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NUCLEAR CHARGE, CONVECTION CURRENT AND MAGNETIZATION CURRENT DENSITIES

by

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Abstract

Nuclear electromagnetic charge and current densities and related topics are discussed. Formulas expressing the multipole-decomposed density distributions in terms of the transition density matrix, geometrical factors and single-particle radial wavefunctions are given in detail. These formulas are used for coding a program, MICRØDENS, written in Fortran-IV, to compute the densities. MICRØDENS also computes the form factors, or the Bessel transforms of the densities. Instructions for the use of the program are provided. Three appendices discuss the densities in connection with several physical processes (gamma-emission, electron scattering and photo nucleon-emission), present the formulas for the computation of the transition density matrix in the most commonly used nuclear models, and give a complete listing of MICRØDENS.

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Densités des charges nucléaires, des courants de convection et des courants de magnétisation

par

H.C. Lee

Résumé

L'auteur de ce rapport fait des commentaires au sujet des densités de courant et de charge électromagnétique nucléaire ainsi qu'au sujet de questions connexes. Il décrit en détail les formules exprimant la répartition des densités à décomposition multipolaire, en fonction de la matrice des densités de transition, de facteurs géométriques et de fonctions ondulatoires radiales à particule unique. Ces formules sont employées pour le codage d'un programme, MICRØDENS, écrit en FORTRAN-IV et destiné à calculer les densités. Par ailleurs, le programme MICRØDENS permet de calculer les facteurs de forme ou les fonctions de Bessel pour les densités. Des instructions sont données pour l'emploi du programme. La première annexe concerne les densités par rapport à plusieurs procédés physiques (émission gamma, diffusion des électrons et émission photo-nucléon), la seconde donne des formules pour calculer la matrice des densités de transition dans les modèles nucléaires les plus couramment utilisés et la troisième est la liste complète des programmes MICRØDENS.

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1. INTRODUCTION

The electromagnetic interaction is one of the best tools that can be used to probe the structure of the nucleus. The reasons for this are manifold. Firstly, it is the best understood interaction among those (strong, electromagnetic and weak) that are used to investigate nuclear structure. Secondly, viewed as an operator, the leading and in many cases the only important portion of the interaction is a one-body operator. From a practical point of view the advancement of experimental technologies in the areas of γ-ray detectors, electron accelerators and photon beam generators in the last two decades or so has produced a great wealth of data from which much information in nuclear structure can be extracted.

The nucleus interacts with the electromagnetic field via its charge and current. From a study of the charge and current densities one can infer certain aspects of nuclear structure. In practice often the charge and current densities are computed in a particular model with specific assumptions. These densities are then used in (electromagnetic) reaction calculations and the results are compared with experimental data. Such a comparison may then lead to the rejection, acceptance or modification of the model used, or some of the assumptions made, or both. This report is mainly concerned with the calculation of nuclear charge and current densities.

Suppose that, under the influence of the electromagnetic interaction, the nucleus goes through a transition from state Ψ_i to state Ψ_f (f may be identical to i), then the transition charge, $\rho^{i\to f}_{(\vec{r})}$, and current, $J^{i\to f}_{(\vec{r})}$, densities are

$$\rho(\vec{r}) = e \sum_k \delta(\vec{r}-\vec{r}_k) g_L^k \{\Psi_f^* \Psi_i\} \tag{1}$$

$$\vec{J}(\vec{r}) = \vec{J}^c(\vec{r}) + \vec{J}^m(\vec{r}) + \vec{J}^{exch}(\vec{r}) \tag{2}$$

$$\vec{J}^c(\vec{r}) = \frac{e\hbar}{i2M} \sum_k \delta(\vec{r}-\vec{r}_k) g_L^k \{\Psi_f^* \vec{\nabla}_k \Psi_i - \Psi_i \vec{\nabla}_k \Psi_f^*\}, \tag{3}$$

$$\vec{J}^m(\vec{r}) = \frac{e\hbar}{2M} \sum_k \delta(\vec{r}-\vec{r}_k) \mu_s^k \vec{\nabla}_k \times \{\Psi_f^* \vec{\sigma}_k \Psi_i\}, \tag{4}$$

where σ_k are the Pauli matrices and we have suppressed the superscripts i→f. In (1), (3) and (4), integration over all internal coordinates other than $\vec{r}_k$ is implied for the expression in the curly brackets; g_L is the nucleon orbital g-factor ($g_L^{proton} = 1$, $g_L^{neutron} = 0$) and μ_s is the magnetic moment of the free nucleon ($\mu_s^{proton} = 2.79$, $\mu_s^{neutron} = -1.91$) in nuclear magnetons. $\vec{J}^c$ is the convection current due to the motion of individual nucleons within the nucleus and $\vec{J}^m$ is the magnetization current generated by the magnetic

moments of the nucleons. $\vec{J}^{exch}$ is the current that will arise from an exchange or a momentum-dependent nuclear interaction term or both. Although the exchange current has been a subject of interest since the early days of nuclear physics[1,2] the nuclear interaction is not sufficiently well known to enable us to treat $\vec{J}^{exch}$ in a general way. In fact $\vec{J}^{exch}$ may require a separate treatment for each individual transition, since it is very model dependent. For example a truncation of the shell model basis may be viewed as being effected by a strongly momentum-dependent (in fact, singular) interaction. In this report $\vec{J}^{exch}$ will be completely ignored. Recently studies of the exchange current can be found in the literature[3-5].

Having decided to consider only the three densities ρ, $\vec{J}^{c}$ and $\vec{J}^{m}$ of which the operative forms are well known, we still must decide on a method to treat the nuclear wavefunctions. Currently in the literature there are many models that are used to describe the many-body nuclear wavefunction. Most models have their own distinctive usefulness and together they form a complementary set. It is therefore easy to conclude that for the purpose of this report one should not commit oneself to any one model but rather adopt a more global approach. A natural

linkage between any many-body wavefunction and a one-body density function is the one-body transition density matrix. In this work we shall assume that the density matrix is known, and begin our evaluation of the charge and current densities from this knowledge.

The plan of this report is as follows. In section 2 we first express the density functions in terms of single-particle density functions and the one-body density matrix. We then expand ρ and $\vec{J}$ in terms of scalar and vector spherical multipoles respectively. This expansion is suitable for finite systems such as the nucleus. The multipole single-particle density functions are expressed in terms of geometric coefficients and single-particle radial functions and their derivatives. The hermitian conjugate and the time-reversal properties of the density operators are discussed in two following subsections. A knowledge of these properties may be used to reduce the complexity of the computation. As well, it establishes the realness of the densities (if the radial wavefunctions are real) and enables one to identify a special selection rule, namely that the electric current densities (both longitudinal and transverse) in an elastic transition (i.e., $\Psi \rightarrow \Psi$) vanish. In the last subsection of section 2 we show how the isoscalar and isovector components of the densities are calculated.

In section 3 we describe a package of computer programs, MICRØDENS, written in FORTRAN-IV for the CDC-6600 installation at Chalk River Nuclear Laboratories, for the computation of the nuclear charge and current densities $\rho(\vec{r})$, $\vec{J}^c(\vec{r})$ and $\vec{J}^m(\vec{r})$. The formulas derived in section 2 are used for the coding. The nuclear form factors, which are essentially the spherical Bessel transforms of the densities, are also computed in MICRØDENS. Spherical harmonic oscillator functions (Hermite polynomials) are used as the radial wavefunctions. The advantages of using these functions are their wide use in structure calculations, their well-known analytical properties, and the fact that a complete set of such functions is determined by a single parameter, the oscillator frequency. A flow chart of the program, adequate instructions for the preparation and the assembly of input cards, and brief descriptions of the functions of all subroutines are provided.

A knowledge of the nuclear charge and current densities as isolated entities is academic, since their properties are manifested only through interacting with external fields. In Appendix A, formulas relating the densities to the external field in several physical processes (γ-decay, electron scattering and photo nucleon-emission) are presented. These may be in the form of transition probabilities or strengths or scattering amplitudes or cross sections. The (e,e')

scattering amplitude in the distorted-wave Born approximation is derived in detail. A new formulation for the amplitude, better than those presently available in the literature, is given. The important concepts of gauge invariance and charge conservation and the related Siegert's theorem[2] are also briefly discussed at the beginning of the Appendix.

In Appendix B we show how the one-body transition density matrix can be extracted from the result of structural calculations in the three most commonly used nuclear models, namely the particle-hole model and its variants, the shell model, and the angular-momentum-projected Hartree-Fock model.

A complete listing of the computer code MICRØDENS and sample outputs are contained in Appendix C.

2. CHARGE AND CURRENT DENSITY DISTRIBUTIONS

2.1 NOTATION AND PHASE CONVENTIONS

We use the Greek alphabet, except λ, which is reserved for the tensor rank, to represent the complete set of quantum numbers defining a single-particle state; we use the corresponding Roman alphabet for the same set excluding the magnetic quantum number. Thus

$$\alpha = (\tau_a n_a \ell_a j_a m_a \ldots) = (a, m_a); \quad \bar{\alpha} = (a, -m_a).$$

The single-particle wavefunction is ℓ-s coupled

$$\psi_\alpha(\vec{r}) = \langle \vec{r} | \alpha \rangle = \sum_{m,\sigma} \langle \ell_a m \tfrac{1}{2} \sigma | j_a m_a \rangle i^{\ell_a} u_a(r) Y^{m_a}_{\ell_a}(\vec{r}) \chi^{\sigma}_{1/2}. \tag{5}$$

Here $u_a(r)$ is the radial wavefunction. The phase i^{ℓ_a} assures that $|\alpha\rangle$ will have the desired property under time-reversal,

$$T|\alpha\rangle = (-)^{j_a - m_a} |\bar{\alpha}\rangle, \tag{6}$$

when $u_a(r)$ is real. $\chi^{\sigma}_{\frac{1}{2}}$ is the spin wavefunction.

Let O_{λ} be a spherical tensorial operator of rank λ. Using the Wigner-Eckart theorem[6] we define the reduced matrix element,

$$\langle f\|O_\lambda\|i\rangle = \sum_{M_i,\mu} \langle J_i M_i \lambda\mu | J_f M_f\rangle \langle f\ M_f|O_{\lambda\mu}|i\ M_i\rangle. \tag{7}$$

We also define a partially reduced matrix element, where only the polar coordinates are integrated over

$$(J_f\|O_\lambda(r)\|J_i) \equiv \frac{1}{r^2}\langle J_f\|\delta(\vec{r}-\vec{r}')O_\lambda(\vec{r}')\|J_i\rangle. \tag{8}$$

In general, if O_λ is a one-body operator, the reduced matrix element can be expressed in terms of reduced matrix elements between single-particle states and the one-body transition density matrix, ρ^{if},

$$(f\|O_\lambda(r)\|i) = \sum_{a,b} \frac{\hat{j}_a}{\hat{\lambda}} \rho^{if}_{ba,\lambda}\ (a\|O_\lambda(r)\|b) \tag{9}$$

where $\hat{j}_a = (2j_a+1)^{1/2}$ etc. and

$$\rho^{if}_{ba,\lambda} \equiv \langle f\|[C^\dagger_a \otimes C_b]_\lambda\|i\rangle;\ [C^\dagger_a \otimes C_b]_{\lambda\mu} = \sum_{m_a,m_b} (-)^{j_b-m_b}\langle j_a m_a j_b -m_b|\lambda\mu\rangle C^\dagger_\alpha C_\beta. \tag{10}$$

$C^\dagger$ and C are respectively the single-particle creation and annihilation operators. We see from (9) that to compute the transition charge or current density it is not necessary to know the wavefunctions of $|i\rangle$ and $|f\rangle$ in their entirety. Only the transition density matrix is needed.

2.2 MULTIPOLE DECOMPOSITION

From now on it will be understood that the transition is from the state $|i\rangle$ to the state $|f\rangle$, and all super- or sub-scripts indicating this fact will be suppressed. Since only certain portions, or multipoles of the density will affect a transition between states of definite angular momentum, it is convenient to decompose the density into various multipoles. We define the multipole charge density ρ_λ and current density $\rho_{\lambda\ell}$ as follows:

$$\rho(\vec{r}) = e \sum_{\lambda\mu} (-i)^\lambda \langle J_i M_i \lambda\mu | J_f M_f \rangle \rho_\lambda(r) Y_\lambda^{\mu *}(\hat{r}) \tag{11}$$

$$\vec{J}^{c,m}(\vec{r})/c = e \sum_{\lambda\ell\mu} (-i)^\ell \langle J_i M_i \lambda\mu | J_f M_f \rangle \rho_{\lambda\ell}^{c,m}(r) \vec{Y}_{\lambda\ell 1}^{\mu *}(\hat{r}) \tag{12}$$

where

$$\vec{Y}_{\lambda\ell 1}^{\mu}(\hat{r}) = \sum_{m\nu} \langle \ell m 1 \nu | \lambda\mu \rangle \, Y_\ell^m(\hat{r}) \, \hat{\varepsilon}_\nu \tag{13}$$

is the vector spherical harmonic. $\hat{\varepsilon}_\nu$, $\nu = \pm 1, 0$ are the spherical unit vectors. The quantities ρ_λ, $\rho_{\lambda\ell}^{c,m}$ to be calculated are now functions of the radial variable only.

2.3 THE CHARGE DENSITY

Recall that the total charge density is given as

$$\rho(\vec{r}) = e \sum_k \delta(\vec{r}-\vec{r}_k) g_L^k \ (\Psi_f^* \Psi_i). \tag{1}$$

Multiplying the right-hand side of (1) and (11) by $i^\lambda Y_\lambda^\mu(\hat{r})$ and integrating over the polar variables and then using (7) and (8) we get

$$\rho_\lambda(r) = \sum_{a,b} \frac{\hat{j}_a}{\hat{\lambda}} \rho_{ba\lambda} \ (a\| i^\lambda y_\lambda(\hat{r}) \| b) \tag{14a}$$

with

$$(a\| i^\lambda y_\lambda(\hat{r}) \| b) = -(-)^{j_b+\frac{1}{2}+\lambda} i^{\ell_b+\lambda-\ell_a} \frac{\hat{\lambda}\,\hat{j}_b}{\sqrt{4\pi}} \begin{pmatrix} j_a & j_b & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} u_a^*(r) \ u_b(n),$$

$$\text{if } \ell_a+\ell_b+\lambda \text{ is even;}$$

$$= 0, \qquad \text{if otherwise.} \tag{14b}$$

The above equation is general. For the special case when the radial function u(r) is taken to be the oscillator function,

$$u_a(r) = d^{-3/2} R_{n_a \ell_a}(r/d), \tag{15}$$

where $R_{n\ell}(x)$ is the (dimensionless) Hermite polynomial[7], d is the oscillator length parameter ($d^{-2} = \frac{M\omega}{\hbar} = 0.02412\ \hbar\omega$ (F^{-2}), and $\hbar\omega$ is the oscillator frequency in MeV).

2.4 THE CONVECTION CURRENT DENSITY

We repeat the expression for $\vec{J}^c$ given in (3),

$$\vec{J}^c(\vec{r}) = \frac{e\hbar}{2iM} \sum_k \delta(\vec{r}-\vec{r}_k) g_L^k (\psi_f^* \vec{\nabla}_k \psi_i - \psi_i \vec{\nabla}_k \psi_f^*). \tag{3}$$

One must always be especially careful whenever evaluating the matrix element of an operator involving the derivative. Consider the integral

$$I = \int d\vec{r}\ \psi_i\ f(r)\ \vec{Y}^{\mu}_{\lambda\ell 1}(\hat{r})\cdot\vec{\nabla}\ \psi_f^* \tag{16a}$$

where $f(r)$ is a function of r only and $\psi_i\psi_f^*\ f(r)r^2$ vanishes at $r\to\infty$. Integrating by parts we get

$$I = -\int d\vec{r}\ \psi_f^*\ \vec{\nabla}\cdot f(r)\ \vec{Y}^{\mu}_{\lambda\ell 1}(\hat{r})\psi_i. \tag{16b}$$

We left multiply both sides of (3) by $f\vec{Y}^{\mu}_{\lambda\ell 1}$, integrate over all space, and use (9) and (12) to obtain

$$\int r^2 dr f(r)\rho^c_{\lambda\ell}(r) = -\frac{\hbar}{2Mc} \sum_{ab} g_L^a \frac{\hat{j}_a}{\hat{\lambda}} \rho_{ba\lambda} \langle a \| i^{1+\ell} (f\vec{Y}_{\lambda\ell 1}\cdot\nabla + \nabla\cdot f\vec{Y}_{\lambda\ell 1}) \| b\rangle. \tag{17}$$

The RHS does not have the desired form since f is being operated upon. We now note that the Hermitian adjoint of $i^{1+\ell}\vec{\nabla}\cdot f\vec{Y}^{\mu}_{\lambda\ell 1}$ is

$$(i^{l+\ell}\vec{\nabla}\cdot f\,\vec{Y}^{\mu}_{\lambda\ell l})^{\dagger} = (-)^{l+\lambda+\mu}\, i^{l+\ell} f^{*}\vec{Y}^{-\mu}_{\lambda\ell l}\cdot\vec{\nabla}. \qquad (18)$$

Using this and the identity

$$\langle\alpha|O|\beta\rangle \equiv \langle\beta|O^{\dagger}|\alpha\rangle^{*}$$

where O is any operator, we get

$$\langle a\|\, i^{l+\ell}\vec{\nabla}\cdot f\vec{Y}_{\lambda\ell l}\,\|b\rangle = (-)^{l+\lambda+j_b-j_a}\frac{\hat{j}_b}{\hat{j}_a}\langle b\|\, i^{l+\ell}\, f\vec{Y}_{\lambda\ell l}\cdot\vec{\nabla}\,\|a\rangle^{*}$$

$$= (-)^{l+\lambda+j_b-j_a}\frac{\hat{j}_b}{\hat{j}_a}\int r^2 dr f(b\|\, i^{l+\ell}\vec{Y}_{\lambda\ell l}\cdot\vec{\nabla}\,\|a)^{*}. \qquad (19)$$

From (17) and (19), we finally get, independent of f

$$\rho^{c}_{\lambda\ell}(r) = -\frac{\hbar}{2Mc}\hat{\lambda}^{-1}\sum_{ab}\rho_{ba\lambda}g^{a}_{L}\{\hat{j}_a(a\|\, i^{l+\ell}\vec{Y}_{\lambda\ell l}\cdot\nabla\|b) - (-)^{\lambda+j_b-j_a}\hat{j}_b(b\|\, i^{l+\ell}\vec{Y}_{\lambda\ell l}\cdot\vec{\nabla}\,\|a)^{*}\}. \qquad (20)$$

From (5) the RHS of (19) has a phase factor $i^{\ell_a+l+\ell-\ell_b}$. Due to the parity of the operator $\vec{Y}^{\mu}_{\lambda\ell l}\cdot\vec{\nabla}$, which is $(-)^{l+\ell}$, the non-vanishing matrix elements must have an even $\ell_a+\ell_b+l+\ell$. Therefore the phase factor mentioned above is real. In other words, $\rho^{c}_{\lambda\ell}(r)$ is real, if the radial wavefunctions and $\rho_{ba\lambda}$ are real. We now introduce the ket $|\ell_a m_a\rangle$ for the spatial part of the single-particle wavefunction,

$$\langle \vec{r} | \ell_a m_a \rangle \equiv Y^{m_a}_{\ell_a}(\hat{r}) u_a(r); \quad \langle \vec{r} | \ell^*_a m_a \rangle = Y^{m_a}_{\ell_a}(\hat{r}) u^*_a(r). \tag{21}$$

The spin wavefunctions can now be contracted out[6)]

$$(a \| i^{1+\ell} \vec{Y}_{\lambda\ell 1} \cdot \vec{\nabla} \| b) = i^{\ell_b+1+\ell-\ell_a} (-)^{j_a+\ell_b+\lambda-\frac{1}{2}} \hat{j}_b \hat{\ell}_a W(\ell_a \ell_b j_a j_b; \lambda \tfrac{1}{2}) (\ell_a \| \vec{Y}_{\lambda\ell 1} \cdot \vec{\nabla} \| \ell_b). \tag{22}$$

Substituting (22) into (20), we finally get

$$\rho^c_{\lambda\ell}(r) = \frac{\hbar}{Mc} \hat{\lambda}^{-1} \sum_{a,b} i^{\ell_b+1+\ell-\ell_a} (-)^{j_a+\frac{1}{2}+\ell_b+\lambda} o_{ba\lambda} g^a_L \hat{j}_a \hat{j}_b W(\ell_a \ell_b j_a j_b; \lambda \tfrac{1}{2})$$

$$\times \tfrac{1}{2} \{ \hat{\ell}_a (\ell_a \| \vec{Y}_{\lambda\ell 1} \cdot \vec{\nabla} \| \ell_b) - (-)^{\lambda} \hat{\ell}_b (\ell^*_b \| \vec{Y}_{\lambda\ell 1} \cdot \vec{\nabla} \| \ell^*_a) \}. \tag{23}$$

The evaluation of the reduced matrix element in (23) is now straightforward; we find

$$(\ell_a \| \vec{Y}_{\lambda\ell 1} \cdot \vec{\nabla} \| \ell_b) = (-)^{\lambda+\ell_b} \frac{\hat{\lambda}\ \hat{\ell}}{\sqrt{4\pi}}$$

$$\sum_{\ell'=\ell_b-1}^{\ell_b+1} (\ell'-\ell_b) \hat{\ell}' \begin{pmatrix} \ell_a & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} W(\ell_b 1 \ell_a \ell; \ell' \lambda) u^*_a(r) D_{\ell_b, \ell'-\ell_b}(r) u_b(r) \tag{24}$$

$$D_{\ell_b, \pm 1}(r) = (\ell_b + \tfrac{1}{2}(1 \pm 1))^{1/2} \left[\frac{d}{dr} \mp \frac{\ell_b + \frac{1}{2}(1 \mp 1)}{r} \right] \tag{25}$$

For $(\ell^*_b \| \vec{Y}_{\lambda\ell 1} \cdot \vec{\nabla} \| \ell^*_a)$, we interchange ℓ_a with ℓ_b, and $u^*_a(r)$ with $u_b(r)$, in (24).

It is not always necessary to compute the second term on the RHS* of (23). We note that $\vec{Y}^{\mu}_{\lambda\lambda 1}$ is proportional to $\vec{L}\ Y^{\mu}_{\lambda}$; it therefore commutes with the gradient operator, $\vec{\nabla}$. Consequently for the current that affects magnetic transitions, $\rho^{c}_{\lambda\lambda}(r)$, the second term is equal to the first term.

Equations (23) and (24) are applicable for any radial wavefunction. When oscillator functions $R_{n\ell}(x)$ are employed, the relations given below are useful. For $\ell > 0$, we have

$$(\frac{d}{dx} + \frac{\ell+1}{x})R_{n\ell}(x) = (\ell+n+\tfrac{1}{2})^{\frac{1}{2}}\ R_{n\ell-1}(x) + (n+1)^{\frac{1}{2}}\ R_{n+1,\ell-1}, \qquad (26a)$$

$$(\frac{d}{dx} - \frac{\ell}{x})R_{n\ell}(x) = (\frac{d}{dx} + \frac{\ell+1}{x})R_{n\ell}(x) - \frac{2\ell+1}{x}\ R_{n\ell}. \qquad (26b)$$

When $\ell = 0$, we have

$$\frac{d}{dx}\ R_{n0}(x) = -(n+\tfrac{3}{2})^{\frac{1}{2}}\ R_{n1}(x) - n^{\frac{1}{2}}\ R_{n-1,1}(x). \qquad (26c)$$

In (26), n is the number of nodes of the oscillator function in the range $0 < r < \infty$.

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*RHS - *right-hand side*

2.5 THE MAGNETIZATION CURRENT DENSITY

We repeat equation (4)

$$\vec{J}^m(\vec{r}) = \frac{e\hbar}{2M} \sum_j \delta(\vec{r}-\vec{r}_j)\mu_s^j \vec{\nabla}_j \times (\Psi_f^* \vec{\sigma}_j \Psi_i), \tag{4}$$

and consider the integral

$$\begin{aligned} I &= i^\ell \int d\vec{r}\ f(r)\ \vec{Y}^\mu_{\lambda\ell 1}(r)\cdot[\vec{\nabla} \times (\Psi_f^* \vec{\sigma} \Psi_i)] \\ &= i^\ell \int d\vec{r}\ \Psi_f^* \vec{\sigma} \Psi_i \cdot \vec{\nabla} \times (f \vec{Y}^\mu_{\lambda\ell 1}). \end{aligned} \tag{27}$$

Using the well-known relations

$$(\vec{\nabla}\times f\ \vec{Y}^\mu_{\lambda\ell 1})_q = \frac{\sqrt{2}}{i} \sum_{m\nu} (-)^k <\ell m 1 -k|\lambda\mu><1\nu 1k|1q>\nabla_\nu(f\ Y^m_\ell) \tag{28}$$

and

$$\begin{aligned} \nabla_\nu f\ Y^m_\ell &= \left(\frac{\ell+1}{2\ell+3}\right)^{\frac{1}{2}} <\ell m|V|\ell+1, m+\nu>\ Y^{m+\nu}_{\ell+1}\ \left(\frac{d}{dr} - \frac{\ell}{r}\right)f \\ &\quad - \left(\frac{\ell}{2\ell-1}\right)^{\frac{1}{2}} <\ell m|V|\ell-1, m+\nu>\ Y^{m+\nu}_{\ell-1}\ \left(\frac{d}{dr} + \frac{\ell+1}{r}\right)f \end{aligned} \tag{29}$$

and calling the left-hand side of (28) $D_q(r,\frac{d}{dr})f$, we rewrite (27) as

$$I = i^{\ell+1} \sum_q (-)^q \int d\vec{r}(\Psi_f^* \sigma_{-q} \Psi_i) D_q(r, \frac{d}{dr}) f$$

$$= -i^{\ell+1} \sum_q (-)^q \int d\vec{r}\ f\ D_q(r, -\frac{d}{dr}) r^2\ \Psi_f^* \sigma_{-q} \Psi_i, \qquad (27')$$

upon integration by parts. Equation (27') has the desired form, since f is not operated upon. From (27'), (28), (7), (9) and (12), and using standard angular momentum recoupling techniques, we have

$$\rho^m_{\lambda\ell}(r) = -\frac{\hbar}{2Mc} \hat{\lambda}^{-1} \sum_{a,b} \hat{j}_a \rho_{ba\lambda} \mu^a_s\ i^{1+\ell} \sqrt{6}$$

$$\times\{(\ell+1)\ W(11\ell+1\ell;1\lambda)(\frac{d}{dr} + \frac{\ell+2}{r})(a\|T_\lambda(Y_{\ell+1}\otimes\sigma)\|b)$$

$$- \ell^{\frac{1}{2}} W(11\ell-1,\ell:1\lambda)(\frac{d}{dr} - \frac{\ell-1}{r})(a\|T_\lambda(Y_{\ell-1}\otimes\sigma)\|b)\}. \qquad (30)$$

$T_\lambda(Y_\ell\otimes\sigma)$ is a rank-λ tensor product of Y_ℓ and $\vec{\sigma}$:

$$T_{\lambda\mu}(Y_\ell\otimes\sigma) = \sum_{mq} <\ell m 1 q|\lambda\mu> Y^m_\ell \sigma_q.$$

With (5), we have

$$(a\|T_\lambda(Y_\ell\otimes\sigma)\|b)$$

$$= (-)^{\ell_a} i^{\ell_b-\ell_a} (\frac{3}{2\pi})^{\frac{1}{2}} \hat{\lambda}\hat{\ell}\hat{j}_b \hat{\ell}_a \hat{\ell}_b \begin{pmatrix} \ell_a & \ell & \ell_b \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} j_a & j_b & \lambda \\ \ell_a & \ell_b & \ell \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix} u^*_a(r) u_b(r). \qquad (31)$$

From (30) and (31), $\ell_a+\ell_b+\ell+1$ must be even, i.e., the phase factor $i^{1+\ell+\ell_b-\ell_a}$ is real, and $\rho^m_{\lambda\ell}$ is real, if u_a and u_b and $\rho_{ba\lambda}$ are real. Since $\ell=\lambda$, $\lambda\pm1$, the two equations above may be further simplified by evaluating the Racah and 9-j coefficients. We finally get

$$\rho^m_{\lambda\ell}(r) = -\frac{h}{2Mc}\sum_{ab} i^{\ell_b-\ell_a+1+\ell}(-)^{\lambda+j_b+\frac{1}{2}}\rho_{ba\lambda}\mu^a_s\frac{\hat{j}_a\hat{j}_b}{\hat{\lambda}\sqrt{4\pi}}\begin{pmatrix} j_a & j_b & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}F^{ab}_{\lambda\ell}(r)u^*_a(r)u_b(r) \qquad (32)$$

$$F^{ab}_{\lambda\lambda}(r) = -\left(\frac{2\lambda+1}{\lambda(\lambda+1)}\right)^{\frac{1}{2}}\left[\frac{\lambda(\lambda+1)}{r} + (x_a+x_b)\left(\frac{d}{dr}+\frac{1}{r}\right)\right] \qquad (33a)$$

$$F^{ab}_{\lambda,\lambda\pm1}(r) = \frac{1}{\lambda+\frac{1}{2}\pm\frac{1}{2}}(x_a-x_b)D_{\lambda,\pm1}(r) \qquad (33b)$$

with $D_{\lambda,\lambda\pm1}(r)$ given by (25), and $x_a = (\ell_a-j_a)(2j_a+1)$.

