \text{energy of the center of mass.} \quad (\text{A-3-6d})$$

From momentum conservation

$$P_\gamma = P_{\text{CM}} = E_\gamma / c. \quad (\text{A-3-7})$$

The excitation energy of the compound system is then given by

$$E_{\gamma_{\text{exc.}}} = E_{\text{Hole}} + E_c = E_\gamma - E_{\text{CM}} \quad (\text{A-3-8})$$

$$= E_\gamma - P_{\text{CM}}^2 / 2(M_p + M_h) \quad (\text{A-3-9})$$

$$= E_\gamma - \frac{1}{2} E_\gamma^2 / (M_p + M_h) c^2. \quad (\text{A-3-10})$$

This work considers only nuclei with $A \geq 12$ for which $(M_p + M_h) c^2$ is greater than 10^4 MeV. Even for the large photon energy of 100 MeV, the second term in Equation A-3-10 is only of the order of 50 keV so to a good approximation the excitation energy is given by

$$E_c = E_\gamma - E_h. \quad (\text{A-3-11})$$

A-4. Channel wave function in the interior region

Let us denote by $u_n(r)$ the reduced radial wave function, $Y_{\ell, m_\ell}(\Omega)$ the spherical harmonic, and χ_{s, m_s} a spinor in spin space. Then, the basis states of the interior region $r \leq a_c$ implied by Equation 1.14, Section 1.3 may be cast in the following form

$$|n_p n_h; j_p j_h; JM\rangle = \sum_{m_p m_h} (-)^{2j_h - j_p - m_p} \hat{j} \begin{pmatrix} j_p & j_h & J \\ m_p & -m_h & -M \end{pmatrix} \\ u_{n_p}(r_p) r_p^{-1} \times u_{n_h}(r_h) r_h^{-1} | (s_p \ell_p) j_p, m_p \rangle | (\ell_h s_h) \\ j_h, m_h \rangle | \tau_h \rangle | \tau_p \rangle, \quad (\text{A-4-1})$$

where the phase convention for hole states has been employed. The kets containing τ characterize the charge of the particle. The isospin formalism is not used so that neutrons and protons are treated separately. The ket $|(S\ell)j, m\rangle$ represents the coupling $\vec{J} = \vec{S} + \vec{\ell}$ and is given by

$$|(S\ell)j, m\rangle = \sum_{m_\ell m_s} (-)^{\ell - S - m} \hat{j} \begin{pmatrix} S & \ell & j \\ m_s & m_\ell & -m \end{pmatrix} Y_{\ell, m_\ell} \chi_{S, m_s}. \quad (\text{A-4-2})$$

It will be necessary for the discussion of matrix elements of the nuclear Hamiltonian to represent these basis states in the channel spin representation. As described in the section on channel notation, we first couple the spin of the particle ($\vec{S}_p$) to the total nuclear spin of the residual nucleus ($\vec{j}_h$) to form the channel spin $\vec{S}$.

$$\psi_{S_p, j_h}^{S, \mu} = \sum_{m_h m_{S_p}} (-)^{2j_h - S_p - m_{S_p}} \hat{S} \begin{pmatrix} S_p & j_h & S \\ m_{S_p} & -m_h & -\mu \end{pmatrix} | (\ell_h S_h) j_h, m_h \rangle$$

$$\times \chi_{S_p, m_{S_p}} \quad (A-4-3)$$

Now we couple the channel spin $\vec{S}$ to the total angular momentum of the particle ($\vec{\ell}_p$) to form the total spin $\vec{J}$ of the compound system.

$$\psi_{\ell_p, S}^{J, M} = \sum_{m_{\ell_p}, \mu} (-)^{\ell_p - S - M} \hat{J} \begin{pmatrix} S & \ell_p & J \\ \mu & m_{\ell_p} & -M \end{pmatrix} \psi_{S_p, j_h}^{S, \mu} Y_{\ell_p, m_{\ell_p}}(\Omega_p).$$

(A-4-4)

Defining

$$\varphi_\alpha = r_h^{-1} u_{n_h}(r_h) | \tau_h \rangle | \tau_p \rangle \quad (A-4-5)$$

as the "internal" function, and employing only the basic angular momentum relations of Section A-1, one obtains

$$| n_p n_h; j_p j_h; JM \rangle \rangle \sum_S K_{\alpha S \ell_p j_p}^J \psi_{\ell_p, S}^{J, M} \varphi_\alpha r_p^{-1} u_{n_p}(r_p) \quad (A-4-6)$$

where

$$K_{\alpha S \ell_p j_p}^J = (-)^{S + \ell_p + j_h + j_p} \hat{S} \hat{j}_p \left\{ \begin{matrix} \ell_p & j & S \\ j_h & 1/2 & j_p \end{matrix} \right\}. \quad (A-4-7)$$

Use has been made of the fact that $S_p = S_h = 1/2$. The recoupling coefficients K fulfill the orthogonality relations

$$\sum_S K_{\alpha S \ell j}^J K_{\alpha' S \ell' j'}^J = \delta_{jj'} \quad (\text{A-4-8})$$

$$\sum_S K_{\alpha S \ell j}^J K_{\alpha' S' \ell' j'}^J = \delta_{SS'} \quad (\text{A-4-9})$$

For the purposes of this work we may write the basis functions in the following form

$$|n_p n_h; j_p j_h; \rangle\rangle = u_{n_p}(r_p) \tilde{\varphi}_c \quad (\text{A-4-10})$$

The explicit form of the "surface function" $\tilde{\varphi}_c$ being given by

$$\begin{aligned} \tilde{\varphi}_c = \sum_S (-)^{S + \ell_p + j_h + j_p} \hat{s}_p \hat{j}_p \left\{ \begin{matrix} \ell_p & J & S \\ j_h & 1/2 & j_p \end{matrix} \right\} \varphi_{\alpha} r_p^{-1} \times \\ \times Y_{\ell_p, S}^{J, M} \end{aligned} \quad (\text{A-4-11})$$

It must be remembered that to be consistent with Equation 1.25, Section 1.3, the wave function defined by Equation A-4-10 must be properly antisymmetrized in particle-hole coordinates.