2.6 PARITY SELECTION RULES

We recall that for transitions affected by the electric or Coulomb field, the parity change from $|i\rangle$ to $|f\rangle$ is "natural" ($(-)^{L_i-L_f} = (-)^{\lambda}$), and for magnetic transitions it is "unnatural" ($(-)^{L_i-L_f} = (-)^{\lambda+1}$). These selection rules must be reflected in the transition densities. In table 1 these rules are summarized.

TABLE 1. PARITY SELECTION RULES

density	type	$L_i+L_f+\lambda$	$\ell_a+\ell_b+\lambda$	$\ell_a+\ell_b+\ell+1$
$\rho_\lambda(r)$	Coulomb	even	even	——
$\rho^{c,m}_{\lambda,\ell=\lambda}(r)$	Magnetic	odd	odd	even
$\rho^{c,m}_{\lambda,\ell=\lambda\pm1}(r)$	Electric	even	even	even

2.7 HERMITIAN PROPERTY OF THE DENSITY OPERATORS

When the Hermitian adjoint of a tensor operator O^{μ}_{λ} is

$$(O^{\mu}_{\lambda})^{\dagger} = (-)^{\lambda+\mu} O^{-\mu}_{\lambda},$$

we shall call O^{μ}_{λ} Hermitian. Conversely, if

$$(O^{\mu}_{\lambda}) = -(-)^{\lambda+\mu} O^{-\mu}_{\lambda}$$

is true, we call O^{μ}_{λ} anti-Hermitian.

The Hermitian property of an operator can be exploited to shorten the calculation of its matrix elements. We define a multipole density operator to be an operator such that its reduced matrix elements between $|\Psi_i>$ and $|\Psi_f>$ give the correct density. From (1), the charge density operator is

$$\rho_{op,\lambda\mu}(\vec{r}) = \frac{1}{r^2} \sum_j g^j_L \, \delta(r-r_j) i^{\lambda} Y^{\mu}_{\lambda}(\hat{r}_j). \tag{34}$$

From (3) and (17), the convection current density operator is

$$\rho^c_{op,\lambda\mu,\ell}(\vec{r}) = -\frac{\hbar}{2Mcr^2} i^{1+\ell} \sum_j g^j_L \{\delta(r-r_j) \vec{Y}^{\mu}_{\lambda\ell 1}(\hat{r}_j) \cdot \vec{\nabla}_j + \vec{\nabla}_j \cdot \delta(r-r_j) \vec{Y}^{\mu}_{\lambda\ell 1}(\hat{r}_j)\}. \tag{35}$$

We cannot immediately write down the magnetization density operator from (4). However, by partial integration, we find

$$\rho^{m}_{op,\lambda\mu,\ell}(\vec{r}) = \frac{\hbar}{2Mc}\, i^{\ell} \sum_{j} \mu_s^j \{\delta(r-r_j)\vec{Y}^{\mu}_{\lambda\ell 1}(\hat{r}_j)\cdot(\vec{\nabla}_j\times\vec{\sigma}_j) + (\vec{\sigma}_j\times\vec{\nabla}_j)\cdot\delta(r-r_j)\vec{Y}^{\mu}_{\lambda\ell 1}(\hat{r}_j)\} \qquad (36)$$

Recalling that

$$\vec{Y}^{\mu}_{\lambda\ell 1}\cdot\vec{A} = \sum_{m,q} \langle \ell m 1 q | \lambda\mu\rangle\, Y^{m}_{\ell}\, A_q$$

and

$$\vec{Y}^{\mu}_{\lambda\ell 1}\cdot(\vec{A}\times\vec{B}) = \frac{\sqrt{2}}{i} \sum_{mrs} \langle \ell m 1 q | \lambda\mu\rangle\langle 1 r 1 s | 1 q\rangle Y^{m}_{\ell}\, A_r B_s,$$

where $\vec{A}$ and $\vec{B}$ are any rank-1 tensors, and $(i^{\ell}Y^{m}_{\ell})^{\dagger} = (-)^{\ell-m} i^{\ell} Y^{-m}_{\ell}$; $(\nabla_q)^{\dagger} = (-)^{1-q}\nabla_q$ and $(\sigma_q)^{\dagger} = (-)^{q}\sigma_{-q}$, it is easily shown that

$$(\rho_{op,\lambda\mu})^{\dagger} = (-)^{\lambda+\mu}\, \rho_{op,\lambda-\mu}, \qquad (37a)$$

and

$$(\rho^{c,m}_{op,\lambda\mu,\ell})^{\dagger} = -(-)^{\lambda+\mu}\, \rho^{c,m}_{op,\lambda-\mu,\ell}. \qquad (37b)$$

That is, the charge density operator is Hermitian and the current density operators are anti-Hermitian. Note that in (35) as well as in (36), either one of the two terms on the RHS by itself does not have definite Hermiticity.

Now consider a tensor O^{μ}_{λ} which has definite Hermiticity, $(O^{\mu}_{\lambda})^{\dagger} = (-)^{p+\mu} O^{-\mu}_{\lambda}$; we find

$$\langle JM|O^{\mu}_{\lambda}|J'M'\rangle = \langle J'M'|(O^{\mu}_{\lambda})^{\dagger}|JM\rangle^{*}$$

$$= (-)^{p-\mu}\langle J'M'|O^{-\mu}_{\lambda}|JM\rangle^{*}$$

leading to

$$\langle J\|O_{\lambda}\|J\rangle = (-)^{p+J-J'}\,\hat{J}'\langle J'\|O_{\lambda}\|J\rangle^{*}. \qquad (38)$$

In the previous sections, we have shown that, when $\rho_{ba\lambda}$ and the radial functions are real†, reduced single-particle matrix elements of $\rho_{\sigma p,\lambda\mu}$ and $\rho^{c,m}_{\sigma p,\lambda\mu,\ell}$ are all real. In this case, from (37,38) we can make the replacement on the LHS of (15), for the charge density

$$\sum_{ab}\rho_{ba,\lambda} \to \sum_{a\geq b}\frac{1}{1+\delta_{ab}}[\rho_{ba,\lambda}+(-)^{\lambda+j_b-j_a}\rho_{ab,\lambda}];\ \underline{\text{for } \rho_{\lambda}(r)}. \qquad (39)$$

Similarly, for the current densities, on the LHS of (23) and (32),

$$\sum_{a,b}\rho_{ba,\lambda} \to \sum_{a\geq b}\frac{1}{1+\delta_{ab}}[\rho_{ba,\lambda}-(-)^{\lambda+j_b-j_a}\rho_{ab,\lambda}];\ \underline{\text{for } \rho^{c,m}_{\lambda\ell}(r)}. \qquad (40)$$

---

† *In the rest of this section, we shall assume this to be the case, unless otherwise stated.*

Equation (40) leads to an interesting result for electric transitions. Consider the pair a=b. Due to the parity selection rule for electric transitions, λ must be even. Therefore we see that the pair a=b cannot generate a convection current which contributes to Eλ transitions. A special case of this property is when $|\psi_i\rangle = |\psi_f\rangle$. For this case it follows immediately from (3) that $\vec{j}^c(\vec{r}) = 0$.

Since the gradient operator is spin independent, we can even make a stronger statement; no convection current can be generated if the spatial wavefunctions of $|i\rangle$ and $|f\rangle$ are identical. Microscopically, this is manifestly true from (23). In the spherical harmonic oscillator model, the spatial wavefunctions of the two states with $j = \ell \pm \frac{1}{2}$ are identical: therefore there is no convection current between such two states. In more realistic (single-particle) models their wavefunctions will in general be different. The difference will be small, however, because it is generated only by the spin-orbit potential, which is a small part of the total potential. This observation, coupled to the fact that only currents can affect γ-transitions (due to gauge invariance, or equivalently, the conservation of charge), seems to lead to the following statement: Eλ transitions between spin-orbit partner states, such as $d_{3/2} \rightarrow d_{5/2}$,

are always weak. On the other hand, we know this conjecture is not supported by experiments. The answer to this apparent paradox lies in the fact that only convection current has been considered so far. Currents generated by exchange and momentum-dependent forces or due to basis truncations (i.e. $\vec{J}^{exch}$) have been ignored. The fact that there are strong E2 transitions in nuclei across the whole periodic table is proof that $\vec{J}^{exch}$ is not negligible. Yet for reasons stated in the Introduction, a global treatment of $\vec{J}^{exch}$ is not feasible. This difficulty is resolved, at least in part, for low energy processes (wave length of photon $\gtrsim$ nucleon size), by the so-called Siegert's theorem[2]. This theorem enables us to side-step the question of currents, and relate the electric transition directly to the nuclear charge distribution. A comprehensive discussion of Siegert's theorem is somewhat outside the scope of this report; however, it is discussed briefly at the beginning of Appendix A.

2.8 TIME-REVERSAL PROPERTY OF THE DENSITY OPERATORS

We shall use the time-reversal properties of the density operators to establish the realness of the densities. Under time-reversal (TR), all momenta and spins change sign, and all c-numbers become their respective complex-conjugates. Let us call the TR transformation T, and for any state $|\psi>$

$$|\psi_T> \equiv T|\psi>. \tag{41}$$

We shall call a state of good angular momentum TR-invariant if under the transformation T, other than gaining a phase $(-)^{J-M}$ only its magnetic quantum number changes sign,

$$T|\gamma JM> = (-)^{J-M}|\gamma J,-M>, \tag{42}$$

where γ is the set of all other quantum numbers. Thus as stated in (6) the single-particle wavefunction given in (5) is TR-invariant, if $u(r)$ is real.

Let O be any operator, and

$$O|\psi> = \sum_n |\phi_n><\phi_n|O|\psi>. \tag{43}$$

We want to find the property of O under TR, which is defined as

$$T O|\psi\rangle = T O T^{-1} T|\psi\rangle \equiv O_T|\psi_T\rangle$$

$$= \sum_n |\phi_{nT}\rangle\langle\phi_n|O|\psi\rangle^*, \tag{44}$$

the second line comes from (43), taking into account that $\langle\phi_n|O|\psi\rangle$ is c-number. It follows that

$$\langle\phi_T|O_T|\psi_T\rangle = \langle\phi|O|\psi\rangle^*. \tag{45}$$

Suppose

$$(O^\mu_\lambda)_T = (-)^{p-\mu}\, O^{-\mu}_\lambda,$$

and let $|JM\rangle$ and $|J'M'\rangle$ be TR-invariant, then from (45)

$$(-)^{J-M-J'+M'+p-\mu}\langle J-M|O^{-\mu}_\lambda|J'-M'\rangle = \langle JM|O^\mu_\lambda|J'M'\rangle^*.$$

Taking the reduced matrix elements on both sides, we have

$$\langle J\|O_\lambda\|J'\rangle^* = (-)^{p-\lambda}\,\langle J\|O_\lambda\|J'\rangle. \tag{46}$$

Therefore $\langle J\|O_\lambda\|J'\rangle$ is real, if $p=\lambda$, and is purely imaginary if $p = \lambda+1$.

From (34), (35) and (36) we find that the charge and current density operators transform similarly under T

$$(\rho_{op,\lambda\mu})_T = (-)^{\lambda-\mu}\ \rho_{op,\lambda-\mu}, \tag{47a}$$

$$(\rho^{c,m}_{op,\lambda\mu,\ell})_T = (-)^{\lambda-\mu}\ \rho^{c,m}_{op,\lambda-\mu,\ell}. \tag{47b}$$

Since we have chosen a phase convention such that the single-particle wavefunctions are TR-invariant (Equation (5)) it follows that all single-particle reduced matrix elements of the density operators are real. This has already been pointed out in Section 2. To establish the realness of the density itself, it remains to show that the many-body states $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are TR-invariant. This can easily be shown by induction, if (5) is true, and if all the coupling coefficients are real. Here we only show it to be true for a two-particle state. Let

$$|ab;JM\rangle = |\alpha\otimes\beta;JM\rangle = \sum_{m_a,m_b} \langle j_a m_a j_b m_b|JM\rangle |\alpha\rangle\ |\beta\rangle.$$

Then from (5),

$$T|ab;JM\rangle = \sum_{m_a,m_b} \langle j_a m_a j_b m_b|JM\rangle (-)^{j_a-m_a}(-)^{j_b-m_b}|\bar{\alpha}\rangle\ |\bar{\beta}\rangle$$

$$= (-)^{J-M} \sum_{m_a,m_b} \langle j_a -m_a\ j_b -m_b|J-M\rangle\ |\bar{\alpha}\rangle\ |\bar{\beta}\rangle$$

$$= (-)^{J-M}|ab;J-M\rangle.$$

Therefore $|JM>$ is TR-invariant. We have thus shown that for the phase convention used here, the charge and current densities are real. A corollary is that the one-body density matrix element $\rho_{ba\lambda}$ is real.

It should be emphasized that Equations (5), (37) and (47) follow strictly from the phase convention adopted in Section 2.1, which is essentially replacing the spherical harmonic Y_ℓ^m by $i^\ell Y_\ell^m$ whenever the former appears. Any other phase-convention, if consistently used, will be equally acceptable but may result in imaginary or complex densities.

The realness of the current, together with the Hermitian property of the current operator, lead to a special selection rule when $|\Psi_f>$ is equal to $|\Psi_i>$. From the identity

$$<\Psi_f|O_{\lambda\mu}|\Psi_i>^* = <\Psi_i|(O_{\lambda\mu})^\dagger|\Psi_f>$$

and (37b), we have

$$(\rho_{\lambda\ell}^{i\to i}(r))^* = \rho_{\lambda\ell}^{i\to i}(r) = -(-)^\lambda \rho_{\lambda\ell}^{i\to i}(r).$$

For magnetic transitions ($\ell=\lambda$), $(-)^\lambda$ must be odd, from the parity selection rule, so $-(-)^\lambda = 1$. Therefore a magnetic transition is allowed. A similar argument shows that the diagonal electric transition is not allowed.

2.9 ISOSPIN DENSITIES

So far we have discussed the charge and current distributions in terms of proton and neutron densities. If the proton and neutron wavefunctions are close approximates to each other, a condition which is certainly fulfilled in all light and intermediate nuclei, then it is convenient to discuss the distributions in terms of isoscalar and isovector densities. Let us call the isoscalar density matrix $\rho^{(0)}_{ba\lambda}$ and the isovector density matrix $\rho^{(1)}_{ba\lambda}$. It is easy to see that

$$\rho^{(0)}_{ba} = \frac{1}{\sqrt{2}} (\rho^{\text{proton}}_{ba\lambda} + \rho^{\text{neutron}}_{ba\lambda}), \tag{48a}$$

$$\rho^{(1)}_{ba} = \frac{1}{\sqrt{2}} (\rho^{\text{proton}}_{ba\lambda} - \rho^{\text{neutron}}_{ba\lambda}). \tag{48b}$$

We can therefore pretend that there is only one kind of particle with orbital g-factor and magnetic moment which is isospin dependent. Thus

$$g^{(T)}_{L} = \frac{1}{\sqrt{2}} (g^{\text{proton}}_{L} + (-)^{T} g^{\text{neutron}}_{L}), \tag{49}$$

$$\mu^{(T)}_{S} = \frac{1}{\sqrt{2}} (\mu^{\text{proton}}_{S} + (-)^{T} \mu^{\text{neutron}}_{S}); \quad T = 0,1. \tag{50}$$

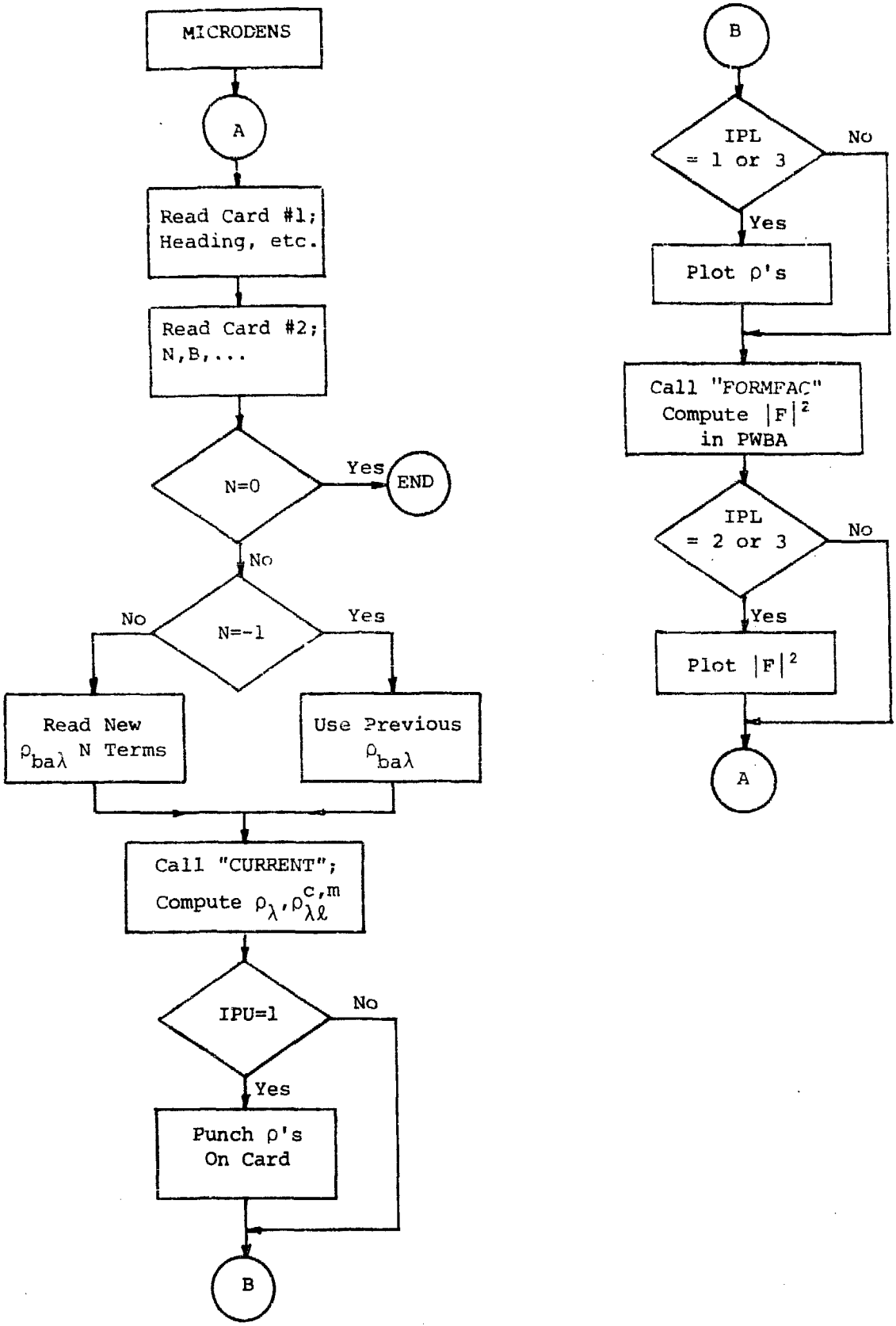
3. THE COMPUTER CODE "MICRØDENS"

3.1 BRIEF DESCRIPTION, FLOW CHART

MICRØDENS is a self-contained package of computer programs, written in the Fortran-IV language, for calculating the charge and current densities, given the one-body transition density matrix. The execution of the program is controlled by input data cards, and the results are printed and/or punched on cards and plotted. The flow chart of the code is given in Fig. 1. The execution begins at point A. Upon the completion of a full cycle of computation, the command returns to point A. The job is terminated upon reading of #2 data card with N=0.

A second part of the program, shown as part B in the flow chart, calculates the Coulomb, electric and magnetic form factors (see Appendix A, Equations (27) and (27c')) corresponding to the one-body transition density matrix.

FIGURE 1. FLOW CHART OF MICRØDENS



3.2 INPUT DATA

For each transition for which the densities are to be calculated, there are three sets of data cards. Each of the first two sets contains only one card. The number of cards in the third set varies.

The contents and format of each card is as follows:

Content/Format

```
card  - NAME, KIND
no. 1   7A10, A10

card  - N,  B,    DX,   NX, DQ, QMAX, VJI, VJF, Z, EFC, EFM, JS, JL, IPL, IPU
no. 2   I4, F6.3, F5.3, I5,          (      7F5.1       ), (      4I2     )

card  - NLJA(1), NLJB(1), IRO(1), RØ(1), NLJA(2),...
no. 3   I3,      I3,      I1,    F8.5,  I3,....
```

NAME is the identifier of the particular calculation. It may be up to seven words (10 characters per word) long, and is used as the heading for all output. KIND may be either one of the three left-adjusted words COULOMB, (ρ_λ computed), ELECTRIC ($\rho^{c,m}_{\lambda,\lambda\pm1}$ computed) and MAGNETIC ($\rho^{c,m}_{\lambda\lambda}$ computed). N is the number of $\rho_{ba\lambda}$ to be read. It therefore determines the number (N/5+1) of cards in set 3. B is the oscillator length parameter (Section 2.3) in Fermies. The meanings of other entries on card No. 2

are clearly explained in the listing of MICRØDENS (see Appendix C), and will not be repeated here. For each pair (a,b), NLJA, NLJB, IRØ and RØ have respectively the following meanings:

$$NLJA = 32*n_a + 2*\ell_a + j_a + \frac{1}{2} - \ell_a,$$

with NLJB similarly defined; IRØ=1(0) if (a,b) is a proton (neutron) pair; and RØ = $\rho_{ba\lambda}$. $n_a \geq 0$ is the principal quantum number minus one.

3.3 PHYSICAL CONSTANTS

We give the names and values of the physical constants used in MICRØDENS:

HBC = $\hbar c$ = 197.33 (MeV.F);

BOHR = $\mu_n/e = \hbar/2Mc$ = 0.105(F), μ_n is the nuclear magneton;

GLP = g_L^p = 1, orbital g-factor for proton;

GLN = g_L^n = 0, orbital g-factor for neutron;

MUSP = μ_s^p = 2.79, magnetic moment for protons in μ_n;

MUSN = μ_s^n = -1.91, magnetic moment for neutron in μ_n.

The effective charge for proton (neutron), in units of e, is GLP+EFCH (GLN+EFCH). EFCH is read as an input parameter on card No. 2.

3.4 COMPUTATION

The charge and current densities are calculated in the subroutine CURRENT. When KIND = COULOMB, the dimensionless density $\tilde{\rho}_\lambda(x) = d^3\rho_\lambda(r)\big|_{r=xd}$ is computed using (14). When KIND = ELECTRIC (or MAGNETIC), $\rho^{c,m}_{\lambda,\lambda\pm1}(x) = d^3\rho_{\lambda,\lambda\pm1}(r)\big|_{r=xd}$ (or $\tilde{\rho}^{c,m}_{\lambda\lambda}(x)$) are calculated using (23-26) and (30-33); d is the oscillator length parameter (see Section 2.3).

In the subroutine FORMFAC, the Coulomb electric and magnetic form factors are computed. These form factors are defined in Appendix A, section 3. They are essentially spherical Bessel transforms of the appropriate densities (see (A.27)). However, in FORMFAC the form factors are not calculated as such, but are directly calculated from the one-body density matrix. For example, if we seek the Bessel transform of the density $(f\|\mathcal{O}_\lambda(r)\|i)$ with kernel $j_\ell(qr)$, then in (9) we replace the partially reduced matrix element $(a\|\mathcal{O}_\lambda(r)\|b)$ by the reduced matrix element $\langle a\|j_\ell(qr)\mathcal{O}_\lambda(r)\|b\rangle$. The point is that for harmonic oscillators such reduced matrix elements can be evaluated analytically (by the routine RADQ) and the form factor thus obtained provides at least a consistency check when compared against the (numerically evaluated) Bessel transform of the appropriate density.

In FORMFAC the form factors are calculated for momentum transfer q = 1 to QMAX(MeV/c), in steps of DQ.

3.5 OUTPUT

The calculated densities and form factors are printed in a format that is self-explanatory (see sample output on p.92).

When IPU=1, the density will also be punched on the card. The first card will contain the first three words of NAME and other relevant information (see card MICRØD.95). Then $\tilde{\rho}^c(x_1)$, $\tilde{\rho}^m(x_1)$, $\tilde{\rho}^c(x_2)$, $\tilde{\rho}^m(x_2)$ ... are punched, in format (6E12.5). NX points are punched, with $x_1=0$, $x_{n+1}-x_n$ = DX. When KIND = COULOMB, $\tilde{\rho}^c(x) = \tilde{\rho}(x)$, and $\tilde{\rho}^m(x) = 0$.

When IPL = 1 or 3, the output includes plots of the density vs. x. When IPL = 2 or 3, the natural-logarithmic of the form factor squared is plotted against q.

3.6 SUBROUTINES AND THEIR FUNCTIONS

Subroutines that are used in MICRØDENS are described in Table 2.

TABLE 2. ROUTINES IN MICRØDENS

Name	*Function*	*Called by*
MICRØD	Main program	
CURRENT	Computes densities	MICRØD
FORMFAC	Computes (e,e') form factors	MICRØD
TLYDEL or TLYDELQ	Computes $(\ell_a \| T_\lambda(Y_\ell \Theta \nabla) \| \ell_b)$ or $\langle \ell_a \| j_\ell(qr) T_\lambda(Y_\ell \Theta \nabla) \| \ell_b \rangle$	FORMFAC, CURRENT
TJYLL	Computes $\langle \ell_a \| j_\ell(qr) T_\lambda(Y_\ell \Theta L) \| \ell_b \rangle$	FORMFAC
RDFUNC	Computes oscillator function $R_a(x)$	CURRENT, TLYDEL
RADQ	Computes the integral $\int_0^\infty x^2 dx\, R_a(x) j_\ell(Qx) R_b(x)$	FORMFAC, TJYLL, TLYDEL
CG000	Computes the 3-j symbol $\begin{pmatrix} \ell_a & \ell_b & \ell \\ 0 & 0 & 0 \end{pmatrix}$	TJYLL, TLYDEL
CLEBS	Computes the 3-j symbol $\begin{pmatrix} a & b & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$	FORMFAC, CURRENT
WCOEF	Computes Racah or 6-j Coefficients	FORMFAC, CURRENT, TJYLL, TLYDEL
LINPLØT	Linear plot	MICRØD
SEMILØG	Semi-log plot	MICRØD

The subroutines LINPLØT and SEMILØG call a system routine PLØT, for plotting purposes. This routine is available at the computing center at Chalk River Nuclear Laboratories only. Users at other computer installations may substitute local versions of plotting routines for PLØT. If this proves impossible, the calls, in MICRØD, to SEMILØG and LINPLØT must be bypassed.

A complete listing of MICRØDENS is given in Appendix C.

CREDITS

The routine RADQ, of which a revised version is used here, was originally written by F.C. Khanna. WCOEF, a high speed program which employs the Regge symmetries to calculate 6-j coefficients, was written by R.Y. Cusson. The two plotting routines LINPLØT and SEMILØG were kindly supplied by M.A. Lone.

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APPENDIX A

In this appendix we present a collection of formulas describing some physical processes most often exploited to probe the nuclear charge and current densities, namely γ-emission, photonuclear-disintegration leading to particle emission, and elastic and inelastic electron scattering. These formulas will all be given explicitly in terms of the density functions ρ_λ, $\rho_{\lambda\ell}^{c,m}$ described in Section 2. Detailed attention will be given only to the development of the formalism for the (e,e') in the distorted wave Born approximation, in view of the fact that this topic has received a less than comprehensive treatment in the literature.

A special property of electromagnetism is its gauge invariance which is closely related to the conservation of charge. A very useful relation which arises from this property is the so-called Siegert's theorem. We shall start the appendix on this topic.

A.1 GAUGE INVARIANCE, CHARGE CONSERVATION AND SIEGERT'S THEOREM

We shall use the compact 4-vector notation $x_\nu = (\vec{x},ct)$, $x^\nu = (\vec{x},-ct)$. The 4-vector electromagnetic potential is $\vec{A}_\nu = (\vec{A},\phi)$, the current is $J_\nu = (\vec{J}/c,\rho)$, and the

gradient is $\partial_\nu = (\vec{\nabla}, -\frac{1}{c}\frac{\partial}{\partial t})$. The gauge invariance of electromagnetism states that Maxwell's equations are invariant under a gauge transformation of the second kind[8],

$$A'_\nu = A_\nu + \partial_\nu \Lambda \tag{A.1}$$

where Λ is any function of x_ν. The gauge invariance is closely related to the conservation of charge. Consider the interaction of A'_ν with current J_ν. We have

$$\int A'_\nu J^\nu \, dx^4 = \int A_\nu J^\nu \, d^4x + \int (\partial_\nu \Lambda) J^\nu \, d^4x$$

$$= \int A_\nu J^\nu \, d^4x - \int \Lambda (\partial_\nu J^\nu) d^4x,$$

integrating by parts. The second term vanishes, however, because charge is conserved:

$$\partial_\nu J^\nu = \frac{1}{c}\left(\vec{\nabla}\cdot\vec{J} + \frac{\partial \rho}{\partial t}\right) = 0. \tag{A.2}$$

The relation above is also called the equation of continuity. The gauge invariance allows us, for example, to work in the Lorentz gauge, expressed by the equation

$$\partial_\nu A^\nu = \vec{\nabla}\cdot\vec{A} + \frac{1}{c}\frac{\partial \phi}{\partial t} = 0$$

We shall see that this is consistent with describing A as being generated by a conserved current, J_ν, via a retarded Green's function[9] G_{ret},

$$A_\nu(r) = -i \int J_\nu(r') G_{ret}(r,r') d^4r' \qquad (A.3)$$

where

$$G_{ret}(r,r') = \frac{1}{|\vec{r}-\vec{r}'|} \delta(t-t' - \frac{1}{c}|\vec{r}-\vec{r}'|).$$

The Lorentz condition is automatically satisfied,

$$\partial_\nu A^\nu(r) = -i \int J^\nu(r') \partial_\nu G_{ret}(r,r') d^4r'$$

$$= +i \int J^\nu(r') \partial'_\nu G_{ret}(r,r') d^4r'$$

$$= -i \int (\partial'_\nu J^\nu(r')) G_{ret}(r,r') d^4r' = 0.$$

Since J_ν is conserved, $\partial_\nu J^\nu = 0$.

From now on we shall restrict our discussion only to fields with definite frequencies

$$A_\nu(r) = A_\nu(\vec{r}) e^{-i\omega t}. \qquad (A.4)$$

Naturally, fields of any time-dependence can be constructed as integrals of such fields. Let us consider a field

created by a source at infinity. In this case Maxwell's equations, in the Lorentz gauge, become

$$\nabla^2 A_\nu + k^2 A_\nu = 0,$$

where $k = \omega/c$. The three independent solutions can be multipole decomposed[6)]

$$\phi(\vec{r}) = a \sum_\lambda \phi_{\lambda 0}(\vec{r}) \tag{A.5a}$$

$$\vec{A}(\vec{r}) = a \sum_\lambda \vec{\mathcal{L}}_{\lambda 0} + \sum_{\lambda,\lambda=\pm 1} b_\mu (\vec{\mathcal{E}}_{\lambda\mu} + \mu \vec{\mathcal{M}}_{\lambda\mu}(r)) \tag{A.5b}$$

with

$$\phi_{\lambda\mu} = [4\pi(2\lambda+1)]^{\frac{1}{2}}\, i^\lambda j_\lambda(kr) Y^\mu_\lambda(\hat{r}) \tag{A.5c}$$

$$\vec{\mathcal{L}}_{\lambda\mu} = (ik)^{-1} \vec{\nabla}\phi_{\lambda\mu} = -i^{1+\lambda} \sqrt{4\pi}\, (\sqrt{\lambda}\, j_{\lambda-1}\, \vec{Y}^\mu_{\lambda,\lambda-1,1} + \sqrt{\lambda+1}\, j_{\lambda+1}\, \vec{Y}^\mu_{\lambda,\lambda+1,1}), \tag{A.5d}$$

$$\vec{\mathcal{E}}_{\lambda\mu} = [k^2\lambda(\lambda+1)]^{-\frac{1}{2}} \vec{\nabla}\times\vec{L}\phi_{\lambda\mu} = i^{1+\lambda}\sqrt{4\pi}\, (\sqrt{\lambda+1}\, j_{\lambda-1}\, \vec{Y}^\mu_{\lambda,\lambda-1,1} - \sqrt{\lambda}\, j_{\lambda+1} \vec{Y}^\mu_{\lambda,\lambda+1,1}), \tag{A.5e}$$

$$\vec{\mathcal{M}}_{\lambda\mu} = (\lambda(\lambda+1))^{-\frac{1}{2}} \vec{L}\phi_{\lambda\mu} = i^\lambda \sqrt{4\pi(2\lambda+1)}\, j_\lambda\, \vec{Y}^\mu_{\lambda\lambda 1} \tag{A.5f}$$

where the direction of the z-axis is along $\vec{k}$, and a and $b_{\pm 1}$ are arbitrary c-numbers. $\vec{\mathcal{L}}_{\lambda\mu}$, $\vec{\mathcal{E}}_{\lambda\mu}$, $\vec{\mathcal{M}}_{\lambda\mu}$ are respectively the longitudinal and transverse electric, and magnetic multipoles. Note that by setting the gauge field Λ in (A.1) to be $\frac{ia}{k}\phi e^{+i\omega t}$, we reduce the gauge transformed ϕ' and $\vec{\mathcal{L}}'$ to zero. Only $\vec{\mathcal{E}}'$ and $\vec{\mathcal{M}}'$ are left, resulting in a two-component field

perpendicular to k. To see this differently we let the field interact with current $J_\nu(r) = J_\nu(\vec{r})e^{i\omega t}$. We get

$$A_\nu J^\nu d^4r = \frac{1}{c}\int \vec{\mathcal{A}}\cdot\vec{J}\, d^4r - \int \phi\rho\, d^4r + (\vec{\xi} \text{ and } \vec{\mathcal{H}} \text{ terms})$$

$$= -\frac{1}{i\omega}\int \phi\vec{\nabla}\cdot\vec{J}\, d^4r + \int \phi\rho\, d^4r + \cdots . \qquad (A.6)$$

From the equations of continuity, and (A.4), we have

$$\nabla\cdot J = -\frac{\partial\rho}{\partial t} = -i\omega\rho. \qquad (A.2')$$

Therefore the first two terms in (A.6) cancel. In other words, due to charge conservation, only the $\vec{\mathcal{E}}$ and $\vec{\mathcal{H}}$ fields are felt by the current.

To proceed further, we expand the fields in powers of kr. Note that since the nucleus is finite $\langle(kr)^n\rangle \lesssim k^n R^n$, where R is the nuclear radius. So for long wave-length photons, $\frac{1}{k} \ll R$, this expansion is meaningful. We keep only the lowest order term. Then

$$\vec{\mathcal{L}}_{\lambda\mu} = \frac{1}{2}\sqrt{\frac{\lambda}{2\lambda+1}}\ \frac{(kr)^{\lambda-1}}{(2\lambda-1)!!}\ \vec{Y}^{\mu}_{\lambda,\lambda-1,1}\ (1 + O(k^2r^2)), \tag{A.7a}$$

$$\vec{\mathcal{E}}_{\lambda\mu} = -\frac{1}{2}\sqrt{\frac{\lambda+1}{2\lambda+1}}\ \frac{(kr)^{\lambda-1}}{(2\lambda-1)!!}\ \vec{Y}^{\mu}_{\lambda,\lambda-1,1}(1 + O(k^2r^2)). \tag{A.7b}$$

Thus, to lowest order

$$\vec{\mathcal{E}}_{\lambda\mu} \approx -\sqrt{\frac{\lambda+1}{\lambda}}\vec{\mathcal{L}}_{\lambda\mu}. \tag{A.8}$$

Using the equations of continuity again, we have

$$\frac{1}{c}\int \vec{\mathcal{E}}_{\lambda\mu}\cdot\vec{J}\ d^3r \approx \sqrt{\frac{\lambda+1}{\lambda}}\ \int \phi_{\lambda\mu}\rho\ d^3r. \tag{A.9}$$

The above relation which states that in the long wave length limit a knowledge of the charge density of matter alone is sufficient to describe the interaction between the matter and the electric potential, is generally referred to as "Siegert's theorem"[2]. The RHS of (A.9) is obviously easier to compute than the LHS. Conceptually it is also easier to grasp, as it is related to static properties of the nucleus.

It should be stressed that in actual calculations, (A.9) will be realized only if (A.2) is explicitly satisfied. For example (A.9) will not be

realized when $\vec{J}^{exch}$ is non-vanishing and not included in $\vec{J}$. Therefore it is always advantageous to use the RHS of (A.9) whenever possible, since unlike (the $\vec{J}^{exch}$ term in) $\vec{J}$ the charge density is known. One of the prescriptions that will guarantee gauge invariance and charge conservation is to replace the operator $\frac{\hbar}{i}\vec{\nabla}$ in (3) by the cannonical momentum operator $[H,\vec{r}]$. This will include in $\vec{J}$ the exchange current due to the explicit dependence of the interaction on momentum. There are other more subtle reasons for the breakdown of (A.2). For example, truncating the basis in a shell model calculation is equivalent to making the two-body interaction effectively momentum-dependent, even if it is not explicitly so. This part of the $\vec{J}^{exch}$ can be either eliminated (or reduced) by enlarging the basis[10] or it can be calculated by perturbation theory. In the literature the latter procedure is referred to as "renormalization" of the density operators[11,4,12].

There is no equivalent of Siegert's theorem for the magnetic interaction $\int \vec{m}_{\lambda\mu}\cdot\vec{J}\, d^4r$. Although the contributions from the magnetization current of (4) almost always dominates this interaction, in some cases[3] the contributions of the exchange current are known to be important.

Siegert's theorem can be generalized so that for the electric interactions explicit reference to the current is deleted for all photon energies. Sachs and Austern[13] used gauge invariance and Foldy[14] used the conservation of charge to achieve this goal. The end results of these two approaches are equivalent but not identical. Essentially they involve different series expansions of the interactions in powers of the photon energy $\hbar\omega$. In both cases the expansions can be identified with the usual multipole expansion only in the long wave-length limit.

The equation of continuity, (A.2), can be expressed in terms of multipole densities. For the Fourier component $J_\nu(r) = J_\nu(\vec{r})e^{i\omega t}$, we have, from (A.2) and (11,12),

$$k\rho_\lambda(r) + \sqrt{\frac{\lambda+1}{2\lambda+1}}\left(\frac{d}{dr} + \frac{\lambda+2}{r}\right)\rho_{\lambda,\lambda+1}(r) + \sqrt{\frac{\lambda}{2\lambda+1}}\left(\frac{d}{dr} - \frac{\lambda-1}{r}\right)\rho_{\lambda,\lambda-1}(r)=0 \qquad (A.2')$$

where $k = \omega/c$.

A.2 GAMMA-EMISSION

The rates of transition from $|\Psi_i\rangle$ to $|\Psi_f\rangle$, or the numbers of photons of energy $\hbar\omega$ emitted per second, are[15)]

$$T^E_{\lambda\mu} = \frac{2k}{\hbar(2\lambda+1)} \left| \int \vec{\mathcal{E}}_{\lambda\mu} \cdot \frac{\vec{J}}{c} \, d^3r \right|^2 \qquad \text{(A.10a)}$$

and

$$T^M_{\lambda\mu} = \frac{2k}{\hbar(2\lambda+1)} \left| \int \vec{\mathcal{M}}_{\lambda\mu} \cdot \frac{\vec{J}}{c} \, d^3r \right|^2 \qquad \text{(A.10b)}$$

respectively due to electric and magnetic λ-pole γ-transitions. Using Siegert's theorem and (11)

$$T^E_{\lambda\mu} = 8\pi e^2 \, (C^f_{i,\lambda\mu})^2 \, \frac{(\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \, \frac{k^{2\lambda+1}}{\hbar} \left(\int_0^\infty r^{\lambda+2} \, \rho_\lambda(r) dr \right)^2 \qquad \text{(A.11a)}$$

in the long wave-length limit. Here $C^f_{i,\lambda\mu} = \langle J_i M_i \lambda\mu | J_f M_f \rangle$. We may also use the current given by (12), in which case

$$T^E_{\lambda\mu} = \frac{8\pi k e^2}{\hbar} \, \frac{1}{2\lambda+1} \, (C^f_{i,\lambda\mu})^2 \left\{ \int_0^\infty r^2 dr \sqrt{\lambda+1} \; j_{\lambda-1}(kr) \rho_{\lambda,\lambda-1}(r) + \sqrt{\lambda} \; j_{\lambda+1}(kr) \rho_{\lambda,\lambda+1}(r) \right\}^2 . \qquad \text{(A.11b)}$$

Similarly

$$T^M_{\lambda\mu} = \frac{8\pi k e^2}{\hbar} \, (C^f_{i,\lambda\mu})^2 \left(\int_0^\infty r^2 dr j_\lambda(kr) \rho_{\lambda\lambda}(r) \right)^2 \qquad \text{(A.11c)}$$

In the long wave-length limit, a condition invariably satisfied in nuclear γ-transitions, we may again expand the spherical Bessel functions and keep the terms lowest order in k. Summing over M_f and μ and averaging over M_i, we define

$$T(\begin{matrix}E\\M\end{matrix}\lambda;i\to f) \equiv \frac{1}{2J_i+1} \sum_{m_i,m_f,\mu} T^{E,M}_{\lambda\mu}(i\to f)$$

$$\equiv \frac{8\pi(\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \frac{k^{2\lambda+1}}{\hbar} B(\begin{matrix}E\\M\end{matrix}\lambda;i\to f). \qquad (A.12)$$

B is called the transition strength. From (A.11)

$$B(E\lambda;i\to f) = e^2 \frac{2J_f+1}{2J_i+1} \left(\int r^{\lambda+2} \rho_\lambda^{i\to f}(r)dr\right)^2, \qquad (A.13a)$$

$$= e^2 \frac{2J_f+1}{2J_i+1} \frac{(2\lambda+1)\lambda}{k^2} \left(\int r^{\lambda+1} \rho^{i\to f}_{\lambda,\lambda-1}(r)dr\right)^2, \qquad (A.13b)$$

$$B(M\lambda;i\to f) = e^2 \frac{2J_f+1}{2J_i+1} \frac{\lambda}{\lambda+1} \left(\int r^{\lambda+2} \rho^{i\to f}_{\lambda\lambda}(r)dr\right)^2. \qquad (A.13c)$$

The strengths are simply moments of the appropriate transition densities. The dimensionality of B(λ) is $e^2L^{2\lambda}$. Note that the RHS of (A.13b) depends explicitly on the photon energy, whereas the expression in (A.13a) does not. This is a reflection of the continuity

equation, which must be satisfied if the equality of (A.13a) and (A.13b) is to be realized. In the literature (A.13a) is invariably used, as its evaluation requires no explicit statement being made of the current.

As for the evaluation of all operators involving the gradient operator, different expressions can be obtained by integrating by parts. We shall use this technique to derive a more familiar expression for B(Mλ). From (20) and (27) (second line) we have

$$\sqrt{\frac{\lambda}{\lambda+1}}\int r^{\lambda+2}\,\rho^{i\to f}_{\lambda\lambda}(r)\,dr$$

$$= \frac{\hbar}{2Mc}\sqrt{\frac{\lambda}{\lambda+1}}\,i^{\lambda}\,\langle\Psi_f\|-2ig_L r^{\lambda}\vec{Y}_{\lambda\lambda 1}\cdot\vec{\nabla}+\mu_s(\vec{\nabla}\times r^{\lambda}\vec{Y}_{\lambda\lambda 1})\cdot\vec{\sigma}\|\Psi_i\rangle. \qquad (A.14)$$

Using the identities†

$$r^{\lambda}\vec{Y}^{\mu}_{\lambda\lambda 1}\cdot\vec{\nabla} = -\sqrt{\frac{1}{\lambda(\lambda+1)}}\;\vec{\nabla}\left(r^{\lambda}Y^{\mu}_{\lambda}\right)\cdot\vec{L},$$

and

$$\vec{\nabla}\times(r^{\lambda}\,\vec{Y}^{\mu}_{\lambda\lambda 1}) = i\sqrt{\frac{\lambda+1}{\lambda}}\;\vec{\nabla}(r^{\lambda}\,Y^{\mu}_{\lambda})$$

we have

$$\sqrt{\frac{\lambda}{\lambda+1}}\int r^{\lambda+2}\rho^{i\to f}_{\lambda\lambda}(r)\,dr = \langle\Psi_f\|\frac{\hbar}{2Mc}\,i^{1+\lambda}\{\frac{2g_L}{\lambda+1}\,\vec{\nabla}(r^{\lambda}Y_{\lambda})\cdot\vec{L}+\mu_s\,\vec{\nabla}(r^{\lambda}y_{\lambda})\cdot\vec{\sigma}\}\|\Psi_i\rangle. \qquad (A.15)$$

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† *The following identities are more general:*

$$\vec{\mathcal{M}}_{\lambda\mu}\cdot\vec{\nabla}/i = -\frac{k}{\sqrt{\lambda(\lambda+1)}}\,\vec{\mathcal{L}}_{\lambda\mu}\cdot\vec{L};\quad\langle\vec{\mathcal{M}}_{\lambda\mu}\cdot(\vec{\nabla}\times\vec{\sigma})\rangle = k\langle\vec{\mathcal{L}}_{\lambda\mu}\cdot\vec{\sigma}\rangle$$

The operators on the RHS are the usual *effective* magnetic λ-pole operators due to charge and spin respectively. The evaluation of the complete matrix element can be found in the literature[6]. However, we may also separate the angular and radial integrations and thereby define the appropriate densities. Using the identity

$$\vec{\nabla}(r^{\lambda}Y^{\mu}_{\lambda}) = \sqrt{\lambda(2\lambda+1)}\; r^{\lambda-1}\; \vec{Y}^{\mu}_{\lambda,\lambda-1,1}$$

and defining the orbital and intrinsic spin densities

$$\rho^{L,i\to f}_{\lambda\ell} = \frac{\hbar}{Mc}\;\frac{1}{\sqrt{\lambda(\lambda+1)}}\;(\Psi_f\|\, i^{\ell} g_L\; \vec{Y}_{\lambda\ell 1}\cdot\vec{L}\|\Psi_i) \qquad (A.16)$$

$$\rho^{S,i\to f}_{\lambda\ell} = \frac{\hbar}{2Mc}\;(\Psi_f\|\, i^{\ell}\; \mu_s\; \vec{Y}_{\lambda\ell 1}\cdot\vec{\sigma}\|\Psi_i), \qquad (A.17)$$

we have

$$B(M\lambda;i\to f) = e^2\;\frac{2J_f+1}{2J_i+1}\;\frac{\lambda}{\lambda+1}\;(2\lambda+1)\Big\{\int_0^{\infty} r^{\lambda+1}(\sqrt{\lambda}\;\rho^{L,i\to f}_{\lambda,\lambda-1} + \sqrt{\lambda+1}\;\rho^{S,i\to f}_{\lambda,\lambda-1})dr\Big\}^2. \qquad (A.13d)$$

We use (9) to evaluate the partially reduced matrix elements. We give the relevant single-particle matrix elements

$$(a\|\, i^{l+\lambda}\vec{Y}_{\lambda\ell 1}\cdot\vec{L}\|\, b) = (-)^{j_a+\ell_b-\lambda-\frac{1}{2}}\;\hat{j}_b\hat{\ell}_a\; W(\ell_a\ell_b j_a j_b;\lambda\tfrac{1}{2})\,(\ell_a\|\, i^{l+\lambda}\vec{Y}_{\lambda\ell 1}\cdot\vec{L}\|\,\ell_b) \qquad (A.18a)$$

$$(\ell_a\|\, i^{1+\lambda}Y_{\lambda\ell 1}\cdot L\|\,\ell_b) = (-)^{\ell+\lambda+\ell_a}\; i^{\ell_b+1+\lambda-\ell_a}\;\Big(\frac{\ell_b(\ell_b+1)}{4\pi}\Big)^{\frac{1}{2}}\;\hat{\ell}\hat{\lambda}(2\ell_b+1)$$

$$\times\; W(\ell_b 1\ell_a\ell;\ell_b\lambda)\begin{pmatrix}\ell_a & \ell & \ell_b\\ 0 & 0 & 0\end{pmatrix} u^{*}_a(r)\; u_b(r) \qquad (A.18b)$$

$$(a\| i^{l+\lambda} \vec{Y}_{\lambda,\lambda\pm1,1}\cdot\vec{\sigma}\| b) = (-)^{\ell_a+\ell_b+j_b+\frac{1}{2}}\, i^{\ell_b+1+\lambda-\ell_a}\, \hat{j}_b \begin{pmatrix} j_a & j_b & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$$

$$\times (x_a+x_b)^{\lambda+1}_{-\lambda}(4\pi^{(\lambda+1)}_{\lambda})^{-\frac{1}{2}}\, u_a^*(r)u_b(r); \qquad \underline{\ell_a+\ell_b+\lambda \text{ odd}}, \tag{A.19a}$$

and

$$(a\| i^{\lambda} \vec{Y}_{\lambda\lambda 1}\cdot\vec{\sigma}\| b) = -(-)^{j_b+\lambda-\frac{1}{2}}\, i^{\ell_b+\lambda-\ell_a}\, \hat{j}_b\hat{\lambda} \begin{pmatrix} j_a & j_b & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$$

$$\times (x_a-x_b)(4\pi\lambda(\lambda+1))^{-\frac{1}{2}}\, u_a^*(r)u_b(r); \qquad \underline{\ell_a+\ell_b+\lambda \quad \text{even}}. \tag{A.19b}$$

In the literature, the transition strength is often expressed in terms of the so-called Weisskopf units[15] (WU). This unit represents a rough estimate of the single-particle strength of a proton in transition and is given as follows:

$$B_{WU}(E\lambda) = \frac{(1.2)^{2\lambda}}{4\pi}\left(\frac{3}{\lambda+3}\right)^2 A^{2\lambda/3}(e^2F^{2\lambda}),$$

$$B_{WU}(M\lambda) = \frac{0.11(1.2)^{2\lambda-2}}{\pi}\left(\frac{3}{\lambda+3}\right)^2 A^{(2\lambda-2)/3}\,(e^2F^{2\lambda}),$$

$$= \frac{10(1.2)^{2\lambda-2}}{\pi}\left(\frac{3}{\lambda+3}\right)A^{(2\lambda-2)/3}\,\mu_n^{\,2}\,F^{2\lambda-2},$$

where $\mu_n = \frac{\hbar e}{2Mc} = 0.105$ eF is the nuclear magneton. A is the atomic mass number of the nucleus. The Weisskopf

unit strengths, in units of $e^2F^{2\lambda}$, for Eλ and Mλ transitions, are respectively plotted in Fig. A.1 and A.2, as functions of A.

Experimental data on transitions are also expressed in terms of the (partial) width, $\Gamma(\lambda) = \hbar T(\lambda)$ and the associated lifetime $\tau(\lambda) = T(\lambda)^{-1}$. $T(\lambda)$ is the rate of transition given in (A.12). We may define the kinematic coefficients $t(\lambda)$ and $c(\lambda)$,

$$\tau(\lambda;i\to f)^{-1} = t(\lambda)\cdot E_\gamma^{2\lambda+1}\cdot B(\lambda;i\to f),$$

$$\Gamma(\lambda;i\to f)^{-1} = C(\lambda)\, E_\gamma^{2\lambda+1}\cdot B(\lambda;i\to f),$$

where $E_\gamma = \hbar ck$ is the transition energy. From (A.12)

$$C(\lambda)\hbar = t(\lambda) = \frac{8\pi(\lambda+1)}{\lambda[(2\lambda+1)!!]^2}\ \frac{c}{(\hbar c)^{2\lambda+1}}\ \left(\frac{e^2}{\hbar c}\right), \text{ if } B(\lambda) \text{ in } e^2F^{2\lambda}$$

$$= \frac{8\pi(\lambda+1)}{\lambda[(2\lambda+1)!!]^2}\ \frac{c}{(\hbar c)^{2\lambda+1}}\ \left(\frac{e^2}{\hbar c}\right)\left(\frac{\hbar}{2Mc}\right)^2 \text{ if } B(\lambda) \text{ in } \mu^2F^{2\lambda-2}.$$

In table A.1, the values for $t(\lambda)$ and $c(\lambda)$ for λ=1 to 5 are listed, with τ in units of psec (10^{-12}sec), Γ in units of eV, and E_γ in units of MeV.

TABLE A.1. VALUES FOR COEFFICIENTS $t(\lambda)$ AND $C(\lambda)$

	$B(\lambda)$ in $e^2F^{2\lambda}$		$B(\lambda)$ in $\mu_n{}^2F^{2\lambda-2}$	
λ	$t(\lambda)$	$C(\lambda)$	$t(\lambda)$	$C(\lambda)$
1	1.60(3)*	1.05	1.76(1)	1.16(-2)
2	1.23(-3)	8.08(-7)	1.36(-5)	8.94(-9)
3	5.72(-10)	3.76(-13)	6.33(-12)	4.16(-15)
4	1.70(-16)	1.12(-19)	1.88(-18)	1.24(-21)
5	3.46(-23)	2.28(-26)	3.83(-25)	2.52(-28)

* *The number in the bracket is the exponent of 10, i.e.* $1.60(3) = 1.60 \times 10^3$.

A.3 ELECTRON SCATTERING

We shall express all momenta and energies in terms of wave numbers, in units of inverse length. The following notations will be used,

$\vec{p}_i; \vec{p}_f$, momenta of the incident and scattered electrons, respectively;

$\varepsilon_i, \varepsilon_f$, initial and final electron energy;

$\vec{q} \equiv \vec{p}_i - \vec{p}_f$, momentum transferred to the nucleus;

$\kappa = \varepsilon_i - \varepsilon_f$, energy transferred to the nucleus;

$\vec{P} \equiv \frac{1}{2}(\vec{p}_i + \vec{p}_f)$,

and

$q_\mu^2 \equiv q^2 - \kappa^2$.

The EM potential which interacts with the nucleus is generated by the electron in motion. We use (A.3) and write $J_\nu^{(e)}$ as

$$J_\nu^{(e)} = e\, \bar{\psi}_f\, \gamma_\nu \psi_i ,$$

where ψ is the electron wavefunction, and γ_ν is the Dirac matrix. From (A.3), (A.4), and integrating the time out, we get the time-independent 4-vector potential

$$\delta(\varepsilon_i - \varepsilon_f - k) A_\nu(\vec{r}) = -e\delta(\varepsilon_i - \varepsilon_f - k) \int d^3r'\, \bar{\psi}_f(\vec{r}')\gamma_\nu \psi_i(\vec{r}')\, \frac{e^{ikR}}{R} . \qquad \text{(A.20)}$$

$R = |r - r'|$. The interaction matrix element, to lowest order, is

$$\langle H_{int} \rangle = \int d^3r \, A_\nu(\vec{r}) \, J^\nu(\vec{r}), \tag{A.21}$$

where $J_\nu(r)$ is the nuclear current. The differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar} \, |\langle H_{int} \rangle|^2 \, \frac{\rho_f}{j_e} \tag{A.22}$$

where ρ_f is the final density of state. Including the nuclear recoil correction

$$\rho_f = \frac{1}{1 + \frac{2\epsilon_f}{M_T} \sin^2 \frac{\theta}{2}} \quad \frac{p_f \epsilon_f}{(2\pi)^3 \hbar c}$$

where θ is the scattering angle in the laboratory frame and M_T is the nuclear mass. j_e is the incident electron flux

$$j_e = c \, p_i / \epsilon_i .$$

(The expression for ρ_f and j_e implies that the electron wavefunctions are normalized in a sphere of unit volume.) Putting everything together, we have

$$\frac{d\sigma}{d\Omega} = \frac{\epsilon_i \epsilon_f p_f}{(2\pi)^2 (\hbar c)^2 p_i} \quad \frac{1}{1 + (2\epsilon_f \sin^2 \frac{\theta}{2})/M_T} \, |\langle H_{int} \rangle|^2 . \tag{A.23}$$

Only $\langle H_{int} \rangle$ remains to be calculated.