APPENDIX B

In calculating the matrix elements of the two body operator V_{ph} in the second quantization formalism one encounters the following particle-hole matrix elements

$$\begin{aligned}
 \langle (j_1 j_2^{-1}) J' M' T' M_T' | V_{ph} | (j_3 j_4^{-1}) J M T M_T \rangle = \\
 - \sum_{\substack{M_1 M_2 \\ M_3 M_4}} (-)^{(j_2 - j_1 - M') + (j_4 - j_3 - M)} \hat{j}_1 \hat{j}_3 \times \\
 \times \begin{pmatrix} j_1 & j_2 & J' \\ m_1 & m_2 & -M' \end{pmatrix} \begin{pmatrix} j_3 & j_4 & J \\ m_3 & m_4 & -M \end{pmatrix} (-)^{(j_2 - m_2) + (j_4 - m_4)} \sum_{\substack{m_{\tau_1} m_{\tau_2} \\ m_{\tau_3} m_{\tau_4}}} (-)^{M_T + M_T'} \hat{T} \hat{T}' \\
 \begin{pmatrix} 1/2 & 1/2 & T' \\ m_{\tau_1} & m_{\tau_2} & -M_T' \end{pmatrix} \begin{pmatrix} 1/2 & 1/2 & T \\ m_{\tau_3} & m_{\tau_4} & -M_T \end{pmatrix} \times \\
 \times (-)^{(1/2 - m_{\tau_2}) + (1/2 - m_{\tau_4})} [(|4|V|32) - (|4|V|23)] . \quad (B-1)
 \end{aligned}$$

Let us examine first the uncoupled direct term

$$(|4|V|32) = (n l j \tau m_1 ; n l j \tau m_4 | V | n l j \tau m_3 ; n l j \tau m_2) \quad (B-2)$$

$$\begin{aligned}
(14|V|32) = & \sum_{i=1}^4 \sum_{\lambda_i \mu_i} (-)^{(1/2-\ell_i-m_i)} \hat{j}_i \begin{pmatrix} \ell_i & 1/2 & j_i \\ \lambda_i & \mu_i & -m_i \end{pmatrix} \times \\
& \times \sum_{\substack{L \ L' \\ M_L \ M_L'}} (-)^{\ell_1+\ell_2+\ell_3+\ell_4+M_L+M_L'} \hat{L} \hat{L}' \begin{pmatrix} \ell_1 & \ell_4 & L \\ \lambda_1 & \lambda_4 & -M_L \end{pmatrix} \begin{pmatrix} \ell_3 & \ell_2 & L' \\ \lambda_3 & \lambda_2 & -M_L' \end{pmatrix} \times \\
& \times \sum_{\substack{S \ S' \\ M_S \ M_S'}} (-)^{M_S+M_S'} \hat{S} \hat{S}' \begin{pmatrix} 1/2 & 1/2 & S \\ \mu_1 & \mu_4 & -M_S \end{pmatrix} \begin{pmatrix} 1/2 & 1/2 & S' \\ \mu_3 & \mu_2 & -M_S' \end{pmatrix} \times \\
& \times \sum_{\substack{T \ T' \\ M_T \ M_T'}} (-)^{M_T+M_T'} \hat{T} \hat{T}' \begin{pmatrix} 1/2 & 1/2 & T \\ m_{\tau_1} & m_{\tau_4} & -M_T \end{pmatrix} \begin{pmatrix} 1/2 & 1/2 & T' \\ m_{\tau_3} & m_{\tau_2} & -M_T' \end{pmatrix} \times
\end{aligned}$$

$$\begin{aligned}
& \times \langle 1/2 \ 1/2 \ S M_S | \langle \ell_1 \ \ell_4 \ L M_L | \langle 1/2 \ 1/2 \ T M_T | \langle R_{n_{\ell_1}}^* (1) R_{n_{\ell_4}}^* (2) | V(1,2) \\
& R_{n_{\ell_3}} (1) R_{n_{\ell_2}} (2) | 1/2 \ 1/2 \ T' M_T' | \ell_3 \ell_2 L' M_L' | 1/2 \ 1/2 \ S' M_S' \rangle . \quad (B-3)
\end{aligned}$$

For the residual interaction we take

$$\begin{aligned}
V(1,2) = & - \frac{V_0 \delta(r_1-r_2) \delta(r_1-a)}{r_1^2 a^2} \delta(\Omega_1-\Omega_2) [a_o + a_\sigma \vec{\sigma}(1) \cdot \vec{\sigma}(2) + a_\tau \vec{\tau}(1) \cdot \vec{\tau}(2) \\
& + a_{\sigma\tau} \vec{\sigma}(1) \cdot \vec{\sigma}(2) \vec{\tau}(1) \cdot \vec{\tau}(2)] . \quad (B-4)
\end{aligned}$$

Then the matrix element appearing in Equation B-3 has the value

$$\begin{aligned}
\langle |V(1,2)| \rangle &= -V_0 \sum_{i=1}^4 \frac{\pi}{R_{n\ell_i}} (a) \langle \ell_1 \ell_4 L M_L | \delta(\Omega_1 - \Omega_2) | \ell_3 \ell_2 L' M'_L \rangle \times \\
&\times [a_0 + a_\sigma (\delta_{S1} - 3\delta_{S0}) + a_\tau (\delta_{T1} - 3\delta_{T0}) + a_{\sigma\tau} (\delta_{S1} - 3\delta_{S0}) (\delta_{T1} - 3\delta_{T0})] \times \\
&\times \delta_{SS'} \delta_{M_S M'_S} \delta_{TT'} \delta_{M_T M'_T} .
\end{aligned} \tag{B-5}$$

The angular matrix element is

$$\langle \ell_1 \ell_4 L M_L | \delta(\Omega_1 - \Omega_2) | \ell_3 \ell_2 L' M'_L \rangle = \frac{\sum_{i=1}^4 \frac{\pi}{R_{n\ell_i}} \hat{\ell}_i}{4\pi} \begin{pmatrix} \ell_1 & \ell_4 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_2 & \ell_3 & L \\ 0 & 0 & 0 \end{pmatrix} \delta_{LL'} \delta_{M_L M'_L} .$$

(B-6)

If we carry out the isospin coupling in Equation B-1 using Equations B-3 and B-5 we get $\delta_{TT'} \delta_{M_T M'_T}$. Employing the Racah algebra of Appendix A and performing a recoupling transformation on the sums over M_L and M_S , one finds that the coupled direct term becomes:

$$\begin{aligned}
&-V_0 \sum_{i=1}^4 \frac{\pi}{R_{n\ell_i}} (a) \frac{\hat{j}_i \hat{\ell}_i}{4\pi} \sum_{SKK'} (-)^{\ell_2 + \ell_4} \hat{S}^2 \hat{K}^2 \hat{K}'^2 F_{ST} \begin{pmatrix} \ell_3 & \ell_4 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & K \\ 0 & 0 & 0 \end{pmatrix} \times \\
&\times \left\{ \begin{matrix} 1/2 & 1/2 & S \\ 1/2 & 1/2 & K' \end{matrix} \right\} \left\{ \begin{matrix} \ell_1 & \ell_2 & K \\ 1/2 & 1/2 & K' \\ j_1 & j_2 & J \end{matrix} \right\} \left\{ \begin{matrix} \ell_3 & \ell_4 & K \\ 1/2 & 1/2 & K' \\ j_3 & j_4 & J \end{matrix} \right\} \delta_{JJ'} \delta_{MM'} \delta_{TT'} \delta_{M_T M'_T}
\end{aligned}$$

where $F_{ST} = a_0 + a_\sigma (\delta_{S1} - 3\delta_{S0}) + a_\tau (\delta_{T1} - 3\delta_{T0}) + a_{\sigma\tau} (\delta_{S1} - 3\delta_{S0})$

$$(\delta_{T1} - 3\delta_{T0}) . \tag{B-7}$$

We can do the sum on S explicitly

$$\sum_S \hat{S}^2 F_{ST} \begin{Bmatrix} 1/2 & 1/2 & S \\ 1/2 & 1/2 & K' \end{Bmatrix} = a_0 + a_\pi (\delta_{T1} - 3\delta_{T0}) - a_\sigma (\delta_{K'1} - 3\delta_{K'0}) \\ - a_{\sigma\pi} (\delta_{T1} - 3\delta_{T0}) (\delta_{K'1} - 3\delta_{K'0}) \quad (B-8)$$

Therefore, the coupled direct term has the form

$$-V_0 \sum_{i=1}^4 \frac{4}{\pi} R_{n\ell_i} (a) \frac{\hat{j}_i \hat{\ell}_i}{4\pi} \sum_{L,S} (-)^{\ell_2 + \ell_4} (2L+1)(2S+1) F_{ST} \begin{pmatrix} \ell_3 & \ell_4 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_2 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} \times \\ \times \begin{Bmatrix} \ell_1 & \ell_2 & L \\ 1/2 & 1/2 & S \\ j_1 & j_2 & J \end{Bmatrix} \begin{Bmatrix} \ell_3 & \ell_4 & L \\ 1/2 & 1/2 & S \\ j_3 & j_4 & J \end{Bmatrix} \delta_{JJ'} \delta_{MM'} \delta_{M_T M_T'} \delta_{TT'}$$

$$F_{ST} = a_0 + a_\pi (\delta_{T1} - 3\delta_{T0}) - a_\sigma (\delta_{S1} - 3\delta_{S0}) - a_{\sigma\pi} (\delta_{S1} - 3\delta_{S0}) (\delta_{T1} - 3\delta_{T0}) \quad (B-9)$$

Let us now examine the exchange term $(14|V|23)$. Since we are exchanging the indices 2 and 3 only we do not expect the result to be very different from the direct term. The primary difference is in the isospin terms.

There are two types of isospin terms in $(14|V|23)$. There will be terms of the form

$$\langle 1/2 \ 1/2 \ T \ M_T | \text{const.} | 1/2 \ 1/2 \ T' \ M_T' \rangle = \delta_{TT'} \delta_{M_T M_T'} \times \text{const.} \quad (B-10)$$

Following these terms back through the Racah algebra we see that their

contribution is a factor of the form

$$2 \delta_{T0} \delta_{TT'} \delta_{M_T M_T'} \quad (B-11)$$

The other type of isospin term has the form

$$\langle 1/2 \ 1/2 \ T \ M_T | \vec{\tau}(1) \cdot \vec{\tau}(2) | 1/2 \ 1/2 \ T' M_T' \rangle = 6(-)^{T'+1} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ & 1/2 & 1/2 & T' \end{Bmatrix}$$

$$\delta_{TT'} \delta_{M_T M_T'} \quad (B-12)$$

The contribution of these terms is a factor

$$2 \delta_{T1} \delta_{TT'} \delta_{M_T M_T'} \quad (B-13)$$

If we follow the calculations through as for the direct term the only other change is the introduction of a phase factor $(-)^{S+1}$ and we obtain for the coupled exchange term