In the plane wave Born approximation, $\bar{\psi}_f(\vec{r}')\psi_i(\vec{r}')$ is proportional to $e^{-i\vec{q}\cdot\vec{r}'}$. Using this property and the relation

$$(\nabla^2_{r'} + k^2)\,\frac{e^{ikR}}{R} = -\delta(\vec{r}'-\vec{r}),$$

and by integrating by parts, we have

$$\langle H_{int}\rangle_{PWBA} = \frac{e}{q_\mu^2}\int \bar{\psi}_f(\vec{r})\gamma_\nu J^\nu(\vec{r})\psi_i(\vec{r})d^3r. \qquad (A.24)$$

The evaluation of the matrix element is straightforward but somewhat tedious; we only give the result for the cross section averaged over initial and summed over final spin projection[16],

$$\frac{d\sigma}{d\Omega} = \frac{\epsilon_i\epsilon_f p_f}{(2\pi)^2(\hbar c)^2 p_i}\,\frac{1}{1+2\epsilon_f/M_T\sin^2\frac{2\theta}{2}}\,\frac{1}{2(2J_i+1)}\sum_{M's}|\langle H_{int}\rangle|^2_{PWBA}$$

$$= \frac{Z^2\alpha^2}{q_\mu^4}\,\frac{p_f}{p_i}\,\frac{2}{1+2\,\epsilon_f/M_T\sin^2\frac{\theta}{2}}\cdot\{V_L(\theta)\sum_{\lambda=0}|F^C_\lambda(q^2)|^2$$

$$+ V_T(\theta)\sum_{\lambda=1}(|F^M_\lambda(q^2)|^2 + |F^E_\lambda(q^2)|^2\} \qquad (A.25)$$

where

$$V_L(\theta) = \frac{1}{2}\frac{q_\mu^4}{q^4}\left[(\varepsilon_i+\varepsilon_f)^2 - q^2\right] \tag{A.26a}$$

$$V_T(\theta) = P^2 - \left(\frac{\vec{P}\cdot\vec{q}}{q}\right)^2 + \frac{1}{2}q_\mu^2. \tag{A.26b}$$

The Coulomb, electric and magnetic form factors, F^C, F^E and F^M, are given by

$$Z\frac{\hat{J}_i\hat{\lambda}}{\hat{J}_f}F_\lambda^C(q^2) = \frac{1}{e}\langle\Psi_f\|\Phi_\lambda\rho_{op}\|\Psi_i\rangle = \sqrt{4\pi}\,\hat{\lambda}\int\rho_{\lambda,\lambda}(r)j_\lambda(qr)r^2dr \tag{A.27a}$$

$$Z\frac{\hat{J}_i\hat{\lambda}}{\hat{J}_f}F_\lambda^E(q^2) = \frac{1}{ec}\langle\Psi_f\|\vec{\mathcal{E}}_\lambda\cdot\vec{J}_{op}\|\Psi_i\rangle$$

$$= \sqrt{4\pi}\int\{\sqrt{\lambda+1}\,\rho_{\lambda,\lambda-1}(r)j_{\lambda-1}(qr) + \sqrt{\lambda}\,\rho_{\lambda,\lambda+1}(r)j_{\lambda+1}(qr)\}r^2dr \tag{A.27b}$$

$$Z\frac{\hat{J}_i\hat{\lambda}}{\hat{J}_f}F_\lambda^M(q^2) = \frac{1}{ec}\langle\Psi_i\|\vec{\mathcal{M}}_\lambda\cdot J_{op}\|\Psi_i\rangle = \sqrt{4\pi}\,\hat{\lambda}\int\rho_{\lambda\lambda}(r)j_\lambda(qr)r^2dr. \tag{A.27c}$$

The multipole fields $\Phi_{\lambda\mu}$, $\vec{\mathcal{E}}_{\lambda\mu}$ and $\vec{\mathcal{M}}_{\lambda\mu}$ are those defined in (A.5) (with k replaced by q) and ρ_λ and $\rho_{\lambda\ell}$ are the nuclear transition densitis defined in Section 2.

When the momentum transfer is small, $qR \lesssim 1$, where R is the nuclear size, we may use Siegert's theorem, resulting in

$$F_\lambda^E(q^2) \approx \frac{k}{q}\sqrt{\frac{\lambda+1}{\lambda}}\,F_\lambda^C(q^2).$$

we have the extra factor k/q which is not equal to unity because in general the exchanged photon will be off the mass-shell.

As in our discussion of the B(Mλ) strength, the orbital and spin densities, defined in (A.16) and (A.17), can be used to compute the magnetic form factor. Thus (see footnote on p.49)

$$\frac{1}{c\epsilon}\langle\psi_f\|\vec{\mathcal{M}}_\lambda\cdot\vec{J}_{op}\|\psi_i\rangle = -\frac{\hbar q}{2Mc}\langle\psi_f\|2q_L\vec{\mathcal{L}}_{\lambda\mu}\cdot\frac{\vec{L}}{\sqrt{\lambda(\lambda+1)}}-\mu_s\vec{\mathcal{E}}_{\lambda\mu}\cdot\vec{\sigma}\|\psi_i\rangle$$

$$=-\sqrt{4\pi}\,q\int[(\sqrt{\lambda}\,\rho^L_{\lambda,\lambda-1}+\sqrt{\lambda+1}\,\rho^s_{\lambda,\lambda-1})j_{\lambda-1}(qr)-(\sqrt{\lambda+1}\,\rho^L_{\lambda,\lambda+1}-\sqrt{\lambda}\,\rho^S_{\lambda,\lambda+1})j_{\lambda+1}(qr)]r^2dr. \qquad \text{(A.27c')}$$

Clearly the LHS of (A.27c) has a simpler appearance. It should also be pointed out that (A.27c) is formally correct for the complete current (including $\vec{J}^{exch}$) density whereas (A.27c') is specialized for $\vec{J}^c$ and $\vec{J}^m$ only. In general the advantage ρ^L and ρ^S have over ρ^c and ρ^m is that the former do not involve the derivative of the nuclear wavefunction. When q is small compared to the nuclear size, only the first two terms on the RHS of (A.27c') need be retained, since $|j_{\lambda+1}(qr)/j_{\lambda-1}(qr)| << 1$. In this case, just as in the case of static Mλ transitions in the long wave-length limit, it is more advantageous to use the orbital and intrinsic spin densities. This is especially so for M1, since $\rho^{L,S}_{1,0}$ are quite simple to calculate.

When the charge of the target is large, or more specifically, when the Coulomb potential energy of the scattered electron is not negligible compared to its kinetic energy, distortions of the incoming and outgoing electron waves must be considered. In this case, the condition leading to the simplified expression of (A.24) is no longer satisfied, and partial wave expansions for both the initial and final electron waves must be carried out.

Although the expression for the (e,e') cross section in the distorted wave Born approximation (DWBA) exist in the literature[17], the derivation is often less than transparent and the end result incomplete. We shall therefore present a complete derivation of the formulas here. Readers who are only interested in the end result shall find them in (A.41) and (A.45).

We shall use the abbreviated notations $\int = \int d^3r'd^3r$, $C^{j_c}_{j_a j_b} = C^{j_c m_c}_{j_a j_b} = \langle j_a m_a j_b m_b | j_c m_c \rangle$, and $\vec{Y}^{\mu}_{\lambda\pm} \equiv \vec{Y}^{\mu}_{\lambda,\lambda\pm1,1}$ and $\vec{Y}^{\mu}_{\lambda} \equiv \vec{Y}^{\mu}_{\lambda\lambda1}$.

We start from (A.20) and (A.21). Using an explicit representation of the Dirac matrices, and expanding[9] out the Green's function, we have

$$H_{int} = -e\int \psi_f^+(\vec{r}')(\rho(\vec{r})-\vec{\alpha}\cdot\vec{J}(\vec{r})/c)\psi_i(\vec{r})\, e^{ikR}/R$$

$$= -4\pi ek \sum_{\lambda=0,\mu} \int \psi_f^+(\rho-\vec{\alpha}\cdot\frac{\vec{J}}{c})\psi_i \; j_\lambda(kr_<)h_\lambda^{(1)}(kr_>)Y_\lambda^{*\mu}(\hat{r}')Y_\lambda^{\mu}(\hat{r}), \qquad (A.28)$$

where $r_<$ ($r_>$) is the smaller (larger) of r' and r, and $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$ is an operator in the electron Hilbert space only. In the following we shall use the abbreviation

$$h_\lambda(r')h_\lambda(r) = j_\lambda(kr_<)h_\lambda^{(1)}(kr_>).$$

For any vectors A and B, we have the identities

$$\sum_{\ell=0}\sum_{m} \vec{A}(\vec{r}')\cdot\vec{B}(\vec{r})Y_\ell^{m*}(\hat{r}')Y_\ell^{m}(\hat{r})h_\ell(r')h_\ell(r)$$

$$= \sum_{\ell=0}\sum_{m,\nu} (-)^\nu (\vec{A}\cdot\hat{\varepsilon}_{-\nu}Y_\ell^{m*}h_\ell)(\vec{B}\cdot\hat{\varepsilon}_\nu Y_\ell^m h_\ell)$$

$$= \sum_{\lambda,\mu}\sum_{\ell=\lambda,\lambda\pm1} \vec{A}\cdot\vec{Y}_{\lambda\ell 1}^{\mu *}(\hat{r}')h_\ell(r')\, h_\ell(r)\, \vec{Y}_{\lambda\ell 1}^{\mu}(\hat{r})\cdot\vec{B} \qquad (A.29a)$$

$$= \sum_{\lambda\mu} \frac{1}{4\pi(2\lambda+1)} \vec{A}\cdot\{\vec{\mathcal{L}}_{\lambda\mu}^*(\hat{r}')\vec{\mathcal{L}}_{\lambda\mu}(\hat{r}) + \vec{\mathcal{E}}_{\lambda\mu}^*(r')\vec{\mathcal{E}}_{\lambda\mu}(r) + \vec{\mathcal{M}}_{\lambda\mu}^*(\hat{r}')\vec{\mathcal{M}}_{\lambda\mu}(\hat{r})\}\cdot\vec{B} \qquad (A.29b)$$

where $\hat{\varepsilon}_{\pm1}$, $\hat{\varepsilon}_0$ are the spherical unit vectors and $\vec{\mathcal{L}}$, $\vec{\mathcal{E}}$, $\vec{\mathcal{M}}$ are the spherical vector tensors defined in (A.5), with j_ℓ replaced by h_ℓ (i.e., $j_\ell(kr_<)$ or $h_\ell^{(1)}(kr_>)$). In the summation over λ, λ starts from 0 for $\vec{\mathcal{L}}$, and from 1 for $\vec{\mathcal{E}}$ and $\vec{\mathcal{M}}$. The reason

for having the two expansions (A.29a) and (A.29b) will be made clear later. Briefly the former will lead to a simpler expression whereas only the latter will allow us to make explicit and easy use of the equation of continuity. Putting (A.29) into (A.28), we have

$$\langle H_{int} \rangle = -4\pi iek \left\{ \int \sum_{\lambda\mu} h_\lambda h_\lambda \, (\psi_f^\dagger (-i)^\lambda Y_\lambda^{*\mu} \psi_i)(\rho \, i^\lambda Y_\lambda^\mu) \right.$$

$$\left. - \sum_{\lambda \ell \mu} h_\ell h_\ell (\psi_f^\dagger (-i)^\ell \, \vec{\alpha} \cdot Y_{\lambda\ell 1}^{*\mu} \psi_i)(i^\ell \, \vec{Y}_{\lambda\ell 1}^\mu \cdot \vec{J}/c) \right\} . \qquad (A.30)$$

We shall do the angular integration for the RHS of (A.30) first. From the definition of the nuclear charge and current densities, (11) and (12), we immediately have

$$\int \rho \, i^\lambda y_\lambda^\mu \, d\Omega_r = e \, C^f_{i,\lambda\mu} \, \rho_\lambda(r),$$

$$\int i^\ell \vec{Y}_{\lambda\ell 1}^\mu \cdot \vec{J}/c \, d\Omega_r = e \, C^f_{i,\lambda\mu} \, \rho_{\lambda\ell}(r). \qquad (A.31)$$

To do the same for the electron part we need explicit expressions for the electron wavefunctions. We follow the notation of Rose[18], and write for the incoming and outgoing functions

$$\psi^{(\pm)\sigma}_{(\vec{p},\vec{r})} = \frac{4\pi}{\sqrt{2}} \sum_{\kappa,m,j} e^{\pm i\delta_\kappa} i^\ell C^{j\nu}_{\ell m \frac{1}{2}\sigma} Y^{m*}_\ell(\hat{p}) \psi^\nu_\kappa(\vec{r}) \tag{A.32a}$$

where δ_κ is the phase-shift, σ is the spin projection, and ψ^ν_κ is a two-component wavefunction,

$$\psi^\nu_\kappa(\vec{r}) = \begin{pmatrix} g_\kappa(r)\phi^\nu_\kappa(\hat{r}) \\ \\ if_\kappa(r)\ \phi^\nu_{-\kappa}(r) \end{pmatrix} \tag{A.32b}$$

$$\phi^\nu_\kappa(\hat{r}) = \sum_{m,\sigma} C^{j_\kappa \nu}_{\ell_\kappa m,\frac{1}{2}\sigma} Y^m_{\ell_\kappa}(\hat{r})\ \chi^\sigma_{\frac{1}{2}} \tag{A.32c}$$

with $j_\kappa = |\kappa| - \frac{1}{2}$, and $\ell_\kappa = \kappa$, if $\kappa > 0$ and $\ell_\kappa = -\kappa - 1$, if $\kappa < 0$. The radial wavefunctions g and f are solutions of the coupled radial Dirac equations[18] and are functions of the electron energy and the nuclear charge distribution:

$$\frac{dg_\kappa}{dr} = (E+m_e-V)f_\kappa - \frac{\kappa+1}{r} g_\kappa \tag{A.32d}$$

$$\frac{df_\kappa}{dr} = \frac{\kappa-1}{r} f_\kappa - (E-m_e-V)g_\kappa \tag{A.32e}$$

where $E = \varepsilon_i$ or ε_k and $V(r)$ are the appropriate static Coulomb potential generated by the nucleus. With (A.32), we have, for any tensor operator O_λ^μ

$$(\psi_f^{\sigma'}|O_\lambda^\mu|\psi_i^\sigma) = 8\pi^2 \sum_{\kappa\kappa' mm'} e^{i(\delta_\kappa+\delta_{\kappa'})} i^{\ell-\ell'} C^{j\nu}_{\ell m \frac{1}{2}\sigma} C^{j'\ell'}_{\ell' m' \frac{1}{2}\sigma} Y_\ell^{m*}(\hat{p}_i) Y_{\ell'}^{m'}(\hat{p}_f) (\psi_{\kappa'}^{\nu'}|O_\lambda^\mu|\psi_\kappa^\nu). \tag{A.33}$$

From (A.32b)

$$(\psi_{\kappa'}^{\nu'}|(-i)^\lambda Y_\lambda^{*\mu}|\psi_\kappa^\nu)$$

$$= (-)^{\lambda+\mu} C^{j'\nu'}_{j\nu,\lambda-\mu} \{g_{\kappa'} g_\kappa(\phi_{\kappa'}\|i^\lambda Y_\lambda\|\phi_\kappa) + f_{\kappa'} f_\kappa(\phi_{-\kappa'}\|i^\lambda Y_\lambda\|\phi_{-\kappa})\} \tag{A.34}$$

and

$$(\psi_{\kappa'}^{\nu'}|(-i)^\ell \vec{\alpha}\cdot\vec{Y}^{\mu*}_{\lambda\ell 1}|\psi_\kappa^\nu) = -i(-)^{\lambda+\mu} C^{j'\nu'}_{j\nu\lambda-\mu}$$

$$\times \{g_{\kappa'} f_\kappa(\phi_{\kappa'}\|i^\ell \vec{\sigma}\cdot\vec{Y}_{\lambda\ell 1}\|\phi_{-\kappa}) - f_{\kappa'} g_\kappa(\phi_{-\kappa'}\|i^\ell \vec{\sigma}\cdot\vec{Y}_{\lambda\ell 1}\|\phi_\kappa)\} \tag{A.35}$$

where $j_\kappa = j_\kappa$, $j' = j_{\kappa'}$. From (14), and (A.19)

$$(\phi_{\pm k'}\|i^\lambda Y_\lambda\|\phi_{\pm\kappa}) = (-)^{j-\frac{1}{2}+\lambda} i^\lambda \frac{\hat{\lambda}\hat{j}}{\sqrt{4\pi}} \begin{pmatrix} j' & j & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}, \quad \ell_\kappa+\ell_{\kappa'},+\lambda \text{ or } \ell_{-\kappa}+\ell_{-\kappa'},+\lambda \text{ even}$$

$$= 0 \qquad \text{otherwise.} \tag{A.36}$$

$$(\phi_{\pm\kappa}\|i^\lambda Y_\lambda\|\phi_{\mp\kappa}) = (-)^{j-\frac{1}{2}+\lambda} i^\lambda \frac{-\hat{\lambda}\hat{j}}{\sqrt{4\pi}} \begin{pmatrix} j' & j & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}, \quad \ell_{\kappa'},+\ell_\kappa+\lambda \qquad \text{odd}$$

$$= 0 \qquad \text{otherwise.} \tag{A.37}$$

$$(\phi_{\pm\kappa}, \| i^{\lambda+1} \vec{\sigma}\cdot\vec{Y}_{\lambda+} \| \phi_{\mp\kappa}) = i \frac{\pm(\kappa'-\kappa)+\lambda+1}{\hat{\lambda}\sqrt{\lambda+1}} (\phi_{\kappa}, \| i^{\lambda} Y_{\lambda} \| \phi_{\kappa}) \tag{A.38}$$

$$(\phi_{\pm\kappa}, \| i^{\lambda-1} \vec{\sigma}\cdot\vec{Y}_{\lambda-} \| \phi_{\mp\kappa}) = -i \frac{\pm(\kappa'-\kappa)-\lambda}{\hat{\lambda}\sqrt{\lambda}} (\phi_{\kappa}, \| i^{\lambda} Y_{\lambda} \| \phi_{\kappa}) \tag{A.39}$$

$$(\phi_{\pm\kappa}, \| i^{\lambda} \vec{\sigma}\cdot\vec{Y}_{\lambda} \| \phi_{\mp\kappa'}) = \mp \frac{\kappa'+\kappa}{\sqrt{\lambda(\lambda+1)}} (\phi_{\kappa}, \| i^{\lambda} Y_{\lambda} \| \phi_{-\kappa}) \tag{A.40}$$

Putting (A.33 - 40) into (A.30a), we get

$$\langle H_{int} \rangle_{DWBA} = -i32\pi^2 e^2 k \sum_{\substack{\lambda\mu\kappa \\ \kappa' m m'}} C^{f}_{i,\lambda_f} e^{i(\delta_\kappa+\delta_{\kappa'})} i^{\ell-\ell'+\lambda} (-)^{j-\frac{1}{2}+\mu} \frac{\hat{\lambda}\hat{j}}{\sqrt{4\pi}} \begin{pmatrix} j' & j & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$$

$$\times C^{j\nu}_{\ell m \frac{1}{2}\sigma} C^{j'\nu'}_{\ell' m' \frac{1}{2}\sigma} C^{j'\nu'}_{j\nu,\lambda-\mu} Y^{m*}_{\ell}(\hat{p}_i) Y^{m'}_{\ell'}(\hat{p}_f)$$

$$\times \int \Big\{ j_\lambda(kr_<) h^{(1)}_\lambda(kr_>) (T^{S}_{\kappa'\kappa\lambda} - i\, T^{M}_{\kappa'\kappa\lambda})$$

$$- \sum_{\ell=\lambda\pm1} j_\ell(kr_<) h^{(1)}_\ell(kr_>) T^{EL}_{\kappa'\kappa\lambda\ell} \Big\} r'^2 dr' r^2 dr \tag{A.41a}$$

where

$$T^{S}_{\kappa'\kappa\lambda} = G^{+}_{\kappa'\kappa}(r') \rho_{\lambda}(r) \tag{A.41b}$$

$$T^{EL}_{\kappa'\kappa\lambda,\lambda-1} = \frac{1}{\hat{\lambda}\sqrt{\lambda}} (\lambda F^{-}_{\kappa'\kappa}(r') - (\kappa'-\kappa) F^{+}_{\kappa'\kappa}(r')) \rho_{\lambda,\lambda-1}(r) \tag{A.41c}$$

$$T^{EL}_{\kappa'\kappa\lambda,\lambda+1} = \frac{1}{\hat{\lambda}\sqrt{\lambda+1}} ((\lambda+1) F^{-}_{\kappa'\kappa}(r') + (\kappa'-\kappa) F^{+}_{\kappa'\kappa}(r')) \rho_{\lambda,\lambda+1}(r) \tag{A.41d}$$

$$T^{M}_{\kappa'\kappa\lambda} = \frac{\kappa'+\kappa}{\sqrt{\lambda(\lambda+1)}} F^{+}_{\kappa'\kappa}(r') \rho_{\lambda\lambda}(r) \tag{A.41 }$$

$$G^{+}_{\kappa',\kappa}(r') = g_{\kappa'}(r')g_{\kappa}(r') + f_{\kappa'}(r')f_{\kappa}(r') \qquad (A.41f)$$

$$F^{\pm}_{\kappa',\kappa}(r') = g_{\kappa'}(r')f_{\kappa}(r') \pm f_{\kappa'}(r')g_{\kappa}(r') \qquad (A.41g)$$

where $\ell = \ell_{\kappa}$, $\ell' = \ell_{\kappa'}$, $j = j_{\kappa}$, $j' = j_{\kappa'}$. Note that for T^{S} and T^{EL}, $\ell+\ell'+\lambda$ must be even, whereas for T^{M}, $\ell+\ell'+\lambda$ must be odd. It follows that other than the phase shift factor $e^{i(\delta_{\kappa}+\delta_{\kappa'})}$, $\langle H_{int} \rangle$ is pure imaginary.

Equation (A.41) has been the basis for essentially all the computer programs written for (e,e') in DWBA. An updated and improved version of one of these, the code DUELS, originally written by the Yale-Duke-Ohio group[19,20], is available at CRNL.

It should be pointed out that in the development above, nowhere was the equation of continuity used. This results in T^{S} being due solely to the scalar multipole, and T^{EL} being due both to the longitudinal and transverse electric multipoles. Consequently T^{S} is not the equivalent of the Coulomb term F^{C} in PWBA. The latter includes the contribution from the longitudinal multipole as well. Similarly, T^{EL} is not the equivalent of F^{E} in PWBA. The latter is due only to the transverse electric multipole. It is desirable to combine the contributions to the scattering from the charge distribution and the longitudinal current. One does not do this for

esthetic reasons alone. For a many-body nucleus (A > 2), the approximation used in calculating the wavefunction often leads to a current which is not conserved, even when the Hamiltonian is formally gauge invariant. Therefore it is advantageous to work in a formalism that does not overly rely on the accuracy of the (irrotational component of the) current. In the following we shall derive an expression for the (e,e') amplitude in which explicit knowledge of the longitudinal current is not needed.

We start from equation 28, and use the shorthand notations for the electron current and density

$$\vec{j}^{\dagger} \equiv \psi_f^{\dagger}(\vec{r}')\vec{\alpha}\,\psi_i(\vec{r}'); \qquad \rho_{(e)}^{\dagger} \equiv \psi_f^{\dagger}(\vec{r}')\psi_i(\vec{r}').$$

In making use of the continuity equation (A.2), we will have to do some integration by parts. Therefore it is necessary to separate the electron and nuclear coordinates. First we recall the integral representation

$$i4\pi k j_\ell(kr_<)h_\ell^{(1)}(kr_>) = 8\int_0^\infty \frac{j_\ell(qr')j_\ell(qr)q^2dq}{q^2-k^2-i\varepsilon}\,. \qquad (A.42)$$

Substituting into (A.28), we get

$$\langle H_{int} \rangle = -8e \int d\vec{r}' \, d\vec{r} \int_0^\infty \frac{q^2 dq}{q^2 - k^2 - i\varepsilon}$$

$$\times \sum_{\ell,m} \left\{ (\rho^\dagger_{(e)}(\vec{r}')\rho(\vec{r}) - \vec{j}^\dagger(\vec{r}')\vec{J}(\vec{r})/c) j_\ell(qr') Y^{m*}_\ell(\hat{r}') j_\ell(qr) Y^m_\ell(\hat{r}) \right\}.$$

The electron and nuclear coordinates are now completely separated. We now use (A.29b) and get

$$\langle H_{int} \rangle = -8e \int d\vec{r}' \, d\vec{r} \int_0^\infty \frac{q^2 dq}{q^2 - k^2 - i\varepsilon} \left\{ \sum_{\ell m} \rho^\dagger_{(e)} \rho j_\ell j_\ell Y^{m*}_\ell Y^m_\ell \right.$$

$$\left. - \sum_{\lambda,\mu} \frac{1}{4\pi(2\lambda+1)} \sum_{\mathcal{R}} (\vec{j}(\vec{r}') \cdot \vec{\mathcal{R}}_{\lambda\mu}(\vec{r}'))^\dagger \, (\vec{J}(\vec{r})/c \cdot \vec{\mathcal{R}}_{\lambda\mu}(\vec{r})) \right\}, \qquad \text{(A.43)}$$

where $\sum_{\mathcal{R}}$ means summing over the three functionals $\vec{\mathcal{L}}$, $\vec{\mathcal{E}}$ and $\vec{\mathcal{M}}$ defined in (A.5). We are especially interested in the term when $\mathcal{R}$ is

$$\vec{\mathcal{L}}_{\lambda\mu}(\vec{r}) = \sqrt{4\pi} \, \hat{\lambda}(iq)^{-1} \vec{\nabla}(j_\lambda(qr) i^\lambda Y^\mu_\lambda(\hat{r})).$$

In this case

$$\frac{1}{4\pi(2\lambda+1)} \int d\vec{r}' (\vec{j}(\vec{r}') \cdot \vec{\mathcal{L}}_{\lambda\mu}(\vec{r}'))^\dagger \int d\vec{r} (J(r)/c \cdot \vec{\mathcal{L}}(\vec{r}))$$

$$= \frac{k^2}{q^2} \int d\vec{r}' \, d\vec{r} \; \rho_\lambda(\vec{r}')^\dagger \rho_\lambda(\vec{r}) \; j_\lambda(qr') j_\lambda(qr) Y^{\mu*}_\lambda(\hat{r}') Y^\mu_\lambda(\vec{r}),$$

where we have integrated by parts, thrown away the vanishing surface terms at infinity, and used (A.2). We get a term which is k^2/q^2 times the scalar term, for each momentum transfer q. Combining this term with the scalar term in (A.43) and recalling that for $\mathcal{R} = \mathcal{L}$ the sum over λ is from $\lambda=0$ on, whereas for $\mathcal{R} = \mathcal{E}$ or $\mathcal{M}$ it is from $\lambda=1$ on, we have

$$\langle H_{int} \rangle = -8e \int d\vec{r}'d\vec{r} \left\{ \int_0^\infty dq \rho^\dagger_{(e)}(\vec{r}')\rho(\vec{r}) \sum_{\ell=0,m} j_\ell(qr')j_\ell(qr) Y^{m*}_\ell(\hat{r}')Y^m_\ell(\hat{r}) \right.$$

$$\left. - \int_0^\infty \frac{q^2 dq}{q^2-k^2-i\varepsilon} \sum_{\lambda=1,\mu} \frac{1}{4\pi(2\lambda+1)} \sum_{\mathcal{R}=\mathcal{E},\mathcal{M}} (\vec{j}(\vec{r}')\cdot\vec{\mathcal{R}}_{\lambda\mu}(\vec{r}'))^\dagger (\vec{J}(\vec{r})/c\cdot\vec{\mathcal{R}}_{\lambda\mu}(\vec{r})) \right\} \tag{A.44}$$

This is a remarkable result. The expression for the Coulomb term (first term in the curly brackets) is similar to that for elastic scattering; that is, for k=0. (Naturally the densities $\rho_{(e)}$ and ρ still depend on the energy loss implicitly.) To proceed, we integrate over q and the angular variables, using (A.50e,f), (A.33-40) and (A.42). In using the last equation for the Coulomb term, we take the limit $k \to 0$,

$$8 \int_0^\infty j_\ell(qr')j_\ell(qr)dq = \frac{4\pi}{2\ell+1} \frac{r_<^\ell}{r_>^{\ell+1}} .$$

The final result is

$$\langle H_{int}\rangle_{DWBA} = -32\pi^3 e^2 \sum_{\substack{\lambda\mu\kappa \\ k'mm'}} C^{f}_{i,\lambda\mu}\, e^{i(\delta_\kappa+\delta_{\kappa'})}\, i^{\ell-\ell'+\lambda}(-)^{j-\frac{1}{2}+\mu}\, \frac{\hat\lambda\hat j}{\sqrt{4\pi}} \begin{pmatrix} j' & j & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$$

$$\times C^{j\nu}_{\ell m\frac{1}{2}\sigma} C^{j'\nu'}_{\ell' m'\frac{1}{2}\sigma'} C^{j'\nu'}_{j\nu\lambda-\mu}\, Y^{m*}_{\ell}(\hat p_i) Y^{m'}_{\ell'}(\hat p_f) \int_0^\infty r'^2 dr' \int_0^\infty r^2 dr$$

$$\times \Bigg\{ \frac{1}{2\lambda+1}\, G^{+}_{\kappa'\kappa}(r')\rho_\lambda(r)\, \frac{r_<^\lambda}{r_>^{\lambda+1}}\, P^{(+)}_{\ell\ell'\lambda}$$

$$+ k\, \frac{\kappa'+\kappa}{\sqrt{\lambda(\lambda+1)}}\, F^{+}_{\kappa'\kappa}(r')\rho_{\lambda\lambda}(r) j_\lambda(kr_<) h^{(1)}_\lambda(kr_>)(1-\delta_{\lambda 0}) P^{(-)}_{\ell\ell'\lambda}$$

$$- ik\frac{\sqrt{\lambda(\lambda+1)}}{\hat\lambda(2\lambda+1)} \Big[(F^{-}_{\kappa'\kappa}(r') - \frac{\kappa'-\kappa}{\lambda} F^{+}_{\kappa'\kappa}(r')) h_{\lambda-1}(kr')$$

$$+ (F^{-}_{\kappa'\kappa}(r') + \frac{\kappa'-\kappa}{\lambda+1} F^{+}_{\kappa'\kappa}(r')) h_{\lambda+1}(kr') \Big]$$

$$\times \Big[\sqrt{\lambda+1}\, \rho_{\lambda,\lambda-1}(r) h_{\lambda-1}(kr) + \sqrt{\lambda}\ \rho_{\lambda,\lambda+1}(r)\ h_{\lambda+1}(kr) \Big] (1-\delta_{\lambda 0}) P^{(+)}_{\ell\ell'\lambda} \Bigg\}, \qquad (A.45)$$

where with $|\lambda'-\lambda| \le 2$

$$h_{\lambda'}(kr')h_\lambda(kr) = \begin{cases} j_{\lambda'}(kr')h^{(1)}_\lambda(kr) + i(2\lambda-1)k^{-3} r'^{\lambda-2}/r^{\lambda+1}\delta_{\lambda'+2,\lambda}; & r' \le r, \\ h^{(1)}_{\lambda'}(kr')j_\lambda(kr) + i(2\lambda+3)k^{-3} r^\lambda/r'^{\lambda+3}\ \delta_{\lambda'-2,\lambda}; & r' > r. \end{cases}$$

The function $P^{(\pm)}$ enforces the parity selection rule,

$$P^{(\pm)}_{\ell\ell'} = \frac{1}{2}\,(1 \pm (-)^{\ell+\ell'+\lambda}).$$

Although in principle they should lead to identical results, (A.45) should be chosen over (A.41) whenever possible. Some of the reasons for advocating this choice have been given earlier. In more practical terms, suppose we are interested in calculating the forward (e,e') amplitude for a natural parity transition. Equation (A.45) only requires that the charge density $\rho_\lambda(r)$ be known whereas (41) requires a knowledge of the current densities $\rho_{\lambda-1}(r)$ and $\rho_{\lambda+1}(r)$ as well. It can be shown that the error incurred in using (A.41) but setting $\rho_{\lambda\pm1}(r) = 0$ is approximately k^2/q^2, where $\vec{q}$ is the (asymtotic) momentum transfer. Therefore the error is small when $k^2/q^2 \ll 1$, and (A.45) offers no practical advantage over (A.41) in such cases. On the other hand, when moderate electron energy beams are used to highly excited nuclear states (such as the giant Eλ resonances), k^2/q^2 can be large, and (A.45) is definitely to be preferred.

Equation (A.45) has the correct limit for elastic scattering, but it is more convenient to use the relation

$$\lim_{k\to 0} kj_\lambda(kr_<)h_\lambda^{(1)}(kr_>) = \frac{-i}{2\lambda+1}\frac{r_<^\lambda}{r_>^{\lambda+1}}$$

for the magnetic term (second term in { }) at the outset. Also in this case the transverse electric (third) term vanishes since $\rho_{\lambda,\lambda\pm1}(r)$ each vanishes individually, as was shown in section 2.8. We also expect the electron kernel to vanish for this term. We note that the electron kernel is an odd function under the permutation $\kappa' \rightleftarrows \kappa$, therefore it must be zero when $\psi_f = \psi_i$.

A.4 (γ,N) REACTIONS

When the absorption of a γ-ray leads only to an internal excitation of the nucleus, the process can be described in terms similar to those describing γ-emission. A more complicated reaction occurs when the nucleus disintegrates. Here we describe the reactions (γ,p) and/or (γ,n).

We first recall the general (non-relativistic) expression for a scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar} |\langle H_{int} \rangle|^2 \frac{\rho(E_f)}{j_i} .$$

$\langle H_{int} \rangle$ is the interaction matrix, in this case

$$H_{int} = \frac{1}{\sqrt{2}} \sum_{\lambda} \sum_{\mu=\pm 1} (\vec{\xi}_{\lambda\mu} + \mu \vec{m}_{\lambda\mu}) \cdot \vec{j}/c \equiv \sum_{\lambda,\mu=\pm 1} O_{\lambda\mu}$$

j_i is the flux of the incoming (unpolarized) beam. For the EM fields given by (A.5), with $b_{+1} = 1/\sqrt{2}$,

$$j_i = k/2\pi\hbar .$$

$\rho_f(E)$ is the number of final states per unit volume per unit energy. For (γ,N) when the wavefunction of the outgoing particle is normalized as

$$\psi^{(+)}_{p_f,\sigma} = 4\pi \sum_{\ell m} u_\ell(r)\ Y^m_\ell(\hat{r})\ Y^{m*}_\ell\ (\hat{p}_f)\chi_\sigma$$

$$\equiv 4\pi \sum_{\ell,m,a} C^{j a^m a}_{\ell m \frac{1}{2}\sigma}\ \psi^{(+)}_\alpha(\hat{r})\ Y^{*m}_\ell(\hat{k}) \qquad (A.46)$$

where $\lim_{r\to\infty} u_\ell(r) = \sin(k\gamma - \frac{\ell\pi}{2} + \text{phase shifts})$, we have (ignoring recoil)

$$\rho_f(E) = \frac{M p_f}{(2\pi\hbar)^3} .$$

Therefore

$$\frac{d\sigma}{d\Omega} = \frac{M}{2\hbar^2}\ \frac{p_f}{hk}\ |\langle H_{int}\rangle|^2 . \qquad (A.47)$$

Let $|\Psi_r\rangle$ be the wavefunction of the residual nucleus.

The total final state is

$$|\Psi_f\rangle = |\psi^{(+)}_{p_f,\sigma}\rangle|\psi_r\rangle$$

$$= 4\pi \sum_{\ell,m,a} C^{\alpha}_{\ell\frac{1}{2}}\ Y^{*m}_\ell\ (\hat{p}_f)|\psi^{(+)}_\alpha\ \psi_r\rangle . \qquad (A.48)$$

Therefore

$$\langle H_{int}\rangle = \frac{1}{\sqrt{2}} \sum_{\lambda,\mu=\pm1} 4\pi \sum_{\ell m a} C^{*}_{\ell\frac{1}{2}} Y^{*m}_{\ell}(\hat{p}_f)\langle\psi^{(+)}_{\alpha}\psi_r|O_{\lambda\mu}|\psi_i\rangle$$

$$= \sum_{\lambda,\mu\pm1} \frac{4\pi}{\sqrt{2}} \sum_{\ell} Y^{*m}_{\ell}(\hat{p}_f) \sum_{ab} \rho^{i\to f}_{ab,\lambda\mu} \frac{\hat{a}}{\hat{\lambda}} \langle a^{(+)}\|O_{\lambda}\|b\rangle \qquad \text{(A.49)}$$

where

$$\rho^{i\to f}_{ab,\lambda\mu} = (-)^{j_b - m_b} C^{\alpha}_{\ell\frac{1}{2}} C^{\lambda\mu}_{\alpha\beta} C^{i}_{J_r,\beta} \langle J_r;b|\}J_i\rangle \qquad \text{(A.50)}$$

is the equivalent of the one-body transition density matrix. $\langle J_r;b|\}J_i\rangle$ is the usual fractional parentage coefficient. We can now use the formulas developed in section 2. We find

$$\langle H_{int}\rangle = \frac{4\pi e}{\sqrt{2}} \sum_{\lambda,\mu=\pm1} \sum_{\ell} Y^{*m}_{\ell}(\hat{p}_f)\sqrt{4\pi}$$

$$\times \{\int r^2 dr\,(\sqrt{\lambda+1}\, j_{\lambda-1}(kr)\rho_{\lambda\lambda-1}(r) + \sqrt{\lambda}\, j_{\lambda+1}(kr)\rho_{\lambda,\lambda+1}(r))$$

$$+ \mu\hat{\lambda}\int r^2 dr\, j_{\lambda}(kr)\rho_{\lambda\lambda}(r)\}. \qquad \text{(A.57)}$$

The similarity among the expressions in (A.51), (A.11), (A.27) and (A.45) that involve the nuclear current densities is quite transparent. In the curly bracket, the first two terms are due to $\vec{\xi}_{\lambda\mu}$ and the last term due

to $\mathcal{M}_{\lambda\mu}$. If the photon wave-length is long, we can again use Siegert's theorem to replace the first two terms by

$$\sqrt{\frac{(2\lambda+1)(\lambda+1)}{\lambda}} \int r^2 dr j_\lambda(kr)\rho_\lambda(r) \approx \sqrt{\frac{\lambda+1}{\lambda}} \frac{k\lambda}{(2\lambda-1)!!} \int r^{\lambda+2}\rho_\lambda(r)dr.$$

When magnetic states M_i and M_f are averaged and summed over, respectively, the parentage states $|J_f;b\rangle$ enter the sum incoherently. Furthermore, when σ is summed over and the cross section integrated over the angle of $\hat{P}_f$, the multipoles contribute incoherently. We get

$$\sigma = \frac{8\pi Mc^2 e^2}{(\hbar c)^2} \frac{P_f}{hk} \sum_{a,b,\lambda} \frac{(2j_a+1)}{(2j_b+1)(2\lambda+1)} |\langle J_r;b|\}J_i\rangle|^2 |\langle a^{(+)}\|O_\lambda\|b\rangle|^2 .$$

The one-body matrix element can be evaluated straightforwardly using (A.5) and the formulas in Section 2, or alternatively, those given in (A.14-19). We only point out that since the radial wavefunction of the outgoing particle is dimensionaless instead of having the normalization $\int |u|^2 r^2 dr = 1$ for bound states, the dimensionality of the matrix element is $L^{3/2}$.

In practice the (γ,N) spectrum (for $A >> 1$) has a broad resonance structure. Thus at least in the giant resonance region ($E_\nu \approx$ 20-30 MeV) cross section is

dominated by the second order effect. That is, the photon is first absorbed by a resonance of the target, and the nucleon is then emitted through the residual nuclear interaction. In this case we have a "second order" term

$$\langle H_{int}^{(2)} \rangle = \frac{1}{\sqrt{2}} \sum_{n,\lambda,\mu=\pm 1} \langle \Psi | (\mathcal{T}_{\lambda\mu} + \mu \mathcal{M}_{\lambda\mu}) \cdot \frac{\vec{J}_{op}}{c} | \Psi_n \rangle \frac{1}{E_f + E_i - E_n + i\Gamma_n/2} \langle \Psi_n | V_{res} | \Psi_f \rangle ,$$

where E_n and Γ_n are respectively the energy and width of the intermediate (resonant) state $|\Psi_n\rangle$. The electronic matrix element can again be expressed in terms of the currents $\rho_{\lambda\ell}^{i\to n}$. The description of the nuclear vertex leading to the particle emission may be quite complex, and is outside the scope of this report.

An alternative to the perturbation treatment is to incorporate the resonance effect into the outgoing wave. This involves the solving of coupled-channel equations, as was done by Buck and Hill[21] and by Raynal et al.[20]. In this case (A.51) is formally retained, with the resonance (or second and higher order) effect included in the (complex) densities $\rho_{\lambda\ell}$.

FIGURE 1. B(Eλ) WEISSKOPF UNITS

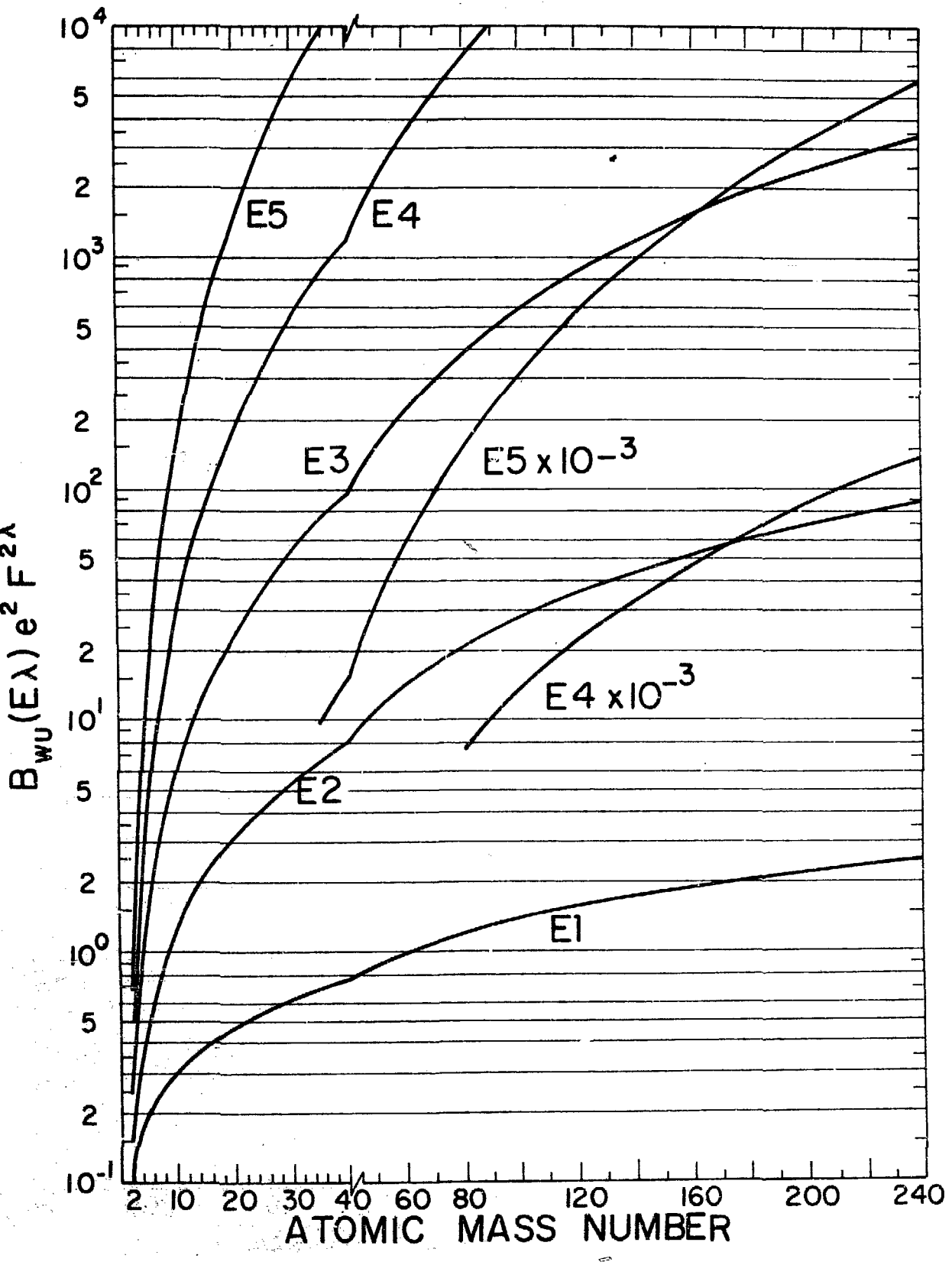
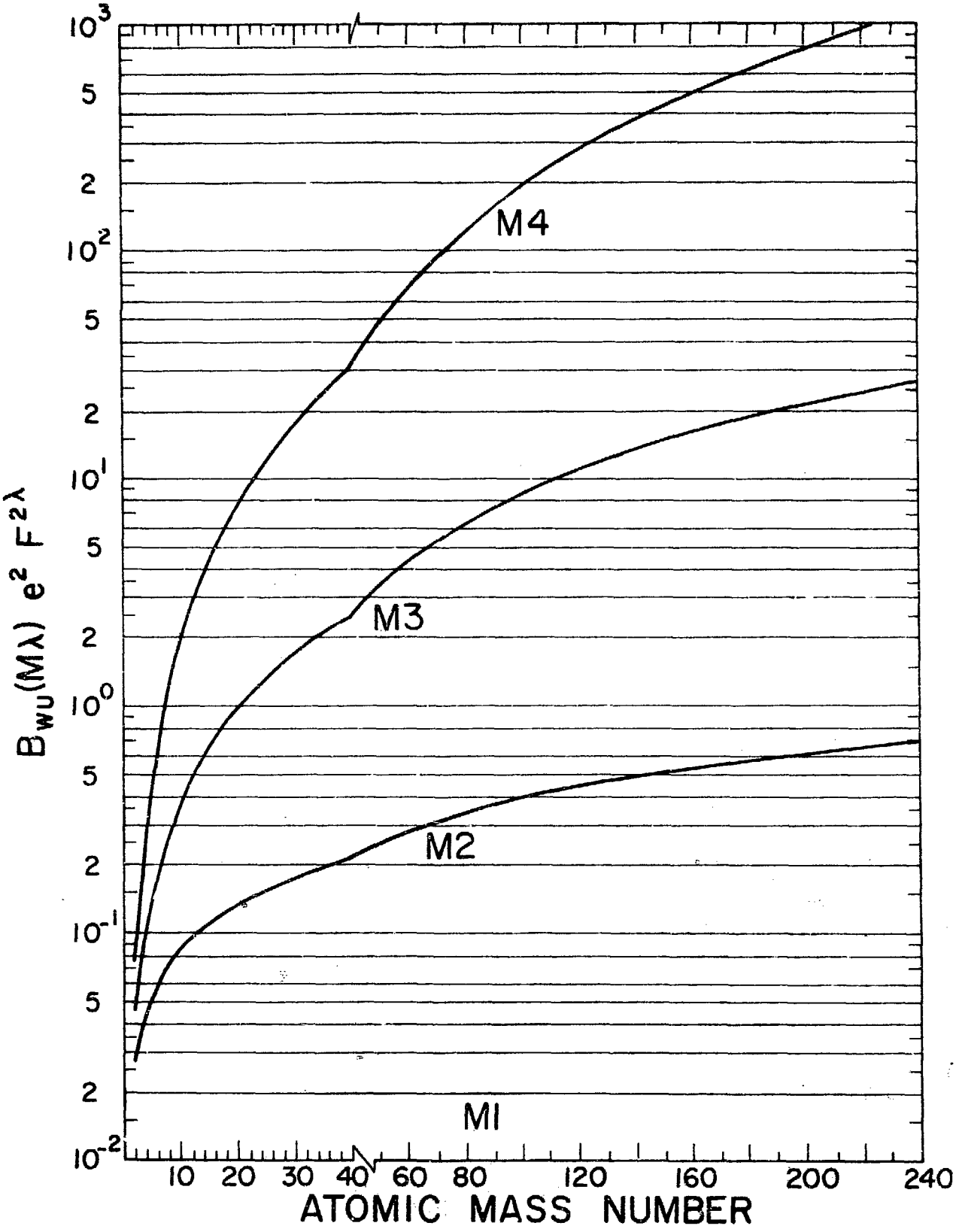


FIGURE 2. B(Mλ) WEISSKOPF UNITS



APPENDIX B

It was shown in Section 2 that the nuclear structural information leading to the one-body charge and current density is contained in the one-body transition density matrix, ρ. The computation of the density matrix depends on the specific microscopic model being used. In some models, such as the shell model and the Hartree-Fock model, the "complete" wavefunction of the nuclear state is obtained. In such cases the computation of ρ can be quite complex. In other models, such as the random-phase approximation and its variants, the transition amplitude instead of the wavefunction is obtained. In such cases the computation of ρ becomes a rather simple matter.

In this appendix we describe methods to calculate ρ in the three most commonly used nuclear models: The particle-hole model, the shell model and the Hartree-Fock model.

B.1 TRANSITION DENSITY MATRIX IN THE PARTICLE-HOLE MODEL

One of the simplest kinds of microscopic model describing nuclear excitations is the particle-hole model. In the Tamm-Dancoff approximation (TDA)

the particle-hole structure of an excited state of spin J, relative to the 0^+ ground state $|0\rangle$ is

$$|\Psi_{JM}\rangle = Q^\dagger_{JM}|0\rangle \equiv \sum_{ph} x^J_{ph}\, A^\dagger_{phJM}|0\rangle \tag{B.1}$$

where

$$A^\dagger_{abJM} = \sum_{mB} C^{JM}_{\alpha\bar{\beta}}\, s_\beta\, C^\dagger_\alpha\, C_\beta; \tag{B.2}$$

p is an orbital not occupied (particle) in $|0\rangle$ and h is an orbital occupied (hole) in $|0\rangle$. The amplitudes x_{ph} are obtained by solving the linearized equation-of-motion[23]

$$\langle\Psi_{JM}|[H,Q_{JM}]|0\rangle = \omega_J\, \langle\Psi_{JM}|Q^\dagger_{JM}|0\rangle. \tag{B.3}$$

The normalization is

$$\sum_{ph} (x^J_{ph})^2 = 1. \tag{B.4}$$

Since $A^\dagger_{abJM}$ is in fact just the transition density operator it is easy to see that in TDA

$$\rho^{0\to J}_{ba\lambda} = \delta_{J\lambda}\, \delta_{ap}\, \delta_{bh}\, x^\lambda_{ph} \qquad \text{(TDA)} \tag{B.5}$$

In the random-phase approximation [23] (RPA), one assumes that there are particle-hole components in the ground state as well and write

$$|\Psi_{JM}> = Q^{\dagger}_{JM}|0> \equiv \sum_{ph} (x^{J}_{ph}\, A^{\dagger}_{phJM} - (-)^{J-M} y^{J}_{ph}\, A_{phJ-M})|0>, \qquad (B.6)$$

and again linearize (B.3). The normalization is now

$$\sum_{ph} ((x^{J}_{ph})^2 - (y^{J}_{ph})^2 = 1.$$

The non-vanishing density matrix elements are

$$\rho^{0\to J}_{hp\lambda} = \delta_{\lambda J}\, x^{\lambda}_{ph}, \qquad (B.7a)$$

$$\rho^{0\to J}_{ph\lambda} = -(-)^{j_p+j_h+\lambda}\, \delta_{\lambda J}\, y^{\lambda}_{ph}. \quad \text{(RPA)} \qquad (B.7b)$$

From (B.7) and the Hermitian properties of the density operators (equations (37) and (39)) we have

$$\rho^{0\to\lambda}_{\lambda}(r) = \sum_{ph} \frac{\hat{j}_p}{\hat{\lambda}} (x_{ph} + y^{\lambda}_{ph})(p\|\rho_{\lambda,0p}\|h) \qquad (B.8a)$$

and

$$\rho^{0\to\lambda}_{\lambda\ell}(r) = \sum_{ph} \frac{\hat{j}_p}{\hat{\lambda}} (x^{\lambda}_{ph} - y^{\lambda}_{ph})(p\|\rho_{\lambda\ell,0p}\|h) \quad . \qquad (B.8b)$$

One should pay attention to the different signs that combine the x and y amplitudes in the charge and current densities.

The particle-hole model is generally applied only to close-shell nuclei. For some medium and heavy nuclei, which have superconducting ground states, the low excited states can be described in terms of two-quasi-particle excitations[24]. In this model the quasi-particle creation ($a_\alpha^\dagger$) and annihilation (a_α) operators are defined as

$$a_\alpha^\dagger = (a_\alpha)^\dagger = u_a c_\alpha^\dagger - (-)^{j_a - m_a} v_a c_{\bar{\alpha}}^\dagger, \tag{B.9}$$

and the angular-momentum-coupled two-quasi-particle operator is defined as

$$A_{abJM}^\dagger = (A_{abJM})^\dagger = \sum_{m_a m_b} C_{\alpha\beta}^{JM} a_\alpha^\dagger a_\beta^\dagger. \tag{B.10}$$

v_a (u_a) is the amplitude that the orbital "a" is occupied (unoccupied) in the BCS ground state. In the quasi-particle random-phase-approximation[22] (QRPA) the excitations are described as

$$|\Psi_{JM}\rangle = Q_{JM}^\dagger |0\rangle = \frac{1}{2} \sum_{ab} (1+\delta_{ab})^{\frac{1}{2}} (x_{ab}^J A_{abJM} - (-)^{J-M} y_{ab}^{JM} A_{abJ-M}) |0\rangle. \tag{B.11}$$

The x and y amplitudes are obtained as usual by solving (B.3), with the normalization

$$\sum_{a \geq b} ((x_{ab}^J)^2 - (y_{ab}^J)^2) = 1.$$

The density matrix in this case becomes

$$\rho_{ba\lambda}^{0\to J} = \delta_{\lambda J} (1+\delta_{ab})^{\frac{1}{2}} (u_a v_b x_{ab}^\lambda + v_a u_b y_{ab}^\lambda). \quad \text{(QRPA)}$$

Similar to (B.8) one can reduce the sum over the pairs (a,b) to that over the ordered pairs (a≥b) by using the symmetry properties of the amplitudes and matrix elements involved, and get

$$\rho_{\lambda}^{0\to\lambda}(r) = \sum_{a\geq b} \frac{\hat{j}_a}{\hat{\lambda}} (1+\delta_{ab})^{-\frac{1}{2}} (u_a v_b + v_a u_b)(x_{ab}^{\lambda} + y_{ab}^{\lambda})(a\|\rho_{\lambda,0p}\|b) \quad \text{(B.13a)}$$

$$\rho_{\lambda\ell}^{0\to\lambda}(r) = \sum_{a\geq b} \frac{\hat{j}_a}{\hat{\lambda}} (1+\delta_{ab})^{-\frac{1}{2}} (u_a v_b - v_a u_b)(x_{ab}^{\lambda} - y_{ab}^{\lambda})(a\|\rho_{\lambda\ell,0p}\|b). \quad \text{(B.14b)}$$

We note that the pair (a=b) does not contribute to the current.

The particle-hole RPA may be generalized so that it becomes applicable to open-shell nuclei with ground states not necessarily of 0^+. For detail the reader is referred to the literature on the equation-of-motion method[25].