$$-2V_0 \sum_{i=1}^4 \frac{1}{\pi} R_{n_{\ell i}} (a) \frac{\hat{j}_i \hat{\ell}_i}{4\pi} \sum_{SKK'} (-)^{\ell_2 + \ell_4 + S + 1} \hat{S}^2 \hat{K}^2 \hat{K}'^2 F_{ST}^1 \begin{pmatrix} \ell_3 & \ell_4 & K \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \begin{pmatrix} \ell_1 & \ell_2 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} 1/2 & 1/2 & S \\ & 1/2 & 1/2 & K' \end{Bmatrix} \begin{Bmatrix} \ell_1 & \ell_2 & K \\ 1/2 & 1/2 & K' \\ j_1 & j_2 & J \end{Bmatrix} \begin{Bmatrix} \ell_3 & \ell_4 & K \\ 1/2 & 1/2 & K' \\ j_3 & j_4 & J \end{Bmatrix} \delta_{JJ'} \delta_{MM'} \delta_{M_T M_T'}$$

$$\text{where } F_{ST}^1 = a_0 \delta_{T0} + a_\sigma \delta_{T0} (\delta_{S1} - 3\delta_{S0}) + a_\tau \delta_{T1} + a_{\sigma\tau} \delta_{T1} (\delta_{S1} - 3\delta_{S0}). \quad (B-14)$$

Again, the sum on S can be done explicitly.

$$\sum_S (-)^{S+1} \hat{S}^2 F'_{ST} \left\{ \begin{matrix} 1/2 & 1/2 & S \\ 1/2 & 1/2 & K' \end{matrix} \right\} = 2a_0 \delta_{T0} \delta_{K'0} + 2a_\tau \delta_{T1} \delta_{K'0} +$$

$$+ 2a_\sigma \delta_{T0} \delta_{K'1} + 2a_{\sigma\tau} \delta_{T1} \delta_{K'1} \quad (B-15)$$

Therefore, the coupled exchange term has the form

$$-V_0 \frac{4}{4\pi} \sum_{i=1}^4 R_{n\ell_i} (a) \frac{\hat{j}_i \hat{\ell}_i}{4\pi} \sum_{L,S} (-)^{\ell_2+\ell_4} (2L+1)(2S+1) F'_{ST} \begin{pmatrix} \ell_3 & \ell_4 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \left\{ \begin{matrix} \ell_1 & \ell_2 & L \\ 1/2 & 1/2 & S \\ j_1 & j_2 & J \end{matrix} \right\} \left\{ \begin{matrix} \ell_3 & \ell_4 & L \\ 1/2 & 1/2 & S \\ j_3 & j_4 & J \end{matrix} \right\} \delta_{JJ'} \delta_{MM'} \delta_{TT'} \delta_{M_T M'_T}$$

$$\text{with } F'_{ST} = a_0 \delta_{T0} \delta_{S0} + a_\tau \delta_{T1} \delta_{S0} + a_\sigma \delta_{T0} \delta_{S1} + a_{\sigma\tau} \delta_{T1} \delta_{S1}. \quad (B-16)$$

Combining the direct term and the exchange term we obtain

$$V_{12:34} = V_0 \frac{4}{4\pi} \sum_{i=1}^4 R_{n\ell_i} (a) \frac{\hat{j}_i \hat{\ell}_i}{4\pi} \sum_{L,S} (-)^{\ell_2+\ell_4} (2L+1)(2S+1) G_{ST} \times$$

$$\times \begin{pmatrix} \ell_3 & \ell_4 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} \times \left\{ \begin{matrix} \ell_1 & \ell_2 & L \\ 1/2 & 1/2 & S \\ j_1 & j_2 & J \end{matrix} \right\} \left\{ \begin{matrix} \ell_3 & \ell_4 & L \\ 1/2 & 1/2 & S \\ j_3 & j_4 & J \end{matrix} \right\} \times$$

$$\times \delta_{JJ'} \delta_{MM'} \delta_{TT'} \delta_{M_T M'_T}$$

$$\text{with } G_{ST} = a_0 + a_\tau (\delta_{T1} - 3\delta_{T0}) - a_\sigma (\delta_{S1} - 3\delta_{S0}) - 5a_{\sigma\tau} (\delta_{S1} \delta_{T1}) +$$

$$+ (3a_{\sigma\tau} - 4a_{\sigma}) \delta_{S1} \delta_{T0} + (3a_{\sigma\tau} - 4a_{\tau}) \delta_{S0} \delta_{T1} - (9a_{\sigma\tau} + 4a_0) \delta_{S0} \delta_{T0}. \quad (B-17)$$

We now take account of the fact that we really want to treat neutrons and protons separately for partial cross section measurements. We can accomplish this by averaging over the charge. Let us consider the two possible particle-hole states

$$\begin{aligned} |nn^{-1}\rangle &= \sum_T (-)^{1/2-m_{\tau 1}} \hat{T} \begin{pmatrix} 1/2 & 1/2 & T \\ m_{\tau 1} & -m_{\tau 1} & 0 \end{pmatrix} \begin{matrix} m_{\tau 1} = -1/2 \text{ for neutrons} \\ m_{\tau 1} = +1/2 \text{ for protons.} \end{matrix} \quad (B-18) \\ |pp^{-1}\rangle & \end{aligned}$$

Thus these states have the form

$$|n n^{-1}\rangle = \frac{1}{\sqrt{2}} |00\rangle - \frac{1}{\sqrt{2}} |10\rangle \quad (B-19a)$$

$$|p p^{-1}\rangle = \frac{1}{\sqrt{2}} |00\rangle + \frac{1}{\sqrt{2}} |10\rangle. \quad (B-19b)$$

The only matrix elements of interest have the forms

$$(1) \langle n n^{-1} | V_{ph} | n n^{-1} \rangle \quad (2) \langle p p^{-1} | V_{ph} | p p^{-1} \rangle \quad (3) \langle p p^{-1} | V_{ph} | n n^{-1} \rangle. \quad (B-20)$$