B.2 TRANSITION DENSITY MATRIX IN THE SHELL MODEL

In the shell model[26], the wavefunction of an n-particle state is described as a linear combination of orthonormal n-particle basis wavefunctions $|\alpha(n)J>$

$$|\Psi_{JM}(n)> = \sum_{\alpha} x_{\alpha}^{J} |\alpha(n)JM> . \qquad (B.15)$$

The (real) amplitudes x_{α}^{J} are obtained by diagonalizing the Hamiltonian sub-matrix

$$H_{\alpha\alpha'}^{J} = <\alpha(n)JM|H|\alpha'(n)JM> .$$

In the j-j coupling scheme, the transition density matrix is

$$\rho_{ab\lambda}^{i\to f} = n \sum_{\alpha_i\alpha_f} x_{\alpha_i}^{J_i} x_{\alpha_f}^{J_f} \sum_{\alpha_p J_p} (-)^{J_p+\lambda-J_f-j_b} \hat{\lambda}\hat{J}_i \, W(j_a j_b J_f J_i;\lambda J_p)$$

$$\times <\alpha_f(n)J_f\{|\alpha_p(n-1)J_p,a><\alpha_p(n-1)J_p,b|\}\alpha_i(n)J_i> . \qquad (B.16)$$

The coefficients of fractional parentage $(cfp)<\alpha_p J_p;a|\}\alpha J>$ are defined in the expansion[6]

$$|\alpha(n)JM> = \sum_{\alpha_p J_p M_p \gamma} C_{J_p M_p \gamma}^{JM} \, |\alpha_p(n-1)J_p M_p><\gamma><\alpha_p(n-1)J_p;c|\}\alpha(n)J> . \qquad (B.17)$$

The values and phases of cfp's depend on the way the many-particle states are built up. In general they can be expressed in terms of single-shell cfp's, i.e. cfp's for which all particles occupied the same orbit a:

$$\langle \alpha(a^n)J|\}\alpha_p(a^{n-1})J_p,a\rangle .$$

Some single-shell cfp's have been tabulated[27,28].

For the particularly simple case when n=2, the basis wavefunctions are

$$|ab;JM\rangle = \sqrt{\frac{1+\delta_{ab}}{2}} \sum_{m_b m_a} C^{JM}_{\alpha\beta} \left(|\alpha\rangle|\beta\rangle - (1-\delta_{ab})|\beta\rangle|\alpha\rangle\right) \qquad (B.18)$$

and the cfp's are

$$\langle a,b|\}abJ\rangle = \sqrt{\frac{1+\delta_{ab}}{2}} = -(-)^{j_a+j_b+J}\langle b,a|\}abJ\rangle . \qquad (B.19)$$

Writing a two-particle state as

$$|\Psi_{JM}(2)\rangle = \sum_{ab} a^J_{ab}|ab;JM\rangle \qquad (B.20)$$

with the normalization

$$\sum_{ab} (a^J_{ab})^2 = 1,$$

the density matrix becomes

$$\rho^{i\to f}_{ba\lambda} = \sum_c \sqrt{1+\delta_{ac}}\,\sqrt{1+\delta_{bc}}\; a^{J_i}_{ca}\, a^{J_f}_{cb} (-)^{j_c+\lambda+J_f-j_b}\, \hat{\lambda}\hat{J}_i\, W(j_a j_b J_f J_i;\lambda j_c) \cdot \qquad (B.21)$$

B.3 TRANSITION DENSITY MATRIX IN THE PROJECTED HARTREE-FOCK APPROXIMATION

In the Hartree-Fock (HF) approximation[21], a variational method is used to minimize the expectation value of the Hamiltonian for a single Slater determinant, $|\chi>$.

$$|\chi> = \prod_{i=1}^{N} C^{\dagger}_{\mu_i} |0>$$

where N is the number of particles and $\{\mu_i\}$ are the set of single-particle HF orbitals. They are related to the set of basis orbital $\{\alpha\}$ by the linear transformation

$$C^{\dagger}_{\mu} = \sum_{\alpha} U_{\alpha\mu} C^{\dagger}_{\alpha}, \qquad \sum_{\alpha} (U_{\alpha\mu})^2 = 1. \qquad (B.22)$$

In general $|\chi>$ does not have a specific angular momentum, but may be expanded in terms of normalized states with good angular momentum,

$$|\chi> = \sum_{JK} n_{JK} |J(K\chi)K>.$$

If the initial state is $|J_i(K_i\chi_i)M_i>$, and the final state is $|J_f(K_f\chi_f)M_f>$, then the transition density matrix is[10]

$$\rho^{i\to f}_{ba\lambda} = (n_{J_fK_f\chi_f}\, n_{J_iK_i\chi_i})^{-1}\,\frac{2J_i+1}{8\pi^2}\sum_{\mu=-\lambda}^{\lambda} C^{J_fK_f}_{J_iK_f-\mu,\lambda\mu}\int d^3\Omega\; D^{J*}_{K_f-\mu_1K_i}(\Omega)$$

$$\times \sum_{m_am_b} C^{\lambda\mu}_{\alpha\beta} <\chi_f|c^\dagger_\alpha c_\beta\, R(\Omega)|\chi_i> \qquad (B.23)$$

where $R(\Omega) = R(\alpha,\beta,\gamma)$ is the rotation operator specified by the Euler angles (α,β,γ), $D(\Omega)$ is the rotation matrix and

$$<\chi_f|c^\dagger_\alpha c_\beta R(\Omega)|\chi_i> = \sum_{\mu\nu} U^i(r)_{\beta\nu}(d^{-1})_{\nu\mu}\; U^{f*}_{\alpha\mu} \qquad (B.24a)$$

$$d_{\mu\nu} = \sum_\alpha U^{f*}_{\alpha\mu}\; U^i(\Omega)_{\alpha\nu} \qquad (B.24b)$$

and

$$U^f_{\alpha\mu}(\Omega) = \sum_\beta \delta_{j_aj_b}\, D^{j_a}_{m_am_b}(\Omega)\; U^f_{\beta\mu}\ , \qquad (B.24c)$$

where U is the transformation of (B.22). In (B.24b), the summations of μ and ν are over occupied orbits (in $|\chi^f>$ and $|\chi^i>$ respectively) only. In general, it is possible to replace the integral in (B.23) by a sum over a certain set of Euler angles, to be determined by the symmetry properties of $|\chi_i>$ and $|\chi_f>$[10].

If the initial and final states are described respectively in terms of linear combinations of projected HF states,

$$|\Psi_i\rangle = |\sigma J_i M_i\rangle = \sum_\sigma x_\sigma^i |J_i(K_\sigma \chi_\sigma) M_i\rangle \tag{B.25a}$$

and

$$|\Psi_f\rangle = |\sigma' J_f M_f\rangle = \sum_{\sigma'} x_{\sigma'}^f, \; |J_f(K_{\sigma'}, \chi_{\sigma'}, |M_f\rangle \tag{B.25b}$$

then

$$\rho_{ba\lambda}^{i\to f} = \sum_{\sigma\sigma'} x_{\sigma'}^f, \; x_\sigma^i \; \rho_{ba\lambda}^{\sigma\to\sigma'} \tag{B.26}$$

where $\rho_{ba}^{\sigma\to\sigma'}$ is given by (B.23).

APPENDIX C

This appendix provides the complete listing of MICRØDENS and the outputs for three sample calculations.

The only comments that need be made on the listing is that the "$" sign is a record separator, and that the subroutines DATE (called at MICRØD.77) and PLØT (called at LINPLØT.37 and SEMILØG.31) are system routines of the CDC-6600 computing system at CRNL. Users at other computer installations may have to use the respective equivalents available locally.

In all three test cases the initial state $|i\rangle$ is the vacuum (0^+) state, and the oscillator length is taken to be 2.0F. Other specifications are given preceding the output for each case.

In the form factor section of the output, quantities listed under the headings F(CHARGE), FC.SQ, F(SPIN), FS.SQ and FTOTAL.SQ are explained in table B.1, where the notations

$$f_{JL}^{c,m}(q) \equiv \int_0^\infty \rho_{JL}^{c,m}(r)\, j_L(qr) r^2 dr, \tag{C.1}$$

$$f_J(q) \equiv \int_0^\infty \rho_J(r)\, j_J(qr) r^2 dr, \tag{C.2}$$

and

$$N = \frac{4\pi(2J_f+1)}{(2J_i+1)Z^2} \tag{C.3}$$

are used. The form factors $F_J^{C,M,E}(q^2)$ are those defined in (A.27).

TABLE C.1

	Heading				
TYPE OF SCAT.	F(CHARGE)	FC.SQ	F(SPIN)	FS.SQ	FTOTAL.SQ
COULOMB	$f_j(q)$	$N\|f_J\|^2$			$F_J^C(q^2)$
MAGNETIC	$f_{JJ}^C(q)$	$N\|f_{JT}^C\|^2$	†	††	$F_J^M(q^2)$
ELECTRIC(L=J-1)	$f_{J,J-1}^C(q)$	$\frac{\sqrt{J+1}}{\hat{J}} f_{J,J-1}^C$	†	††	
ELECTRIC(L=J+1)	$f_{J,J+1}^C(q)$	$N\left\|\frac{\sqrt{J+1}}{\hat{J}} f_{J,J-1}^C + \frac{\sqrt{J}}{\hat{J}} f_{J,J+1}^C\right\|^2$	†	††	$F_J^E(q^2)$

† Same as under F(CHARGE), but replace superscript c by m.

†† Same as under FC.SQ, but replace superscript c by m.

C.1 LISTING OF MICRØDENS

MICROD

```
      PROGRAM MICROD(INPUT,OUTPUT,PUNCH,PLOT)                                   MICROD     2
      DIMENSION C(50),S(50),RO(50),NLJA(50),NLJB(50),NAME(7),IRO(50),           MICROD     3
     1   SNAME(3),XX(50),TC(50),TS(50)                                          MICROD     4
      COMMON/CFACTOR/GLP,GLN,MUSP,MUSN,EFC(2),EFM(2),BOHR,TRI                   MICROD     5
      EQUIVALENCE (C,NLJA), (S,NLJB)                                            MICROD     6
      REAL MUSP,MUSN                                                            MICROD     7
      DATA GLP,GLN,MUSP,MUSN/1.,0.,2.79,-1.91/                                  MICROD     8
      DATA PI,BOHR,HBC/3.1415 92653, 0.105, 197.33/                             MICROD     9
      DATA MODE/10LELECTRIC  /                                                  MICROD    10
*     BOHR = 0.5*HBAR/M(NUCLEON)*C (FERMI)                                      MICROD    11
      X= HCOEF(1.,1.,1.,1.,1.,1.)                                               MICROD    12
*                                                                               MICROD    13
  100 READ 1002, NAME,KIND                                                      MICROD    14
*                                                                               MICROD    15
*     IPL=0 NO PLOT.  EXL IS = LARGER EXPONENT OF 10 FOR SEMILOG PLOT           MICROD    16
*     IPL = 1  DENSITY PLOT ONLY.    = 2  FORMFACTORS ONLY  =3 BOTH             MICROD    17
*     DENSITY AND FORMFACTORS.  NC IS THE NUMBER OF CYCLES OOR SEMILOG P        MICROD    18
*                                                                               MICROD    19
      READ  1003, N,A,DX,NX,DQ,QMAX,VJI,VJF,Z,EFC,EFM,JS,JL,IPL,IPU             MICROD    20
*                                                                               MICROD    21
*     N             LENGTH OF RO ARRAY TO BE READ IN                          MICROD    22
*     A             OSCILLATOR LENGTH IN FERMIES                              MICROD    23
*     DX            INCREMENT IN X, X= R/A                                    MICROD    24
*     NX            NO. OF X VALUES FOR WHICH DENSITY BE CALCULATED           MICROD    25
*                   FIRST POINT IS X=0.  IF NX.LT.2 DENSITY NOT COMPUTED      MICROD    26
*     DQ            INCREMENT IN MOMENTUM TRANSF Q IN MEV/C                   MICROD    27
*     QMAX          MAXIMUM VALUE FOR Q                                       MICROD    28
*     VJI,VJF       SPIN OF INITIAL AND FINAL STATE. IF LEFT BLANK            MICROD    29
*                   VJI IS SET TO 0 AND VJF= MULTIPOLARITY                    MICROD    30
*     JS,JL         SMALLEST AND LARGEST MULTIPOLE TO BE CONSIDERED           MICROD    31
*     IPL           PLOT OPTION. =1, PLOT(LINEAR) DENSITY ONLY                MICROD    32
*                                =2, PLOT(SEMI-LOG) FORM FACTORS ONLY         MICROD    33
*                                =3, PLOT BOTH                                MICROD    34
*     IPU           PUNCH OPTION.  =1, PUNCH DENSITY. =0, NO PUNCH            MICROD    35
*     EFC           CHARGE ENHANCEMENT FOR PROTON(1) AND NEUTRON(2)           MICROD    36
*     EFM           MAGNETIC MOMENT ENHANCEMENT                               MICROD    37
c                                                                               MICROD    38
*     IF N=0 JOB TERMINATES.  IF N= -1 USE RO-ARRAY OF LAST CASE                MICROD    39
*     KIND MAY BE 10LCOULOMB   , OR 10LELECTRIC  , OR 10LMAGNETIC  .            MICROD    40
*                                                                               MICROD    41
      IF ( N.EQ. 0 ) GOTO 99 $ PRINT 1004                                       MICROD    42
      PRINT 1003, N,A,DX,NX,DQ,QMAX,VJI,VJF,Z,EFC,EFM,JS,JL,IPL,IPU             MICROD    43
*                                                                               MICROD    44
      PRINT1012, NAME,KIND  $ IF (N.EQ. -1) GOTO 15 $ NOLD= N                   MICROD    45
*                                                                               MICROD    46
*     READ IN AND CONSTRUCT DENSITY ARRAY IRO                                   MICROD    47
*                                                                               MICROD    48
      READ 1005,( (NLJA(I),NLJB(I),IRO(I),RO(I)), I= 1, N)                     MICROD    49
      PRINT1005,( (NLJA(I),NLJB(I),IRO(I),RO(I)), I= 1, N)                     MICROD    50
*                                                                               MICROD    51
*     NLJ = 32*N+ 2*L + (J+0.5- L)                                              MICROD    52
*     CONSTRUCT THE WORD IRO AS FOLLOWS                                         MICROD    53
*          FIRST 22(0 - 21) BITS STORES ABS(RO)*1.E05                           MICROD    54
*          NEXT 8 BITS(22 - 29) STORES NLJB                                     MICROD    55
*          NEXT 8 BITS(30 - 37) STORES NLJA                                     MICROD    56
*          THE 59TH BIT STORES ISO ( =1 FOR PROTON, =0 FOR NEUTRON)             MICROD    57
*          THE SIGN OR 60TH BIT HAS THE SIGN OF RO.                             MICROD    58
*                                                                               MICROD    59
      DO 1 I= 1, N $ IR= ABS(RO(I))*1.E05 $ IS=1 $ IF(RO(I).LT.0) IS= 0         MICROD    60
      IS= SHIFT(IS,59) $ ISO= SHIFT(IRO(I),58) $ IR= IS .O. ISO .O. IR          MICROD    61
    1 IRO(I)= IR .O. SHIFT(NLJA(I),30) .O. SHIFT(NLJA(I),22)                    MICROD    62
      PRINT 1006, (IRO(I), I= 1, N)                                             MICROD    63
   15 N= NOLD $ IF (KIND -MODE) 11, 12, 13                                      MICROD    64
*     COULOMB                                                                   MICROD    65
   11 ICO= -2 $ JML= 0 $ GOTO 14                                                MICROD    66
*     TRANSVERSE ELECTRIC                                                       MICROD    67
   12 ICO= 0 $ JML= 1 $ GOTO 14                                                 MICROD    68
*     MAGNETIC                                                                  MICROD    69
   13 ICO= 0 $ JML = 0                                                          MICROD    70
   14 DO 2 J= JS,JL,2 $ LS= J- JML $ LL= J+ JML $ DO 2 L= LS,LL,2               MICROD    71
      C(1)= S(1)= RO(1)= 0 $ PRINT 1007, NAME,KIND,J,L                          MICROD    72
      Z2= SQRT( J/(J+J+1.) ) $ Z1= SQRT( (J+1.)/(J+J+1.) )                      MICROD    73
      TRI= 1. $ IF(J.GT.L) TRI= -1.                                             MICROD    74
      IF (VJI.LT..1) VJF= J                                                     MICROD    75
*     LABELS FOR PLOT ROUTINES                                                  MICROD    76
      CALL DATE(SNAME(3))  $  SNAME(2)=10HLAM+1000GR                            MICROD    77
      SNAME(1)=10000*A + J                                                      MICROD    78
```

MICROD (CONTINUED)

```
*
*     FIRST COMPUTE CHARGE AND SPIN DENSITIES
*
      IF (NX .LT. 2 ) GOTO 3
      X=XX(1)=0 $ DO 3 I=2,NX $ X=XX(I)=X+DX
      CALL CURRENT(C(I),S(I),ICD,J,L,X,IRO,N,B) $ RO(I)= C(I)+ S(I)
 3    PRINT 1001, X,C(I),S(I),RO(I)
      IF(IPU.EQ.0) GO TO 5
      PUNCH 1008, (NAME(I), I= 1,3),KIND,J,L,DX,NX,B
      PUNCH 2000, ( (C(I),S(I)), I= 1, NX )
    5 CONTINUE
      IF(IPL.EQ.1.OR.IPL.EQ.3) CALL LINPLOT(XX,C,S,DX,NX,NAME,SNAME)
*
*     NOW CALCULATE FORM FACTORS IN BORN APPROXIMATION
*
 8    DO 7 I= 1, 150
 7    C(I)= 0
      PRINT 1009, NAME,KIND,J,L
      XNORM= 4.*PI*(VJF+VJF+1.)/(VJI+VJI+1.)///7
      NQ= QMAX/DQ $ Q=1.-DQ $ DO 4 I= 1,NQ $ XX(I)=Q=Q+ DQ $ QH= Q/HBC
      CALL FORMFAC(CC,SS,ICD,J,L,QH*B,IRO,N,B)
      IF     (L-J) 21,22,23
 21   TC(I)=        Z1*CC $ TS(I)=        Z1*SS $ GOTO 4
 23   C(I)= TC(I)+ Z2*CC $ S(I)= TS(I)+ Z2*SS $ Y= C(I)+ S(I)
      C(I)= C(I)*C(I)*XNORM $ S(I)= S(I)*S(I)*XNORM $ RO(I)=Y*Y*XNORM
      GOTO 4
 22   C(I)= CC*CC*XNORM $ S(I)= SS*SS*XNORM
      Y= CC+ SS$ Y= Y*Y $ RO(I)= Y*XNORM
 4    PRINT 1010, Q,QH,CC,C(I),SS,S(I),RO(I)
      Y= -1. $ DO 6 I= 1, 150
 6    Y= AMAX1(Y, C(I) ) $ EXL= ALOG10(Y+Y)
      IF (IPL.EQ.2 .OR. IPL.EQ.3 )
     1    CALL SEMILOG(XX,C,S,RO,DQ,NQ,NAME,SNAME,EXL,-6)
 2    CONTINUE          $ GOTO 100
 99   CONTINUE
1002 FORMAT(8A10)
1003 FORMAT(I4,1X,2F5.3,I5,9F5.1,4I2)
1004 FORMAT(1H1)
1005 FORMAT( 5(2I3,I1,F8.5) )
1006 FORMAT( 4(5X020) )
1007 FORMAT(////7A10/5X,A10* J=*I1* L=*I1*,  X=R/B, DENSITY TIMES B-CUB
     1ED IS PRINTED*//      8X*X*13X*CHARGE*15X*SPIN*15X*TOTAL*/)
1008 FORMAT(3A10,X,A10* J=*I1* L=*I1* DX=*F4.2* NX=*I2* B=*F5.3*(F)*)
1001 FORMAT(5X,F6.2,3E20.5)
2000 FORMAT( 6E12.5 )
1009 FORMAT(////7A10,5X*BORN APPROX *A10* J=*I1* L=*I1* FORM FACTORS*//
     1 6X*Q(MEV/C)    Q(1/FM)*5X*F(CHARGE)*8X*FC.SQ*9X*F(SPIN)*
     2 9X*FS.SQ*8X*FTOTAL.SQ*/)
1012 FORMAT(1X////8A10/)
1010 FORMAT(5X,2F10.3,6E15.5)
      END
```

MICROD 73
MICROD 80
MICROD 81
MICROD 82
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MICROD 127
MICROD 128
MICROD 129

CURRENT

```
      SUBROUTINE CURRENT(CHARGE,SPIN,ICO,J,L,X,IROA,N,9)                    CURRENT    2
*                                                                           CURRENT    3
*      ROUTINE CALCULATES CURRENT DENSITIES CORRESPONDING TO THE SINGLE      CURRENT    4
*     PARTICLE DENSITY MATRIX, IROA.  CHARGE IS THE DENSITY OF THE          CURRENT    5
*     GRADIENT OPERATOR.  SPIN IS THE PURE IMAGINARY PART OF THE DENSITY    CURRENT    6
*     OF THE GRADIENT-CROSS-SPIN(PAULI) OPERATOR.                           CURRENT    7
*     IRO = SIGN(RO)*(SHIFT(J,55) + SHIFT(NLJA,30) + SHIFT(NLJB,22)         CURRENT    8
*                  + ABS(RO)*1.E05 )                                        CURRENT    9
*     RO =RO(RA,J)  . NLJ= SHIFT(N,5) + L*2+ JL, JL= J+ .5.                 CURRENT   10
*     X IS DIMENSIONALESS                                                   CURRENT   11
*     N IS THE LENGTH OF THE DENSITY ARRAY IROA                             CURRENT   12
*     ICO = -1     COMPUTE CHARGE ONLY                                      CURRENT   13
*         =  0     COMPUTE BOTH CHARGE AND SPIN                             CURRENT   14
*         = +1     COMPUTE SPIN ONLY                                        CURRENT   15
*     (FOR DETAIL SEE H.C.LEE,...NUCLEAR CHARGE, CONVECTION CURRENT AND     CURRENT   16
*     MAGNETIZATION CURRENT DENSITIES...AECL REPORT NO. 4839, NOV 1974)     CURRENT   17
*                                                                           CURRENT   18
*     CHANGED TO TIME-REVERSAL INVARIANT PHASE( FEB 2 1974 ) ADDITIONAL     CURRENT   19
*     PHASE (LB+ J- LA)/2 FOR ELECTRIC AND ( LB+ J- LA+ 1)/2 FOR MAG.       CURRENT   20
*                                                                           CURRENT   21
      COMMON/CFACTOR/GLP,GLN,MUSP,MUSN,EFC(2),EFM(2),BOHR,TRI               CURRENT   22
      REAL MUSP,MUSN,MUS    $ LOGICAL SLNAB,SJL                             CURRENT   23
      DIMENSION IROA(1) $ LOGICAL IPASS                                     CURRENT   24
      DATA IPASS,ESP/.F.,1.E-5/                                             CURRENT   25
      DATA PI/3.1415 92653/, I22,I8/177777778,3778/                         CURRENT   26
      SJL= J .NE. L                                                         CURRENT   27
    1 CHARGE= SPIN= 0 $ IF (IABS(J-L) .GT. 1 .OR. J .LT. 1 ) RETURN         CURRENT   28
*     FIRST RECOVER QUANTUM NUMBERS AND DENSITY MATRIX ELEMENT FROM IRO     CURRENT   29
      DO 11 I= 1, N $ IRO= IROA(I) $ ISO= SHIFT(IRO,-59)                    CURRENT   30
      ISO= ISO.A.1 $ S= ISO $ ISO= IRO.A.I22 $ RO= (S+S- 1.)*ISO*ESP        CURRENT   31
      ISO= SHIFT(IRO,-58) $ ISO= ISO .A. 1                                  CURRENT   32
*     ISO= 1 , PROTON,   = 0 , NEUTRON                                      CURRENT   33
      GL= ISO*(GLP+ EFC(1))+ (1- ISO)*(GLN+ EFC(2))                         CURRENT   34
      MUS= ISO*(MUSP+ EFM(1))+ (1- ISO)*(MUSN+ EFM(2))                      CURRENT   35
      IRO= SHIFT(IRO, -22) $ IJUMP= 1                                       CURRENT   36
    2 NLJ= IRO .A. I8 $ JA= NLJ .A. 1  $ NLJ= NLJ/2 $ LA= NLJ .A. 15        CURRENT   37
      JA= LA+JA $ NLJ= SHIFT(NLJ,-4) $ NA= NLJ .A. 7 $ GOTO (3,31) IJUMP    CURRENT   38
    3 LB= LA $ JB= JA $ NB= NA $ IRO= SHIFT(IRO,-8) $ IJUMP=2$ GOTO 2       CURRENT   39
*     HAVE Q.N. AND RO, NOW COMPUTE DENSITY.  FIRST CHARGE                  CURRENT   40
   31 SLNAB= NA.EQ.NB .A. (LA.EQ.LB)                                        CURRENT   41
      IF  (SLNAB .A. SJL .A. (JA.EQ.JB) ) GOTO 11                           CURRENT   42
      IFAS= LB+ J- LA $ IF (ICO.GT.-2) GOTO 4                               CURRENT   43
*     THIS SECTION COMPUTES COULOMB TRANSITION DENSITY                      CURRENT   44
      IFAS= JB+ J+ IFAS/2 $ IFAS= IFAS .A. 1 $ FAS= 1- IFAS- IFAS           CURRENT   45
      FAS= FAS*SQRT( JA*JB/PI)                                              CURRENT   46
      CHARGE= CHARGE- FAS*RO*GL*CLEBS(JA,JB,J)                              CURRENT   47
     1      *RDFUNC(NA,LA,X)*RDFUNC(NB,LB,X)                               CURRENT   48
      GOTO 11                                                               CURRENT   49
    4 I6= LA+ LB $ IF (MOD(I6+L,2).EQ.0) GOTO 11 $ I5= JA+ JB- 1            CURRENT   50
      IF (I5.LT.J .OR. IABS(JA-JB).GT.J) GOTO 11                            CURRENT   51
      IF (SLNAB .A. SJL) GOTO 12                                            CURRENT   52
      IF (I6.LT.J .OR. IABS(LA-LB).GT.J) GOTO 12 $ IF (ICO) 5,5,6           CURRENT   53
    5                I1= I5+ I6 $ I5= I5+ J $ I2= JA+ LB+ J                 CURRENT   54
      IFA= I2+ ( IFAS+1-IABS(J-L) )/2 $ IFA= IFA .A. 1                      CURRENT   55
      I3= LA+ JA $ I4= LB+ JB $ I6= I6+ J $ FAS= 1- IFA- IFA                CURRENT   56
      FAS= FAS*2.*SQRT(JA*JB/(J+J+1.))*GL                                   CURRENT   57
*     RACAH IS W(JA,JB,LA,LB,J,1/2)                                         CURRENT   58
      TDQE= TDQE= SQRT(LA+LA+1.)*TLYDEL(NA,LA,NB,LB,J,L,X)                  CURRENT   59
      IF (SLNAB) GOTO 13 $ IFA= (J+1) .A. 1                                 CURRENT   60
      TDQE= SQRT(LB+LB+1.)*TLYDEL(NB,LB,NA,LA,J,L,X)*(1-IFA-IFA)            CURRENT   61
   13 CHARGE= CHARGE-RO*FAS*FWCOEF(I1,I2,I3,I4,I5,I6)*(TDQ+ TDQE)*0.5       CURRENT   62
   12 IF (ICO) 11,6,6                                                       CURRENT   63
*     NOW COMPUTE SPIN                                                      CURRENT   64
    6 RA= RDFUNC(NA,LA,X) $ RB= RDFUNC(NB,LB,X)                             CURRENT   65
      DRAB= 0 $ IF (LA.GT.0) GOTO 7                                         CURRENT   66
      RNO= 0 $ IF (NA.GT.0) RNO= SQRT(FLOAT(NA))*RDFUNC(NA-1,1,X)           CURRENT   67
      RNO=-SQRT(NA+1.5)*RDFUNC(NA,1,X)- RNO+ RDFUNC(NA,0,X)/X               CURRENT   68
      DRAB= DRAB+ RB*RNO $ GOTO 8                                           CURRENT   69
    7 DRAB= DRAB+ RB*( SQRT(LA+ NA+ 0.5)*RDFUNC(NA, LA-1, X)                CURRENT   70
     1               + SQRT(NA+ 1.)*RDFUNC(NA+1, LA-1, X) )                 CURRENT   71
    8 IF (LB.GT.0) GOTO 9                                                   CURRENT   72
      RNO= 0 $ IF (NB.GT.0) RNO= SQRT(FLOAT(NB))*RDFUNC(NB-1,1,X)           CURRENT   73
      RNO=-SQRT(NB+1.5)*RDFUNC(NB,1,X)- RNO+ RDFUNC(NB,0,X)/X               CURRENT   74
      DRAB= DRAB+ RA*RNO $  GOTO 10                                         CURRENT   75
    9 DRAB= DRAB+ RA*( SQRT(LB+ NB+ 0.5)*RDFUNC(NB, LB-1, X)                CURRENT   76
     1               + SQRT(NB+ 1.)*RDFUNC(NB+1, LB-1, X) )                 CURRENT   77
   10 RAB= RA*RB/X $ DRAB= DRAB- (LA+ LB)*RAB                               CURRENT   78
```

CURRENT (CONTINUED)

```
      RA= (LA- JA+ 0.5)*(JA+ JA) $ RB= (LB- JB+ 0.5)*(JB+ JB)                    CURRENT     79
*     RAB= RA*RB/X , DRAB= D/DX( RA*RB*X*X)/X**2 , RA= XA , RB= XB              CURRENT     80
      S=  JA*JB/PI     $ IF (J-L) 20, 21, 22                                    CURRENT     81
*     FOR RO(J,J+1)                                                             CURRENT     82
   20 S= S/(J+1.)/(J+ J+ 1.)                                                    CURRENT     83
      S= SQRT(S)          *(RA- RB)*(DRAB- (J+2.)*RAB ) $ GOTO 23               CURRENT     84
*     FOR RO(J,J)                                                               CURRENT     85
   21 S=SQRT(S/(J*J+ J1)*( (RA+RB)*( RAB- DRAB)- (J*J+ J)*RAB) $ GOTO 23        CURRENT     86
*     FOR RO(J,J-1)                                                             CURRENT     87
   22 S= S/J/(J+ J+ 1.)                                                         CURRENT     88
      S= SQRT(S)    *(RA- RB)*(DRAB+ (J- 1.)*RAB )                              CURRENT     89
   23 IFA= J+ JB+ ( IFAS+1- IABS(J-L) )/2 $ IFA= IFA .A. 1                      CURRENT     90
      SPIN= SPIN+(1- IFA- IFA       )*CLEBS(JA,JB,J)*S*RO*MUS                   CURRENT     91
   11 CONTINUE $ IF (ICO .EQ. -2) RETURN                                        CURRENT     92
      CHARGE= 2.*BOHR*TRI*CHARGE/8 $ SPIN= BOHR*TRI*SPIN/8 $ RETURN             CURRENT     93
      END                                                                       CURRENT     94
```

TLYDEL

```
      FUNCTION TLYDEL(NA,LA,NB,LB,LAM,L,X)                                      TLYDEL      2
*     ROUTINE CALCULATES REDUCED MATRIX ELEMENT OF TENSORIAL OPERATOR            TLYDEL      3
*     OF ORDER LAM FORMED BY THE VECTOR COUPLING OF THE SPHERICAL               TLYDEL      4
*     HARMONIC OF ORDER L TO THE GRADIENT OPERATOR. ONLY THE ANGLES             TLYDEL      5
*     ARE INTEGRATED OVER.  THE RADIAL FUNCTIONS ARE ASSUMED TO  HARMONI        TLYDEL      6
*     OSCILLATOR FUNCTIONS.  X = R/B IS DIMENSIONALESS, B= OSC. LENGTH.         TLYDEL      7
*     THE BRINK AND SACTHLER, NOT THE TIME-REVERSAL-INVARIANT PHASE             TLYDEL      8
*     IS USED.                                                                  TLYDEL      9
*                                                                               TLYDEL     10
      LOGICAL RHO                                                               TLYDEL     11
      DATA PI/3.1415 92653/                                                     TLYDEL     12
      RHO= .T. $ GOTO 11 $ ENTRY TLYDELG $ RHO = .F.                            TLYDEL     13
   11 I4= LA+ LB+ L $ TLYDEL= 0 $ GOTO 1                                        TLYDEL     14
*     FOLLOWING ENTRY POINT DO TESTING OF TRIANGULAR RELATIONS.                 TLYDEL     15
      ENTRY TLYDET $ TLYDEL= 0 $ IF (MOD(I4,2).NE.1) RETURN                     TLYDEL     16
      IF (IABS(LAM-L) .GT. 1) RETURN                                            TLYDEL     17
      IF (LAM .GT. LA+LB .OR. LAM .LT. IABS(LA-LB)) RETURN                      TLYDEL     18
    1 I5= LAM+ LB $ FAS= 1- 2*MOD(I5,2)                                         TLYDEL     19
      Z= (LAM+LAM+1)*(L+L+1)/4./PI $ I2= I5+ L+ LB- 1 $ I3= LB+ LB              TLYDEL     20
      I5= I5+LA $ I6= L+LAM+ 1 $ I1= I4 + 1 $ I4= I4- 1                         TLYDEL     21
      FAS= FAS*SQRT(Z) $ IF (RHO) FAS= FAS*RDFUNC(NA,LA,X)                      TLYDEL     22
      IF (LB.GT.0) GOTO 13 $ IF (RHO) GOTO 2                                    TLYDEL     23
      RMO= 0 $ IF (NB.GT.0) RMO=SQRT(FLOAT(NB))*RADQ(NA+1,LA,NB,1,L,X)          TLYDEL     24
      RMO= -SQRT(NB+1.5)*RADQ(NA+1,LA,NB+1,1,L,X)- RMO                          TLYDEL     25
      GOTO 15                                                                   TLYDEL     26
    2 RMO= 0 $ IF (NB.GT.0) RMO= SQRT(FLOAT(NB))*RDFUNC(NB-1,1,X)               TLYDEL     27
      RMO= -SQRT(NB+1.5)*RDFUNC(NB,1,X)- RMO                                    TLYDEL     28
      GOTO 15                                                                   TLYDEL     29
   13 IF (RHO) GOTO 3                                                           TLYDEL     30
      RMO= SQRT(     LB+NB+ .5  )*RADQ(NA+1,LA,NB+1,LB-1,L,X)                   TLYDEL     31
     1   + SQRT( NB+ 1.)*RADQ(NA+1,LA,NB+2,LB-1,L,X)          $ GOTO 14         TLYDEL     32
    3 RMO= SQRT(LB+NB+.5)*RDFUNC(NB,LB-1,X)                                     TLYDEL     33
     1    + SQRT(NB+1.)*RDFUNC(NB+1,LB-1,X)                                    TLYDEL     34
   14 CONTINUE                                                                  TLYDEL     35
      LPA= LA+L $ LMA= IABS(LA-L)                                               TLYDEL     36
      IF (LPA+1 .LT. LB .OR. LMA+1 .GT. LB) GOTO 4                              TLYDEL     37
      TLYDEL=-SQRT(LB*(I3-1.))*CG000(LA,L,LB-1)                                 TLYDEL     38
*     RACAH IS W(LB,1,LA,L,LB-1,LAM)                                            TLYDEL     39
      TLYDEL= TLYDEL*FWCOEF(I1,I2,I3,I4,I5,I6)*RMO                              TLYDEL     40
    4 IF (LPA-1 .LT. LB .OR. LMA-1 .GT. LB) GOTO 5                              TLYDEL     41
      IF (RHO) GOTO 6                                                           TLYDEL     42
      RMO= RMO- (I3+1)*X/(L+L+1.)                                               TLYDEL     43
     1 *( RADQ(NA+1,LA,NB+1,LB,L-1,X)+ RADQ(NA+1,LA,NB+1,LB,L+1,X))             TLYDEL     44
      GOTO 15                                                                   TLYDEL     45
    6 RMO= RMO-          (I3+1)*RDFUNC(NB,LB,X)/X                             TLYDEL     46
   15 CONTINUE                                                                  TLYDEL     47
      RMO= RMO*SQRT((LB+1.)*(I3+3))*CG000(LA,L,LB+1)                            TLYDEL     48
*     RACAH IS W(LB,1,LA,L,LB+1,LAM)                                            TLYDEL     49
      TLYDEL= TLYDEL+ RMO*FWCOEF(I1,I2+2,I3+2,I1,I5,I6)                         TLYDEL     50
    5 TLYDEL= TLYDEL*FAS $ RETURN                                               TLYDEL     51
      END                                                                       TLYDEL     52
```

FORMFAC

```
      SUBROUTINE FORMFAC(CHARGE,SPIN,ICO,J,L,Q,IRQA,N,B)                    FORMFAC    2
*                                                                           FORMFAC    3
*     COMPUTE FORM FACTORS                                                  FORMFAC    4
*     ROUTINE SIMILAR TO CURRENT, EXCEPT THAT THE DELTA FUNTION IN          FORMFAC    5
*     X IS REPLACED BY THE SPHERICAL BESSEL FUNCTION OF ORDER J.            FORMFAC    6
*     FOR MAGNETIC FORM FACTOR, USE THE RELATION                            FORMFAC    7
*        MAG*(D+ CURL(MU)) = -K*( -LONG*L/SQRT(J*J+J) + ELEC*MU )           FORMFAC    8
*       D = K**9 , X = R/B , K IS THE MOMENTUM-TRANSFER.                    FORMFAC    9
*                                                                           FORMFAC   10
      COMMON/CFACTOR/GLP,GLN,MUSP,MUSN,EFC(2),EFM(2),BOHR,TRI               FORMFAC   11
      REAL MUSP,MUSN,MUS      $ LOGICAL SLNAB,SJL                           FORMFAC   12
      DIMENSION IRQA(1) $ LOGICAL IPASS                                     FORMFAC   13
      DATA IPASS,ESP/.F.,1.E-5/                                             FORMFAC   14
      DATA PI/3.1415 92653/, I22,I8/177777778,3778/                         FORMFAC   15
      SJL= J.NE.L                                                           FORMFAC   16
    1 CHARGE= SPIN= 0 $ IF (IABS(J-L) .GT. 1 .OR. J .LT. 1 ) RETURN         FORMFAC   17
      Z1= J*(J+ J+ 1) $ Z1= 1./SQRT(Z1)                                     FORMFAC   18
      Z2= (J+ 1)*(J+ J+ 1) $ Z2= 1./SQRT(Z2)                               FORMFAC   19
*     FIRST RECOVER QUANTUM NUMBERS AND DENSITY MATRIX ELEMENT FROM IRQ     FORMFAC   20
      DO 11 I= 1, N $ IRQ= IRQA(I) $ ISQ= SHIFT(IRQ,-59)                    FORMFAC   21
      ISQ= ISQ.A.1 $ S= ISQ $ ISQ= IRQ.A.I22 $ RQ= (S+S- 1.)*ISQ*ESP        FORMFAC   22
      ISQ= SHIFT(IRQ,-58) $ ISQ= ISQ .A. 1                                  FORMFAC   23
*     ISQ= 1 , PROTON,  = 0 , NEUTRON                                       FORMFAC   24
      GL= ISQ*(GLP+ EFC(1))+ (1- ISQ)*(GLN+ EFC(2))                         FORMFAC   25
      MUS= ISQ*(MUSP+ EFM(1))+ (1- ISQ)*(MUSN+ EFM(2))                      FORMFAC   26
      IRQ= SHIFT(IRQ, -22) $ IJUMP= 1                                       FORMFAC   27
    2 NLJ= IRQ .A. I8 $ JA= NLJ .A. 1  $ NLJ= NLJ/2 $ LA= NLJ .A. 15        FORMFAC   28
      JA= LA+JA $ NLJ= SHIFT(NLJ,-4) $ NA= NLJ .A. 7 $ GOTO (3,31) IJUMP    FORMFAC   29
    3 LB= LA $ JB= JA $ NB= NA $ ISQ= SHIFT(IRQ,-8) $ IJUMP=2$ GOTO 2       FORMFAC   30
*     HAVE Q.N. AND RQ, NOW COMPUTE DENSITY.  FIRST CHARGE                  FORMFAC   31
   31 SLNAB= NA.EQ.NB .A. (LA.EQ.LB)                                        FORMFAC   32
      IF  (SLNAB .A. SJL .A. (JA.EQ.JB) ) GOTO 11                           FORMFAC   33
      IFAS= LB+ J- LA $ IF (ICO.GT.-2) GOTO 4                               FORMFAC   34
*                                                                           FORMFAC   35
*     THIS SECTION COMPUTES COULOMB FORM FACTOR                             FORMFAC   36
*                                                                           FORMFAC   37
      IFAS= JB+ J+ IFAS/2 $ IFAS= IFAS .A. 1 $ FAS= 1- IFAS- IFAS           FORMFAC   38
      FAS= FAS*SQRT( JA*JB/PI)                                              FORMFAC   39
      CHARGE= CHARGE- FAS*RQ*GL*CLEBS(JA,JB,J)                              FORMFAC   40
     1      *RADQ(NA+1,LA,NB+1,LB,J,Q)                                     FORMFAC   41
      GOTO 11                                                               FORMFAC   42
    4 I6= LA+ LB $ IF (MOD(I6+L,2).EQ.0) GOTO 11 $ I5= JA+ JB- 1            FORMFAC   43
      IF (I5.LT.J .OR. IABS(JA-JB).GT.J) GOTO 11                            FORMFAC   44
      IF (SLNAB .A. SJL) GOTO 7                                             FORMFAC   45
      IF (I6.LT.J .OR. IABS(LA-LB).GT.J) GOTO 7 $ IF (ICO) 5,5,6            FORMFAC   46
    5                 I1= I5+ I6 $ I5= I5+ J $ I2= JA+ LB+ J              FORMFAC   47
      IFA= I2+ ( IFAS+1-IABS(J-L) )/2 $ IFA= IFA .A. 1                      FORMFAC   48
      I3= LB+ JA $ I4= LB+ JB $ I6= I6+ J $ FAS= 1- IFA- IFA                FORMFAC   49
      FAS= FAS*2.*SQRT( (LA+LA+1.)*JA*JB/(J+J+1.) )                         FORMFAC   50
*     RACAH IS W(LA,LB,JA,JB,J,1/2)                                         FORMFAC   51
      FAS= FAS*RQ*Q*FWCOEF(I1,I2,I3,I4,I5,I6)*GL $ IF(J.NE.L) GOTO 10       FORMFAC   52
      IF (LA+ LB.GE.J+1 .A. IABS(LA-LB).LE.J+1)                             FORMFAC   53
     1CHARGE= CHARGE- FAS*  Z1*TJYLL(NA,LA,NB,LB,J,J+1,Q)                   FORMFAC   54
      IF (LA+ LB.GE.J-1 .A. IABS(LA-LB).LE.J-1)                             FORMFAC   55
     1CHARGE= CHARGE- FAS*  Z2*TJYLL(NA,LA,NB,LB,J,J-1,Q)                   FORMFAC   56
      GOTO 7                                                                FORMFAC   57
   10 IFA= (J+1) .A. 1 $ TDQ= TLYDELQ(NA,LA,NB,LB,J,L,Q)                    FORMFAC   58
      TDQ= TDQ+ (1-IFA-IFA)*SQRT( (LB+LB+1.)/(LA+LA+1.) )                  FORMFAC   59
     1      *TLYDELQ(NB,LB,NA,LA,J,L,Q)                                    FORMFAC   60
   12 CHARGE= CHARGE- 0.5*FAS*TDQ/Q                                         FORMFAC   61
    7 IF (ICO) 11, 6, 6                                                     FORMFAC   62
*     NOW COMPUTE SPIN                                                      FORMFAC   63
    6 IF (J .EQ. L) GOTO 8                                                  FORMFAC   64
*     ELECTRIC MATRIX ELEMENT, L = J+1 OR J-1                               FORMFAC   65
      S= JA*JB*2./PI/(J+L+1.)/(J+J+1.) $ S= (L- J)*SQRT(S)                  FORMFAC   66
      XAB= (LA- JA+ 0.5)*(JA+ JA) - (LB- JB+ 0.5)*(JB+ JB)                  FORMFAC   67
      S= S*XAB*RADQ(NA+1,LA,NB+1,LB,J,Q)   $   GOTO 9                       FORMFAC   68
*     MAGNETIC MATRIX ELEMENT, L = J                                        FORMFAC   69
    8 S= JA*JB*J/PI/(J+ 1.) $ S= SQRT(S)/(J+J+1.)                           FORMFAC   70
      XAB= (LA- JA+ 0.5)*(JA+ JA) + (LB- JB+ 0.5)*(JB+ JB)                  FORMFAC   71
      S= S*( (XAB+ J+ 1.)*RADQ(NA+1,LA,NB+1,LB,J+1,Q)                       FORMFAC   72
     1    - (J+ 1.)/J*(XAB- J)*RADQ(NA+1,LA,NB+1,LB,J-1,Q) )              FORMFAC   73
    9 IFA= J+ JB+ ( IFAS+1- IABS(J-L) )/2 $ IFA= IFA .A. 1                  FORMFAC   74
      SPIN= SPIN-(1- IFA- IFA      )*CLEBS(JA,JB,J)*S*RQ*Q*MUS              FORMFAC   75
   11 CONTINUE $ IF (ICO .EQ. -2) RETURN                                    FORMFAC   76
      CHARGE= 2.*BOHR*TRI*CHARGE/B $ SPIN= BOHR*TRI*SPIN/B $ RETURN         FORMFAC   77
      END                                                                   FORMFAC   78
```

RADQ

```
      FUNCTION RADQ(NP,LP,NF,LF,L,Q)                                    RADQ      2
C                                                                       RADQ      3
C          PROGRAM CALCULATES THE RADIAL INTEGRAL                       RADQ      4
C          (NP,LP|| JL(QP) ||NF,LF)                                     RADQ      5
C          WHERE JL(P) IS THE SPHERICAL BESSEL FUNCTION OF ORDER L      RADQ      6
C          AND Q IS A DIMENSIONALESS QUANTITY.                          RADQ      7
C          NFACT(N) IS EQUAL TO FACTORIAL OF (N-1),                     RADQ      8
C          NDFACT(N) IS EQUAL TO DOUBLE FACTORIAL OF N,                 RADQ      9
C          GMMA(N) IS EQUAL TO GAMMA(N-.5)                              RADQ     10
C                                                                       RADQ     11
      DIMENSION GMMA(100),NFACT(50),NDFACT(100)                         RADQ     12
      LOGICAL IPASS                                                     RADQ     13
      DATA IPASS/.FALSE./                                               RADQ     14
      ENTRY RAQ                                                         RADQ     15
      IF((-1)**(LP+LF+L))10,10,21                                       RADQ     16
   21 IF(NF.LE.0)GOTO4$ IF(NP.LE.0)GOTO4$ IF(IPASS)GOTO2$ IPASS=.TRUE.  RADQ     17
      PI=3.14159265359$ B=SQRT(PI)$ X=-.5$ GMMA(1)=B$ DO3 I=2,100$X=X+1. RADQ     18
    3 GMMA(I)=X*GMMA(I-1)$ NFACT(1)=1$ DO5 I=2,50                       RADQ     19
    5 NFACT(I)=(I-1)*NFACT(I-1)$ NDFACT(1)=1$ NDFACT(2)=2$ DO7 I=3,100  RADQ     20
    7 NDFACT(I)=I*NDFACT(I-2)                                           RADQ     21
    2 RNF=NFACT(NF)                                                     RADQ     22
      RNP=NFACT(NP)                                                     RADQ     23
      RLF=NDFACT(2*LF+1)                                                RADQ     24
      RLP=NDFACT(2*LP+1)                                                RADQ     25
      RF=NDFACT(2*LF+2*NF-1)                                            RADQ     26
      RP=NDFACT(2*LP+2*NP-1)                                            RADQ     27
      IF(Q.LT.1.E-06) Q=1.E-06                                          RADQ     28
      A=((2.**(LF-NF+3))/B)*(RF/RNF)*(1./RLF**2)                        RADQ     29
      C=((2.**(LP-NP+3))/B)*(RP/RNP)*(1./RLP**2)                        RADQ     30
      AC=SQRT(A*C)                                                      RADQ     31
      SUM1=0.0                                                          RADQ     32
      DO 1 K=1,NF                                                       RADQ     33
      KT=K-1                                                            RADQ     34
      RK=NFACT(KT+1)                                                    RADQ     35
      RNK=NFACT(NF-KT)                                                  RADQ     36
      RFK=NDFACT(2*LF+2*KT+1)                                           RADQ     37
      S=((-1.)**KT*2.**KT*RNF*RLF)/(RK*RNK*RFK)                         RADQ     38
      SUM2=0.0                                                          RADQ     39
      DO 6 KP=1,NP                                                      RADQ     40
      KS=KP-1                                                           RADQ     41
      RKP=NFACT(KS+1)                                                   RADQ     42
      RNKP=NFACT(NP-KS)                                                 RADQ     43
      RFKP=NDFACT(2*LP+2*KS+1)                                          RADQ     44
      M=2*(KT+KS)+LF+LP+2                                               RADQ     45
      XS=FLOAT(M-L)*0.5-1.                                              RADQ     46
    9 NNS=XS                                                            RADQ     47
      I=FLOAT(L+M)*0.5+1.                                               RADQ     48
      XA=B*Q**L*GMMA(I)*EXP(-Q**2/4.)/(2.**(L+2)*GMMA(L+2))             RADQ     49
*                                                                       RADQ     50
*     FOLLOWING TO ST. NO.11 COMPUTE CONFL. HYPER-G 1F1(-NNS,L+1.5,QSQ/4) RADQ     51
*                                                                       RADQ     52
      QSQ4=Q*Q/4. $ SUMM= SUMN= 1. $ NSTP= NNS $ NSB= 1                 RADQ     53
      IF (NNS) 12, 11, 13                                               RADQ     54
   12 NSTP= QSQ4+ 5                                                     RADQ     55
   13 XD= -NNS $ XN= L+ 1.5                                             RADQ     56
   14 DO 8 NS= NSB, NSTP $ SUMN= SUMN*XD*QSQ4/XN/NS                     RADQ     57
      SUMM= SUMM+ SUMN $ XD= XD+ 1. $ XN= XN+ 1.                        RADQ     58
    8 CONTINUE $ IF ( (NNS.GT.0) .OR. (ABS(SUMN/SUMM).LT.1.E-6) )GOTO11 RADQ     59
      NSB= NSTP+ 1 $ NSTP= NSTP+ 5 $ GOTO 14                            RADQ     60
   11 SUM2=SUM2+XA*SUMM*(-1.)**KS*2.**KS*RNP*RLP/(RKP*RNKP*RFKP)        RADQ     61
    6 CONTINUE                                                          RADQ     62
      SUM1=SUM1+S*SUM2                                                  RADQ     63
    1 CONTINUE                                                          RADQ     64
      XLP=LP                                                            RADQ     65
      XLF=LF                                                            RADQ     66
      XL=L                                                              RADQ     67
      RAD1= RADQ= AC*SUM1                                               RADQ     68
      RETURN                                                            RADQ     69
   10 PRINT20                                                           RADQ     70
   20 FORMAT(10X*MESSAGE FROM RADQ----L+LP+LAMDA IS ODD, RADQ FAILS*)   RADQ     71
      RAD1= RADQ= 0.                                                    RADQ     72
      RETURN                                                            RADQ     73
    4 PRINT100                                                          RADQ     74
  100 FORMAT(10X*MESSAGE FROM RADQ ---*/                                RADQ     75
     1      10X*ERROR IN THE PRINCIPLE QUANTUM NUMBER OF THE OSCILLA-    RADQ     76
     2TOR WAVE FUNCTION. THE W.F. WITH ZERO NODE MUST HAVE N=1. *)      RADQ     77
      RETURN                                                            RADQ     78
      END                                                               RADQ     79
```

TJYLL

```
      FUNCTION TJYLL(NA,LA,NB,LB,LAM,L,Q)                                    TJYLL      2
*                                                                            TJYLL      3
*     REDUCED MATRIX ELEMENT OF T(LAM)( Y(L), L ) * J(L,Q)                   TJYLL      4
*        T(LAM)   IS  SPHERICAL TENSOR OF RANK LAM                           TJYLL      5
*        Y(L)     IS  SPHERICAL HARMONICS OF ORDER L                         TJYLL      6
*        L        IS  THE ORBITAL ANGULAR MOMENTUM OPERATOR                  TJYLL      7
*        J(L,Q)   IS  SPHERICAL BESSEL FUNCTION OF ORDER L, ARGUEMENT Q      TJYLL      8
*        Q = MOMENTUM-TRANSFER*LENGTH-PARAMETER, DIMENSIONLESS               TJYLL      9
*     ONLY ENTRY POINT TJYLT TEST ALL TRIANGULAR AND PARITY SELECTION        TJYLL     10
*     RULES.                                                                 TJYLL     11
*                                                                            TJYLL     12
      DATA PI/3.14159 92653/                                                 TJYLL     13
      TJYLL= 0 $ GOTO 1 $ ENTRY TJYLT $ TJYLL= 0                             TJYLL     14
      IF (IABS(J-L) .GT. 1) RETURN                                           TJYLL     15
      IF (LA+LB.LT.LAM .OR. IABS(LA-LB).GT.LAM) RETURN                       TJYLL     16
      IF (LA+LB.LT.L   .OR. IABS(LA-LB).GT.L  ) RETURN                       TJYLL     17
      IF (MOD(LA+LB+L,2).EQ.1) RETURN                                        TJYLL     18
*     FIRST COMPUTE ARGUEMENTS FOR FAST RACAH                                TJYLL     19
 1    I2= LB+ L+ LAM $ I3= LB+ LB+ 1 $ I4= LA+ LB+ L                         TJYLL     20
      I5= LA+ LB+ LAM $ I6= L+ LAM+ 1                                        TJYLL     21
*     COMPUTE GOEMETRIC FACTORS                                              TJYLL     22
      TJYLL= (LB+ LB+1)*(L+ L+ 1)*(LAM+ LAM+ 1)                              TJYLL     23
      TJYLL= 0.5*SQRT(TJYLL/PI)*I3                                           TJYLL     24
*     COMPUTE PHASE                                                          TJYLL     25
      TJYLL= TJYLL*(1- 2*MOD(LAM+ LB, 2) )                                   TJYLL     26
*     NOW COMPUTE THE REST, RACAH IS W(LB,1,LA,L,LB,LAM)                     TJYLL     27
      TJYLL= TJYLL*FWCOEF(I4+1,I2,I3,I5,I6)                                  TJYLL     28
      TJYLL= TJYLL*RADQ(NA+1,LA,NB+1,LB,L,Q)*CGOOO(LA,L,LB)                  TJYLL     29
      RETURN                                                                 TJYLL     30
      END                                                                    TJYLL     31
```

RDFUNC

```
      FUNCTION RDFUNC(N,L,X)                                                 RDFUNC     2
C     NORMALIZED H.O.RADIAL-FUNCTION UPTO NOSC=20 (NOSC=2*N+L)               RDFUNC     3
      DIMENSION FL(11),GL(21)                                                RDFUNC     4
      LOGICAL IPASS$ DATA IPASS/.F./                                         RDFUNC     5
      DATA N1MAX,L1MAX/11,21/                                                RDFUNC     6
      N1= N+1$ L1= L+1$ RDFUNC=0$ IF(N.LT.0.OR.L.LT.0) RETURN                RDFUNC     7
      NL= N+L+1$ IF(N1.GT.N1MAX.OR.NL.GT.L1MAX) GO TO 5                      RDFUNC     8
      IF(IPASS) GO TO 2$ IPASS= .T.$ FL(1)=0.$ GL(1)= ALOG(0.5)              RDFUNC     9
      DO 1 M = 2 , L1MAX$ A= M-1$ IF(M.GT.N1MAX) GO TO 1                     RDFUNC    10
      FL(M)= FL(M-1)+ALOG(A)                                                 RDFUNC    11
 1    GL(M)= GL(M-1)+ALOG(A+0.5)                                             RDFUNC    12
      A= 2./SQRT(3.141593)                                                   RDFUNC    13
 2    XSQ= X*X                                                               RDFUNC    14
C     EVALUATE LAGUERRE POLYNOMINAL POLAG(N,L+1/2,XSQ)                       RDFUNC    15
      POLAG= EXP(GL(NL)-GL(L1)-FL(N1))$ IF(N.EQ.0) GO TO 4$ B= 1.            RDFUNC    16
      DO 3 M=1,N$ B= -B*XSQ                                                  RDFUNC    17
 3    POLAG= POLAG+B*EXP(GL(NL)-GL(L1+M)-FL(N1-M)-FL(M+1))                   RDFUNC    18
 4    B= EXP(FL(N1)-GL(NL))$ B= SQRT(A*B)                                    RDFUNC    19
      RDFUNC= B*(X**L)*EXP(-0.5*XSQ)*POLAG$ RETURN                           RDFUNC    20
 5    PRINT6,N,L$ RETURN                                                     RDFUNC    21
 6    FORMAT(/1X,*XXXXX  N=*,I2,2X,*L=*,I2,2X,*N OR L TOO LARGE*,            RDFUNC    22
     11* CANNOT CALCULATE RADFNC.CHANGE DIMENSION AND DATA  XXXXX*)          RDFUNC    23
      END                                                                    RDFUNC    24
```