Forms 1 and 2 imply the result

$$\frac{1}{2} (G_{S1} + G_{S0}) \quad (B-21a)$$

while form 3 gives

$$\frac{1}{2} (G_{S0} - G_{S1}). \quad (B-21b)$$

The result of Equation B-21 has the form

$$\begin{aligned}
 G_S^{m_\tau m'_\tau} = & a_0 (\delta_{m_\tau m'_\tau} - 2\delta_{S0}) - a_\tau [(4\delta_{m_\tau m'_\tau} - 2)\delta_{S0} + (2 - \delta_{m_\tau m'_\tau})] - \\
 & - a_\sigma [(2 + \delta_{m_\tau m'_\tau})\delta_{S1} - 3\delta_{S0} \delta_{m_\tau m'_\tau}] - a_{\sigma_\tau} [(6 - 3\delta_{m_\tau m'_\tau})\delta_{S0} + \\
 & + (5\delta_{m_\tau m'_\tau} - 4)\delta_{S1}] .
 \end{aligned} \tag{B-22}$$

Finally, we obtain the coupled matrix elements of V_{ph} as

$$\begin{aligned}
 V_{12;34} = & V_0 \sum_{i=1}^4 R_{n\ell_i} (a) \frac{\hat{j}_i \hat{\ell}_i}{4\pi} \sum_{L,S} (-)^{\ell_2 + \ell_4} (2L+1)(2S+1) G_S^{m_\tau m'_\tau} \times \\
 & \times \begin{pmatrix} \ell_3 & \ell_4 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} \ell_1 & \ell_2 & L \\ 1/2 & 1/2 & S \\ j_1 & j_2 & J \end{matrix} \right\} \left\{ \begin{matrix} \ell_3 & \ell_4 & L \\ 1/2 & 1/2 & S \\ j_3 & j_4 & J \end{matrix} \right\}
 \end{aligned} \tag{B-23}$$

with

$$G_S^{m_\tau m'_\tau} \text{ as given by Equation B-22.}$$

APPENDIX C

To obtain the proton wave functions for r less than or equal to the radius of the well, we must solve the differential Equation 3.3 with the potential $V(r)$ as defined by Equation 3.6a. The differential equation then has the form

$$\begin{aligned} & \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{L(L+1)}{r^2} + \frac{2\mu}{\hbar^2} \left(\frac{Z_1 Z_2 e^2}{2r_W^3} \right) r^2 \right] R_{n,L}(r) = \\ & \frac{2\mu}{\hbar^2} \left\{ \left(\frac{3Z_1 Z_2 e^2}{2r_W} \right) - V_{SW} + d_L [J(J+1) - L(L+1) - S(S+1)] \right. \\ & \left. + b_L L(L+1) - E \right\} R_{n,L}(r). \end{aligned} \quad (C-1)$$

If we let

$$\gamma^2 = \frac{2\mu}{\hbar^2} \left(\frac{Z_1 Z_2 e^2}{2r_W^3} \right) \quad (C-2)$$

$$\begin{aligned} 4\alpha\gamma^2 &= \frac{2\mu}{\hbar^2} \left\{ V_{SW} + E - \frac{3Z_1 Z_2 e^2}{2r_W} - d_L [J(J+1) - L(L+1) - S(S+1)] \right. \\ & \left. - b_L L(L+1) \right\} \end{aligned} \quad (C-3)$$

then, Equation C-1 takes the form

$$\left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{L(L+1)}{r^2} - \gamma^2 r^2 + 4\alpha\gamma^2 \right] R_{n,L}(r) = 0. \quad (C-4)$$

If we make the transformation

$$R_{n,L}(r) = e^{-i \gamma^2 r^2 / 2} r^L L_L(r) \quad (C-5)$$

the differential equation satisfied by $W_L(r)$ is

$$W_L'' + W_L' \left[-2i\gamma^2 r + \frac{2(L+1)}{r} \right] + W_L [4\alpha\gamma^2 - i\gamma^2(2L+3)] = 0. \quad (C-6)$$

The solution of Equation C-6 is the confluent hypergeometric function

$$W_L(r) = {}_1F_1 \left(\frac{2L+3}{4} + i\alpha; L+3/2; i\gamma^2 r^2 \right). \quad (C-7)$$

Therefore, the function $R_{n,L}(r)$ takes the following form

$$R_{n,L}(r) = e^{-i\gamma^2 r^2/2} r^L {}_1F_1 \left(\frac{2L+3}{4} + i\alpha; L+3/2; i\gamma^2 r^2 \right). \quad (C-8)$$

A multiplicative constant will not alter the solution but for reasons that will become apparent we take the solution of Equation C-1 to be

$$R_{n,L}(\gamma r) = e^{-i\gamma^2 r^2/2} \left(\frac{\pi\alpha}{4} \right)^{1/2} (\gamma r)^L \times {}_1F_1 \left(\frac{2L+3}{4} + i\alpha; L+3/2; i\gamma^2 r^2 \right). \quad (C-9)$$

From the properties of the ${}_1F_1$ function one can show that

$$R_{n,L}^*(\gamma r) = R_{n,L}(\gamma r) \quad (C-10)$$

so that $R_{n,L}$ is real. In the limit of zero charge (i.e. Z_1 or Z_2 approaches zero)

$$R_{n,L}(\gamma r) = j_L(kr) \quad (C-11a)$$

$$\text{with } k^2 = \frac{2\mu}{\hbar^2} \{ E + V_{SW} - d_L [J(J+1) - L(L+1) - S(S+1)] - b_L \times L(L+1) \} \quad (C-11b)$$

and thus $R_{n,L}$ becomes the regular spherical Bessel function as it should.

The constant $(\frac{\pi\alpha}{4})^{L/2}$ appearing in Equation C-9 is exactly the proportionality factor necessary to achieve Equation C-11. If we let

$$x = \gamma^2 r^2 / 2 \quad (C-12a)$$

then the function $R_{n,L}(\gamma r)$ takes the following forms

$$R_{n,L}(x) = \left(\frac{\pi\alpha}{4}\right)^{L/2} e^{-ix} (2x)^{L/2} {}_1F_1\left(\frac{2L+3}{4} + i\alpha; L + 3/2; 2ix\right) \quad (C-12b)$$

$$= \left(\frac{\pi\alpha}{4}\right)^{L/2} (2x)^{L/2} S\left(\frac{2L+3}{4} + i\alpha; \frac{2L+3}{4} - i\alpha; ix, -ix\right) \quad (C-12c)$$

$$= \left(\frac{\pi\alpha}{4}\right)^{L/2} (2x)^{L/2} \sum_{N=0}^{\infty} \frac{(x)^N}{N!} R_N\left(\frac{2L+3}{4} + i\alpha, \frac{2L+3}{4} - i\alpha; i, -i\right) \quad (C-12d)$$

where the S-function and the polynomials R_N are the generalizations to two variables of e^{-x} and x^N as investigated by B. C. Carlson (108,109). To avoid confusion between $R_{n,L}$ and the R- polynomials, R_N , we define the function $S_L(\alpha, x)$ to be $R_{n,L}$ and using the properties of the R_N polynomials we find

$$S_L(\alpha, x) = R_{n,L}(x) = \left(\frac{\pi\alpha}{4}\right)^{L/2} (2x)^{L/2} \sum_{N=0}^{\infty} \frac{x^N}{N!} R_N \quad (C-13a)$$

$$R_0 = 1, \quad R_1 = -2\alpha/(L + 3/2) \quad (C-13b)$$

$$(L + 3/2 + N)R_{N+1} = -2\alpha R_N - NR_{N-1} \quad (N = 1, 2, \dots). \quad (C-13c)$$

with x defined by Equation C-12a. An integral representation for the S_L - function is obtained from the integral representations of the ${}_1F_1$ - function:

$$S_L(\alpha, x) = \left(\frac{\pi\alpha}{4}\right)^{L/2} (2x)^{L/2} \Gamma(L+3/2) (2)^{1/2-L} / \left|\Gamma\left(\frac{2L+3}{4} + i\alpha\right)\right|^2 x \\ \times \int_0^1 (1-\varphi^2)^{\frac{2L-1}{4}} \cos \left[x\varphi + \alpha \ln \left(\frac{1+\varphi}{1-\varphi} \right) \right] d\varphi. \quad (C-14)$$

It may be noted that the S_L - function can be related to the regular Coulomb function of order $(2L-1)/4$

$$S_L(\alpha, x) \sim F_{(2L-1)/4}(\alpha, x). \quad (C-15)$$

With this correspondence in mind, the following properties of S_L can be obtained by applying the procedures outlined for $F_L(\eta, \rho)$ by Lowan and Horenstein (57):

$$\alpha^2 S_L(\alpha, x) - \left[\frac{\alpha}{2x} - \frac{8\alpha^2}{(2L+3)(2L+7)} \right] S_{L+2}(\alpha, x) + \\ + \frac{1}{(2L+5)(2L+9)} \left[1 + \left(\frac{4\alpha}{2L+7} \right)^2 \right] S_{L+4}(\alpha, x) = 0 \quad (C-16a)$$

$$\frac{dS_L(\alpha, x)}{dx} - \left[\frac{L}{2x} - \frac{4\alpha}{(2L+3)} \right] S_L(\alpha, x) + \frac{[(2L+3)^2 + (4\alpha)^2]}{\alpha(2L+5)(2L+3)^2} x \\ \times S_{L+2}(\alpha, x) = 0 \quad (C-16b)$$

$$\left[\frac{4}{\pi(2\alpha)^L} \right]^{1/2} \int_0^\infty e^{-px} x^{(L+1)/2} S_L(\alpha, x) dx = \\ \Gamma(L+3/2) e^{2\alpha \tan^{-1} p/(1+p^2)} (2L+3)/4 \quad (C-16c)$$

$$\left[\frac{4}{\pi(2\alpha)L} \right]^{1/2} \int_0^\infty e^{-px} \frac{d}{dx} \{ x^{(L+1)/2} S_L(\alpha, x) \} dx =$$

$$\Gamma(L+3/2) p e^{2\alpha \tan^{-1} p / (1+p^2)^{(2L+3)/4}} \quad (C-16d)$$

$$\left[\frac{4}{\pi(2\alpha)L} \right]^{1/2} \int_0^\infty e^{-px} x^{(L+3)/2} S_L(\alpha, x) dx =$$

$$\frac{\Gamma(L+5/2) p e^{2\alpha \tan^{-1} p}}{(1+p^2)^{(2L+3)/4}} - \frac{2\alpha \Gamma(L+3/2) e^{2\alpha \tan^{-1} p}}{(1+p^2)^{(2L+3)/4}}. \quad (C-16e)$$

Equations C-16c - C-16e are valid for $\text{Re } p < 0$.

APPENDIX D

To obtain the normalization of the Weyl function $\tilde{w}_c(r)$ as defined by Equation 2.6, set $\gamma = \Delta E_c/E_c$ and use the fact that

$$w_c(r) \sim \sin(k_c r + \delta - L\pi/2)/r.$$

$$\text{Then, } \tilde{w}_c(r) = W_c \int_{E_c}^{E_c(1+\gamma)} dE \sin\left(\frac{2\mu_c}{\hbar^2} E^{1/2} r + \delta - L\pi/2\right)/r. \quad (D-1)$$

Define $\alpha = \sqrt{2\mu_c/\hbar^2} r$; $\beta = \delta - L\pi/2$ and make the transformation

$x = \alpha E^{1/2} + \beta$. With the two further restrictions that

$$x\gamma \ll 1 \quad (D-2)$$

$$(1+\gamma)^{1/2} \sim 1 + \frac{1}{2}\gamma \quad (D-3)$$

the following expression for $\tilde{w}_c(r)$ is obtained

$$\tilde{w}_c(r) = (2W_c/\alpha^2 r)(x^2 \gamma/2) \sin(x) + \theta(\gamma^2) \quad (D-4a)$$

$$= (W_c \gamma/\alpha^2 r) \sin(x) [\alpha^2 E + 2\alpha\beta E^{1/2} + \beta^2] + \theta(\gamma^2) \quad (D-4b)$$

$$\therefore \tilde{w}_c(r) \approx (W_c \gamma/r) E \sin(x + \beta). \quad (D-4c)$$

In terms of the original variables this is

$$\tilde{w}_c(r) = W_c \Delta E \sin(k_c r + \delta - L\pi/2)/r. \quad (D-5)$$

Since the matching condition $\tilde{w}_c(r) = w_c(r)$ must hold in the non-modified region,

$$W_c = \frac{1}{\Delta E}. \quad (D-6)$$

APPENDIX E

The angular distribution $P(\theta, E)$ may be obtained from the following considerations. If α defines the set of quantum numbers

$$\alpha = \{n_h, \ell_h, j_h\}$$

then the asymptotic outgoing part of the nuclear wave function defined in Section 1.2 for a fixed α , ν is

$$\Psi_{\alpha}^{\nu} = - \sum_{\ell_p j_p} V_{\alpha \ell_p j_p}^{J, \nu} e^{i \delta_J^{\nu}} O_c \tilde{\phi}_c \quad (E-1)$$

where O_c , the outgoing radial function, has the asymptotic form

$$O_c \sim \exp [i(k_c r - \ell_p \pi/2 - \eta_{\alpha} \ln 2k_c r)]. \quad (E-2)$$

The outgoing part of the total wave function is found by summing Equation E-1 over all ν values with an appropriate function of ν and E inserted to account for the perturbation approach used for the photon channels.

$$\begin{aligned} \Psi_{\alpha}^{\nu} = & - \sum_{\nu \ell_p j_p} g(\nu, E) V_{\alpha \ell_p j_p}^{J, \nu} e^{i \delta_J^{\nu}} \times \\ & \times \exp [i(k_c r - \ell_p \pi/2 - \eta_{\alpha} \ln 2k_c r)] \tilde{\phi}_{\alpha \ell_p j_p}. \end{aligned} \quad (E-3)$$

The angular distribution $P(\theta, E)$ is defined as

$$P(\theta, E) = \int \Psi_{\alpha}^{\dagger} r_p^2 \Psi_{\alpha} d\tau_h \quad (E-4)$$

where $d\tau_h$ implies an integration over all coordinates of the residual nucleus since these are not experimentally measured in the laboratory.

$$P(\theta, E) = \sum_{\nu \ell p j p} \sum_{\nu' \ell p' j p'} g^*(\nu', E) g(\nu, E) V_{\alpha \ell' p' j' p}^{J, \nu'} V_{\alpha \ell p j p}^{J, \nu} \\ e^{-i\delta_J^{\nu'}} e^{-i\delta_J^{\nu}} e^{-i\ell' p \pi/2} e^{-i\ell p \pi/2} \int \tilde{\phi}_{\alpha \ell' p' j' p}^* \tilde{\phi}_{\alpha \ell p j p} r p^2 d\tau_h. \quad (E-5)$$

Making use of the identities:

$$\sum_{\nu, \nu'} e^{i(\delta_J^{\nu} - \delta_J^{\nu'})} f(\nu, \nu') = \sum_{\nu, \nu'} \cos(\delta_J^{\nu} - \delta_J^{\nu'}) f(\nu, \nu') \quad (E-6a)$$

$$\sum_{\ell p \ell p'} e^{i(\ell p' - \ell p)\pi/2} f(\ell p, \ell p') = \sum_{\ell p \ell p'} \cos[(\ell p' - \ell p)\pi/2] \times$$

$$\times f(\ell p, \ell p') \quad (E-6b)$$

the angular distribution can be written as

$$P(\theta, E) = \sum_{\nu \ell p j p} \sum_{\nu' \ell p' j p'} g^*(\nu', E) g(\nu, E) V_{\alpha \ell p j p}^{J, \nu'} V_{\alpha \ell' p' j' p}^{J, \nu'} \\ \cos(\delta_J^{\nu} - \delta_J^{\nu'}) \times \cos[(\ell p' - \ell p)\pi/2] \int \tilde{\phi}_{\alpha \ell p' j p'}^* \tilde{\phi}_{\alpha \ell p j p} r p^2 d\tau_h. \quad (E-7)$$

Using the definition of $\tilde{\phi}_{\alpha \ell j}$ as defined by Equation A-4-11, one finds with the Racah algebra of Section A-1, that

$$\begin{aligned}
\int \tilde{\varphi}_{\alpha \ell p' j p'}^* \varphi_{\alpha \ell p j p} r_p^2 d\tau_h = \sum_{S,L} (-)^{j_p + j'_p + 2j_h} (2S+1) \hat{j}_p \hat{j}'_p \times \\
\times \left\{ \begin{matrix} \ell_p & J & S \\ j_h & 1/2 & j_p \end{matrix} \right\} \left\{ \begin{matrix} \ell_p & J & S \\ j_h & 1/2 & j_p \end{matrix} \right\} (-)^{S+L+M} (2J+1) \frac{\hat{\ell}_p \hat{\ell}'_p}{4\pi} (2L+1) \times \\
\times \begin{pmatrix} \ell_p & \ell'_p & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J & J & L \\ M & -M & 0 \end{pmatrix} \left\{ \begin{matrix} J & \ell'_p & S \\ \ell_p & J & L \end{matrix} \right\} P_L(\cos \theta). \quad (E-8)
\end{aligned}$$

The sum on S can be performed explicitly. Since the projection quantum number M is not measured experimentally, we average over all M values. For the case of $E1$ radiation, $J = 1$ and M has only the two values ± 1 . Thus Equation E-8 reduces to

$$\begin{aligned}
\int \tilde{\varphi}^* \tilde{\varphi} r_p^2 d\tau_h = \frac{1}{2} \sum_L \sum_{M=-1,+1} (-)^{-1/2+j_h+M} \frac{(3)(2L+1)}{4\pi} \hat{j}_p \hat{j}'_p \times \\
\times \hat{\ell}_p \hat{\ell}'_p \begin{pmatrix} \ell_p & \ell'_p & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & L \\ M & -M & 0 \end{pmatrix} \left\{ \begin{matrix} j'_p & j_p & L \\ \ell_p & \ell'_p & 1/2 \end{matrix} \right\} \left\{ \begin{matrix} j'_p & j_p & L \\ 1 & 1 & j_h \end{matrix} \right\} P_L(\cos \theta). \quad (E-9)
\end{aligned}$$

The sum on M gives

$$\sum_{M=\pm 1, -1} (-)^M \begin{pmatrix} 1 & 1 & L \\ M & -M & 0 \end{pmatrix} = - \begin{pmatrix} 1 & 1 & L \\ 1 & -1 & 0 \end{pmatrix} [1 + (-)^L]. \quad (E-10)$$

Using Equation E-10 in Equation E-9, the final form of $P(\theta, E)$ is given by

$$\begin{aligned}
P(\theta, E) = \sum_L B_L P_L(\cos \theta) \\
B_L = \sum_{\nu} \sum_{\ell_p j_p \nu'} \sum_{\ell'_p j'_p} g^*(\nu', E) g(\nu, E) v^{1, \nu'}_{\alpha \ell'_p j'_p} v^{1, \nu}_{\alpha \ell_p j_p} \times \\
\times \cos(\delta_1^{\nu} - \delta_1^{\nu'}) \cos[(\ell'_p - \ell_p)\pi/2] (-)^{j_h + 1/2} \frac{(3)(2L+1)}{4\pi} \hat{j}_p \hat{j}'_p \hat{\ell}_p \hat{\ell}'_p \times \\
\times \left\{ \begin{matrix} j'_p & j_p & L \\ 1 & 1 & j_h \end{matrix} \right\} \frac{1}{2} [1 + (-)^L] \times \begin{pmatrix} \ell_p & \ell'_p & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & L \\ 1 & -1 & 0 \end{pmatrix} \left\{ \begin{matrix} j'_p & j_p & L \\ \ell_p & \ell'_p & 1/2 \end{matrix} \right\}. \quad (E-11)
\end{aligned}$$

Since the angular distribution of the partial cross sections is proportional to $P(\theta, E)$

$$\frac{d\sigma_{\alpha}}{d\Omega} = q P(\theta, E) \quad q, \text{ a constant} \quad (\text{E-12})$$

$$\int \frac{d\sigma_{\alpha}}{d\Omega} d\Omega = 4\pi q B_0 \quad (\text{E-13})$$

$$\text{where} \quad 4\pi B_0 = \sum_{\ell p \ j p} \left| \sum_{\nu} g(\nu, E) e^{i\delta_{\ell}^{\nu}} \frac{1, \nu}{\alpha \ \ell p \ j p} \right|^2. \quad (\text{E-14})$$

The total cross section is found by summing Equation E-13 over all values of α .

$$\sigma_T = \sum_{\alpha} \int \frac{d\sigma_{\alpha}}{d\Omega} d\Omega = q \sum_{\nu} |g(\nu, E)|^2. \quad (\text{E-15})$$

By Equation 2.13 of Section 2, we have

$$\sigma_T = 4\pi^2 (e^2/\hbar c) (\hbar\omega) \sum_{\nu} |M_{\nu}|^2. \quad (\text{E-16})$$

Thus the constant q and the function $g(\nu, E)$ are given by

$$q = 4\pi^2 (e^2/\hbar c) (\hbar\omega) \quad (\text{E-17a})$$

$$g(\nu, E) = M_{\nu}. \quad (\text{E-17b})$$

Therefore the partial cross sections take the form

$$\int \frac{d\sigma_{\alpha}}{d\Omega} d\Omega = 4\pi^2 \left(\frac{e^2}{\hbar c}\right) (\hbar\omega) \sum_{\ell p \ j p} \left| \sum_{\nu} e^{i\delta_{\ell}^{\nu}} \frac{1, \nu}{\alpha \ \ell p \ j p} M_{\nu} \right|^2. \quad (\text{E-18})$$

The angular distribution normalized to $B_0 = 1$ is

$$\begin{aligned}
 P(\theta, E) &= \sum_L B_L P_L(\cos \theta) \\
 B_L &= N \sum_{\nu \ell_p j_p} \sum_{\nu' \ell'_p j'_p} M_{\nu} M_{\nu'} V_{\alpha \ell_p j_p}^{1, \nu} V_{\alpha \ell'_p j'_p}^{1, \nu'} \cos(\delta_1^{\nu} - \delta_1^{\nu'}) \times \\
 &\times \cos[(\ell'_p - \ell_p)\pi/2] (-)^{j_h + 1/2} (3)(2L+1) \hat{j}_p \hat{j}'_p \hat{\ell}_p \hat{\ell}'_p \frac{1}{2} \times \\
 &\times [1 + (-)^L] \begin{pmatrix} \ell_p & \ell'_p & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & L \\ 1 & -1 & 0 \end{pmatrix} \left\{ \begin{matrix} j'_p & j_p & L \\ \ell_p & \ell'_p & 1/2 \end{matrix} \right\} \left\{ \begin{matrix} j'_p & j_p & L \\ 1 & 1 & j_h \end{matrix} \right\} \quad (E-19a)
 \end{aligned}$$

where

$$N = \frac{4\pi^2 (e^2/\hbar c) (\hbar\omega)}{\int \frac{d\sigma}{d\Omega} d\Omega} \quad (E-19b)$$