CLEBS

```
      FUNCTION CLEBS(A,B,J)                                                    CLEBS      2
*                                                                              CLEBS      3
*     COMPUTE 3-J COEFFICIENT (JA,JB,J/0.5,-0.5,0)                             CLEBS      4
*     JA,JB ASSUMED TO HALF-INTEGERS.  A= JA*0.5                               CLEBS      5
*     (FORMULA FROM BRINK AND SATCHLER, P.112 )                                CLEBS      6
*                                                                              CLEBS      7
      DIMENSION FACL(100) $ INTEGER A,B $ LOGICAL PASS                         CLEBS      8
      DATA PASS/.F./                                                           CLEBS      9
      IF (PASS) GOTO 1 $ PASS= .T. $ FACL(1)= 0 $ X= 1.                        CLEBS     10
      DO 10 K= 1, 99 $ FACL(K+1)= FACL(K)+ ALOG(X)                             CLEBS     11
   10 X= X+ 1.                                                                 CLEBS     12
*     FACL(K+1) IS EQUAL TO LOG OF K-FACTORIAL                                 CLEBS     13
    1 K= A+ B+ J- 1 $ IF (K .GT. 98) GOTO 2                                    CLEBS     14
      X= FACL(A+B-J)+ FACL(A-B+J+1)+ FACL(B-A+J+1)- FACL(K+2)                  CLEBS     15
      K= J+ MOD(K,2) $ X= 0.5*X+ FACL( (K+B+A+1)/2 )                           CLEBS     16
     1  - FACL( (A+B-K+1)/2 ) - FACL( (A+K-B+1)/2 )- FACL((B+K-A+1)/2 )         CLEBS     17
      X= EXP(X)*2./SQRT(4.*A*B)                                                CLEBS     18
      CLEBS= -(1- 2*MOD( (A+B+K-1)/2, 2) )*X $ RETURN                          CLEBS     19
    2 PRINT 100 $ STOP                                                         CLEBS     20
  100 FORMAT(/1X10H**********,*MESSAGE FROM FUNCTION CLEBS, JA+JB+J GT        CLEBS     21
     1 98. INCREASE DIMENSION OF FACL IF NECESSARY*10H**********)              CLEBS     22
      END                                                                      CLEBS     23
```

CG000

```
      FUNCTION CG000(IA,IB,IC)                                                 CG000      2
C     SUBROUTINE TO CALCULATE THE 3-J SYMBOL (A,B,C/0,0,0)                     CG000      3
C     THE TRIANGULAR INEQUALITIES ARE ALREADY SATISFIED.                       CG000      4
C     ALSO (-1)**(A+B+C)=+1 HAS BEEN SATISFIED.                                CG000      5
      DIMENSION FL(130)                                                        CG000      6
      DATA IPASS/0/                                                            CG000      7
      IF(IPASS.EQ.1) GOTO23 FL(1)=0$DO 01 K=2,130$ A=K-1                       CG000      8
    1 FL(K)=FL(K-1)+ALOG(A)$ IPASS=1                                           CG000      9
    2 CG000=.0                                                                 CG000     10
      IF(IC.GT.(IA+IB).OR.IC.LT.IABS(IA-IB)) RETURN                            CG000     11
      IF((-1)**(IA+IB+IC).NE.1) RETURN                                         CG000     12
      IAB=IA+IB                                                                CG000     13
   40 IG2=IAB+IC                                                               CG000     14
      IG2P=IG2+2                                                               CG000     15
      IG=IG2/2                                                                 CG000     16
      ICP=IC+1                                                                 CG000     17
      IACMBP=IA-IB+ICP                                                         CG000     18
      IBCMAP=IB-IA+ICP                                                         CG000     19
      IABMCP=IAB-IC+1                                                          CG000     20
   70 IGP1=IG+1                                                                CG000     21
      IGMAP1=IGP1-IA                                                           CG000     22
      IGMBP1=IGP1-IB                                                           CG000     23
      IGMCP1=IGP1-IC                                                           CG000     24
      IGD2=IG/2                                                                CG000     25
      NSIG=IG-IGD2-IGD2                                                        CG000     26
      SIG=1-NSIG-NSIG                                                          CG000     27
      X=FL(IGP1)-FL(IGMAP1)-FL(IGMBP1)-FL(IGMCP1)                              CG000     28
      DLG=.5*(FL(IACMBP)+FL(IBCMAP)+FL(IABMCP)-FL(IG2P))                       CG000     29
      YLG=X+DLG                                                                CG000     30
      Y=EXP(YLG)                                                               CG000     31
      TJ=SIG*Y                                                                 CG000     32
      CG000=TJ                                                                 CG000     33
      RETURN                                                                   CG000     34
      END                                                                      CG000     35
```

WCOEF

```
      FUNCTION WCOEF(A,B,C,D,E,F)                                          WCOEF      2
*  THIS PROGRAM, WRITTEN BY R.Y.CUSSON AND J.H.SCHMIDT IN SEPT. 1971,       WCOEF      3
*  USES REGGES FORMULA (NUOVO CIMENTO,VOL11(1959),P116) TO EVALUATE THE     WCOEF      4
*  RACAH COEFFICIENT W(A,B,C,D,E,F)=(-1)**(A+B+C+D)*SIXJ(A,B,E/D,C,F) .     WCOEF      5
*                                                                           WCOEF      6
*  SINCE MANY PROGRAMS WHICH USE RACAH COEFFICIENTS ALSO USE CLEBSCH -      WCOEF      7
*  GORDANS, COMMON BLOCK CGRACAH HAS BEEN SET UP SO TABLES OF LOGS AND      WCOEF      8
*  SQUARE ROOTS DO NOT HAVE TO BE CALCULATED EACH TIME THE FUNCTIONS        WCOEF      9
*  ARE CALLED. NOTE THAT ALOGF(0) IS SOMETIMES REQUIRED IN THE              WCOEF     10
*  CALCULATIONS AND SO ALOGF0=ALOGF(0)=0.                                   WCOEF     11
*                                                                           WCOEF     12
*  COMMON BLOCK RACASYS IS INCLUDED TO ENSURE THAT ALL ITS ELEMENTS ARE     WCOEF     13
*  STORED SEQUENTIALLY IN CORE. THIS IS IMPORTANT FOR EQUIVALENCING.        WCOEF     14
*                                                                           WCOEF     15
*  COMMON BLOCK XRACAH IS USED IN CALCULATING X-COEFFICIENTS.               WCOEF     16
                                                                           WCOEF     17
      COMMON/CGRACAH/INITIAL,ALOGF0,ALOGF(80),SQRF(80)                     WCOEF     18
      COMMON/RACASYS/X1,X2,X3,Y1,Y2,Y3,Y4,IX1,IX2,IX3,IY1,IY2,IY3,IY4      WCOEF     19
      COMMON/XRACAH/JOUT,JXSWTCH                                           WCOEF     20
      DIMENSION RV(7),IV(7)                                                WCOEF     21
      EQUIVALENCE (RV,X1),(IV,IX1,VA),(IX2,VB),(IY1,VC),(IY2,VD),          WCOEF     22
     1 (IY3,VE),(IY4,VF)                                                   WCOEF     23
      DATA INITIAL/0/,ALOGF0/0./,JXSWTCH/0/                                WCOEF     24
 400  FORMAT(*  ILLEGAL PARAMETERS IN WCOEF(*,6F5.1,*)*)                   WCOEF     25
*  ENSURES THAT ALOGF AND SQRF ARE SET UP ONLY ONCE IN EACH PROGRAM         WCOEF     26
      IF (INITIAL .NE. 0) GO TO 20                                         WCOEF     27
      ALOGF(1)=0.                                                          WCOEF     28
      SQRF(1)=1.    $    SM=1.                                            WCOEF     29
      DO 25 J=2,80                                                         WCOEF     30
      SM=SM+1.                                                             WCOEF     31
      SQRF(J)=SQRT(SM)                                                     WCOEF     32
 25   ALOGF(J)=ALOGF(J-1)+ALOG(SM)                                         WCOEF     33
      INITIAL = 1                                                          WCOEF     34
 20   SIXJ=1.     $     IFAS=0     $     WCOEF=0.                         WCOEF     35
*  SET UP THE REGGE SYMBOL                                                 WCOEF     36
      Y4= A+B     $     Y3=C+D       $     Y2=E+F                         WCOEF     37
      X1=Y4+Y3    $     X2=A+D+Y2    $     X3=B+C+Y2                      WCOEF     38
      Y1=Y4+E     $     Y2=Y3+E      $     Y3=A+C+F     $     Y4=B+D+F     WCOEF     39
*   CHECK THAT THE REGGE SYMBOL CONTAINS ONLY NON-NEGATIVE INTEGERS         WCOEF     40
      DO 1 K=1,7                                                           WCOEF     41
      J=ABS(RV(K))                                                         WCOEF     42
      IF (FLOAT(J) .NE. RV(K)) GO TO 998                                   WCOEF     43
 1    IV(K)= J                                                             WCOEF     44
*  CHECK FOR TRIANGLE AND IN RANGE CONDITION .                             WCOEF     45
      GO TO 201                                                            WCOEF     46
      ENTRY FWCOEF                                                         WCOEF     47
*  CALLING SEQUENCE IS F=FWCOEF(IX1,IX2,IY1,IY2,IY3,IY4)  WHERE            WCOEF     48
*          IX1 = A+B+C+D                 IY2=C+D+E                      WCOEF     49
*          IX2 = A+D+E+F                 IY3=A+C+F                      WCOEF     50
*          IY1 = A+B+E                   IY4=B+D+F                      WCOEF     51
*  IF PARAMETERS ARE LEGAL THE VALUE OF WCOEF(A,B,C,D,E,F) IS RETURNED      WCOEF     52
*  WCOEF MUST BE CALLED FIRST TO INITIALISE /CGRACAH/                       WCOEF     53
*  NOTE - IF FWCOEF IS CALLED, NO ARGUMENT CHECKING IS DONE                 WCOEF     54
      VA=A$ VB=B$ VC=C$ VD=D$ VE=E$ VF=F                                   WCOEF     55
      IX3= IY1+IY2+IY3+IY4-IX1-IX2                                         WCOEF     56
 201  IY0= MAX0(IY1,IY2,IY3,IY4)                                           WCOEF     57
      IX0= MIN0(IX1,IX2,IX3)                                               WCOEF     58
```

WCOEF (CONTINUED)

```
      IF (IY0 .GT. 78) GO TO 998                                          WCOEF     59
      X=IX0-IY0+1                                                         WCOEF     60
      IF (X .LT. 1.) GO TO 996                                            WCOEF     61
      IFAS=IX1                                                            WCOEF     62
      IF (IX0 .LT. 0) GO TO 999                                           WCOEF     63
*   THE EXPRESSION (IY0 .AND. 1) SIMPLY CHECKS IF IY0 IS ODD OR EVEN      WCOEF     64
      K=IY0 .AND. 1                                                       WCOEF     65
*  NOTE   DELC IS EVALUATED AS FOLLOWS                                    WCOEF     66
*          DELC=(1)-(2)+((3)-(4))                                         WCOEF     67
*  WHERE       (1)=SUM OF SMALLER LOGS                                    WCOEF     68
*              (2)=SUM OF SMALLER LOGS                                    WCOEF     69
*              (3)=MOST LIKELY TO BE THE LARGEST LOG                      WCOEF     70
*              (4)=SUM OF LARGE LOGS                                      WCOEF     71
      DELC=((ALOGF(IX1-IY1)+ALOGF(IX1-IY2)+ALOGF(IX1-IY3)+ALOGF(IX1-IY4)  WCOEF     72
     1       +ALOGF(IX2-IY1)+ALOGF(IX2-IY2)+ALOGF(IX2-IY3)+ALOGF(IX2-IY4)  WCOEF     73
     2 +ALOGF(IX3-IY1)+ALOGF(IX3-IY2)+ALOGF(IX3-IY3)+ALOGF(IX3-IY4))*.5)   WCOEF     74
     3     - (ALOGF(IY0-IY1)+ALOGF(IY0-IY2)+ALOGF(IY0-IY3)+ALOGF(IY0-IY4)  WCOEF     75
     4       +ALOGF(IX1-IY0)+ALOGF(IX2-IY0)+ALOGF(IX3-IY0))+(ALOGF(IY0+1)  WCOEF     76
     5       -.5*(ALOGF(IY1+1)+ALOGF(IY2+1)+ALOGF(IY3+1)+ALOGF(IY4+1)))    WCOEF     77
      DELC=(1-K-K)*EXP(DELC)                                              WCOEF     78
*   INITIALISE THE SUM                                                    WCOEF     79
      SM=1.                                                               WCOEF     80
      IF (X .LE. 1.) GO TO 13                                             WCOEF     81
      Z0=IX0+3                                                            WCOEF     82
      K=IX0+1   $  X1=IX1-K  $  X2=IX2-K  $  X3=IX3-K                     WCOEF     83
      K=K+1     $  Y1=K-IY1  $  Y2=K-IY2  $  Y3=K-IY3  $  Y4=K-IY4        WCOEF     84
*   THE SUM IS DONE RECURSIVELY WITHOUT ALOGF                             WCOEF     85
*  NOTE BECAUSE OF THE DEFINITION OF X, THE SUM FROM 2 TO X IS THE        WCOEF     86
*  SAME AS THE SUM FROM IY0 TO IX0                                        WCOEF     87
      XK=2.                                                               WCOEF     88
 15   SM= 1.-SM*(Z0-XK)*(X1+XK)*(X2+XK)*(X3+XK)/                          WCOEF     89
     1 ((Y1-XK)*(Y2-XK)*(Y3-XK)*(Y4-XK))                                  WCOEF     90
      XK=XK+1.                                                            WCOEF     91
      IF (XK .LE. X) GO TO 15                                             WCOEF     92
*   SIXJ IS THE USUAL 6-J SYMBOL OF WIGNER .                              WCOEF     93
 13   SIXJ= DELC*SM                                                       WCOEF     94
 999  IFAS=IFAS .AND. 1                                                   WCOEF     95
      WCOEF=SIXJ*(1-IFAS-IFAS)                                            WCOEF     96
 997  RETURN                                                              WCOEF     97
*  JXSWTCH DETERMINES WHETHER OR NOT WCOEF WAS CALLED BY XCOEF. IF IT     WCOEF     98
*  WAS, NO ERROR MESSAGE IS PRINTED BY WCOEF                              WCOEF     99
 998  IF (JXSWTCH .EQ. 0) GO TO 996                                       WCOEF    100
      JOJT=1   $   JXSWTCH=0                                              WCOEF    101
      GO TO 997                                                           WCOEF    102
 996  PRINT 400,A,B,C,D,E,F                                               WCOEF    103
      GO TO 997                                                           WCOEF    104
      END                                                                 WCOEF    105
```

LINPLOT

```
      SUBROUTINE LINPLOT(X,Y,Z,DX,N,NAME,SNAME)                                 LINPLOT     2
      DIMENSION X(50),Y(50),Z(50),NAME(4),SNAME(3)                              LINPLOT     3
      DATA FORM1/6H(F7.4)/,FORM2/10H(F10.2A10)     /,FORM3/6H(F5.2)/            LINPLOT     4
      DATA FORM4/6H(4A10)/                                                      LINPLOT     5
*     FIND MAX ABSOLUTE VALUE FOR ARRAY Y AND Z                                 LINPLOT     6
      AM=0.0                                                                    LINPLOT     7
      DO 1 I=1,N                                                                LINPLOT     8
    1 AM=AMAX1(AM,ABS(Y(I)),ABS(Z(I)))                                          LINPLOT     9
      IF(AM)6,6,7                                                               LINPLOT    10
    6 PRINT 8,NAME                                                              LINPLOT    11
      GO TO 9                                                                   LINPLOT    12
    8 FORMAT(*0*,5A10,* ARRAYS ARE ZERO*)                                       LINPLOT    13
*     SELECT VERTICAL SCALE FACTORAPPLICABLE WHEN AM IS LESS THAN 1             LINPLOT    14
    7 AM=2*AM  $ NP=0                                                           LINPLOT    15
    2 IF(AM.GT.1) GO TO 3  $  NP = NP +1  $ AM = AM*10 $ GO TO 2                LINPLOT    16
    3 AM=AINT(AM+1.0)   $  AM=AM*10.0**(-NP)                                    LINPLOT    17
*     UPPER AND LOWER LIMITS FOR AXIS                                           LINPLOT    18
      YMAX= AM/2.$  YMIN = - YMAX $ XMIN = 0.0 $ XMAX = INT(X(N) + 1.0)         LINPLOT    19
*     PLOTTING THE FRAME                                                        LINPLOT    20
      TICX = 10* DX   $ TICY = AM*0.1  $ XL = XMAX/(10*DX)                      LINPLOT    21
      CALL PLOT(1,XL,10.0,XMIN,XMAX,YMIN,YMAX,TICX,TICY)                        LINPLOT    22
*     PLOTTING THE ARRAYS  BOTH ON THE SAME FRAME                               LINPLOT    23
      CALL PLOT(2,1,8,X,Y,N) $ CALL PLOT(2,1,0,X,Z,-N)                          LINPLOT    24
*     LABELS ON  Y AXIS                                                         LINPLOT    25
      DO 4 I=1,11     $  XLOC= XMIN -0.8*TICX                                   LINPLOT    26
      ARR = YLOC = YMIN + (I-1)*TICY                                            LINPLOT    27
    4 CALL PLOT(3,FORM1,1.0,0,XLOC,YLOC,ARR,1)                                  LINPLOT    28
*     IDENTIFICATION ON UPPER AXIS                                              LINPLOT    29
      XLOC=XMIN   $  YLOC= YMAX + 0.2 * TICY                                    LINPLOT    30
      CALL PLOT(3,FORM4,1.0,0,XLOC,YLOC,NAME,4)                                 LINPLOT    31
      XLOC= XMIN+3.5*TICX$    CALL PLOT(3,FORM2,1.0,0,XLOC,YLOC,SNAME,3)        LINPLOT    32
*     LABELS ON XAXIS                                                           LINPLOT    33
      YLOC= YMIN - 0.2*TICY  $ IXL= INT(XL) +1                                  LINPLOT    34
      DO 5 I= 1,IXL     $ XLOC = XMIN + (I-1)*TICX - 0.3*TICX                   LINPLOT    35
      ARP = XMIN + (I-1)*TICX                                                   LINPLOT    36
    5 CALL PLOT(3,FORM3,1.0,0,XLOC,YLOC,APR,1)                                  LINPLOT    37
    9 RETURN                                                                    LINPLOT    38
      END                                                                       LINPLOT    39
```

SEMILOG

```
      SUBROUTINE SEMILOG(X,Y,Z,YZ,DO,N,NAME,SNAME,EXL,NC)                       SEMILOG     2
      DIMENSION X(50),Y(50),Z(50),YZ(50),NAME(4),SNAME(3)                       SEMILOG     3
      DATA FORM/10H(F10.2A10)/                                                  SEMILOG     4
      DATA FORM4/6H(4A10)/                                                      SEMILOG     5
      DATA FORMX/8HO(MEV) /,FORMY/10HFORMFACTOR  /,FORMSL/6H(F5.1)/             SEMILOG     6
*     SET LIMITS FOR PLOT  YMAX = 10EXP EXL, CYCLES = NC                        SEMILOG     7
      XMIN=0$XMAX=X(N)$TIC=5.*DO$XL=XMAX/TIC$YL=10                              SEMILOG     8
      CALL SMLOGY(XL,YL,XMIN,XMAX,TIC,EXL,NC,FORMX,8,FORMY,12,FORMSL,5)         SEMILOG     9
*     F(CHARGE) SYMBOL 7 FOR NEGATIVE VALUES AND 8 FOR POSITIVE                 SEMILOG    10
      DO 1 I=1,N                                                                SEMILOG    11
      IF(Y(I)-0.)2,3,4                                                          SEMILOG    12
    2 SYMB1=7$Y(I)=ALOG10(ABS(Y(I)))$GO TO 5                                    SEMILOG    13
    4 SYMB1=8 $ Y(I)=ALOG10(Y(I)) $ GO TO 5                                     SEMILOG    14
    3 Y(I) = -10 $ SYMB1= 8                                                     SEMILOG    15
    5 CALL PLOT(2,1,SYMB1,X(I),Y(I),1)                                          SEMILOG    16
    1 CONTINUE                                                                  SEMILOG    17
*     F(SPIN) SYMBOL 1 FOR NEG AND 2 FOR POSITIVE                               SEMILOG    18
      DO 11 I=1,N                                                               SEMILOG    19
      IF(Z(I)-0.) 6,7,8                                                         SEMILOG    20
    6 SYMB2=1 $ Z(I) = ALOG10(ABS(Z(I)))  $ GO TO 9                             SEMILOG    21
    7 SYMB2=2 $ Z(I) = -10 $ GO TO 9                                            SEMILOG    22
    8 SYMB2=2  $ Z(I) = ALOG10(Z(I))                                            SEMILOG    23
    9 CALL PLOT(2,1,SYMB2,X(I),Z(I),1)                                          SEMILOG    24
   11 CONTINUE                                                                  SEMILOG    25
      SYMB3=6$ DO 12 I=1,N                                                      SEMILOG    26
   12 YZ(I)=ALOG10(YZ(I))                                                       SEMILOG    27
      CALL PLOT(2,1,SYMB3,X,YZ,N)                                               SEMILOG    28
*     WRITE LABEL                                                               SEMILOG    29
      YLOC=EXL+0.05 $ XLOC=0.0 $ CALL PLOT(3,FORM4,1,0,XLOC,YLOC,NAME,4)        SEMILOG    30
      XLOC=4.0 $ CALL PLOT(3,FORM,1,0.,XLOC,YLOC,SNAME,3)                       SEMILOG    31
      RETURN                                                                    SEMILOG    32
      END                                                                       SEMILOG    33
```

Case No. 1: $|f> = |(\pi 1S_{1/2})(\pi 0d_{5/2})^{-1};2^{+}>$; Coulomb transition

```
  1 2.000 .100    48 20.0300.0 -0.0 -0.0 20.0 -0.0 -0.0 -0.0 -0.0 2 2-0-0


TEST CASE NO.1, 2+,P(0D5/2)-P(1S1/2),B=2.0(F)                          COULOMB
33  51 1.00000
    600000004101203032 40

TEST CASE NO.1, 2+,P(0D5/2)-P(1S1/2),B=2.0(F)
    COULOMB    J=2 L=2,  X=R/B, DENSITY TIMES B-CUBED IS PRINTED
```

X	CHARGE	SPIN	TOTAL
.10	.43376E-02	0.	.43376E-02
.20	.16499E-01	0.	.16499E-01
.30	.34102E-01	0.	.34102E-01
.40	.53721E-01	0.	.53721E-01
.50	.71563E-01	0.	.71563E-01
.60	.84192E-01	0.	.84192E-01
.70	.89150E-01	0.	.89150E-01
.80	.85337E-01	0.	.85337E-01
.90	.73108E-01	0.	.73108E-01
1.00	.54086E-01	0.	.54086E-01
1.10	.30768E-01	0.	.30768E-01
1.20	.60192E-02	0.	.60192E-02
1.30	-.17422E-01	0.	-.17422E-01
1.40	-.37343E-01	0.	-.37343E-01
1.50	-.52299E-01	0.	-.52299E-01
1.60	-.61682E-01	0.	-.61682E-01
1.70	-.65646E-01	0.	-.65646E-01
1.80	-.64922E-01	0.	-.64922E-01
1.90	-.60589E-01	0.	-.60589E-01
2.00	-.53856E-01	0.	-.53856E-01
2.10	-.45867E-01	0.	-.45867E-01
2.20	-.37585E-01	0.	-.37585E-01
2.30	-.29723E-01	0.	-.29723E-01
2.40	-.22736E-01	0.	-.22736E-01
2.50	-.16852E-01	0.	-.16852E-01
2.60	-.12120E-01	0.	-.12120E-01
2.70	-.84685E-02	0.	-.84685E-02
2.80	-.57537E-02	0.	-.57537E-02
2.90	-.38042E-02	0.	-.38042E-02
3.00	-.24494E-02	0.	-.24494E-02

3.10	-.15367E-02	0.	-.15367E-02
3.20	-.93982E-03	0.	-.93982E-03
3.30	-.56058E-03	0.	-.56058E-03
3.40	-.32623E-03	0.	-.32623E-03
3.50	-.18529E-03	0.	-.18529E-03
3.60	-.10274E-03	0.	-.10274E-03
3.70	-.55632E-04	0.	-.55632E-04
3.80	-.29424E-04	0.	-.29424E-04
3.90	-.15204E-04	0.	-.15204E-04
4.00	-.76769E-05	0.	-.76769E-05
4.10	-.37885E-05	0.	-.37885E-05
4.20	-.18275E-05	0.	-.18275E-05
4.30	-.86186E-06	0.	-.86186E-06
4.40	-.39742E-06	0.	-.39742E-06
4.50	-.17921E-06	0.	-.17921E-06
4.60	-.79038E-07	0.	-.79038E-07
4.70	-.34095E-07	0.	-.34095E-07

TEST CASE NO.1, 2+,P(005/2)-P(1S1/2),B=2.0(F) BORN APPROX COULOMB

Q(MEV/C)	Q(1/FM)	F(CHARGE)	FC.SQ	F(SPIN)	FS.SQ	FTOTAL.SQ
1.000	.005	-.66919E-05	.70343E-11	0.	0.	.70343E-11
21.000	.106	-.29015E-02	.13224E-05	0.	0.	.13224E-05
41.000	.208	-.10542E-01	.17456E-04	0.	0.	.17456E-04
61.000	.309	-.21551E-01	.72954E-04	0.	0.	.72954E-04
81.000	.410	-.33974E-01	.18130E-03	0.	0.	.18130E-03
101.000	.512	-.45652E-01	.32738E-03	0.	0.	.32738E-03
121.000	.613	-.54626E-01	.46873E-03	0.	0.	.46873E-03
141.000	.715	-.59465E-01	.55545E-03	0.	0.	.55545E-03
161.000	.816	-.59477E-01	.55567E-03	0.	0.	.55567E-03
181.000	.917	-.54760E-01	.47103E-03	0.	0.	.47103E-03
201.000	1.019	-.46101E-01	.33385E-03	0.	0.	.33385E-03
221.000	1.120	-.34766E-01	.18986E-03	0.	0.	.18986E-03
241.000	1.221	-.22233E-01	.77648E-04	0.	0.	.77648E-04
261.000	1.323	-.99311E-02	.15492E-04	0.	0.	.15492E-04
281.000	1.424	.96700E-03	.14688E-06	0.	0.	.14688E-06

Case No. 2: $|f> = |(\pi 1S_{1/2})(\pi 0d_{5/2})^{-1};2^{+}>$; Electric transition

```
  1 2.000 .100    48 20.0300.0 -0.0 -0.0 20.0 -0.0 -0.0 -0.0 -0.0 2 2-0-0


TEST CASE NO.2, 2+,P(0D5/2)-P(1S1/2),B=2.0(F)                          ELECTRIC
33  51 1.00000
    600000004101203032 40
```

TEST CASE NO.2, 2+,P(0D5/2)-P(1S1/2),B=2.0(F)
ELECTRIC J=2 L=1, X=R/B, DENSITY TIMES B-CUBED IS PRINTED

X	CHARGE	SPIN	TOTAL
.10	-.72207E-02	.19957E-01	.12737E-01
.20	-.13846E-01	.37180E-01	.23335E-01
.30	-.19354E-01	.49414E-01	.30060E-01
.40	-.23362E-01	.55256E-01	.31894E-01
.50	-.25662E-01	.54382E-01	.28699E-01
.60	-.26239E-01	.47426E-01	.21188E-01
.70	-.25247E-01	.35981E-01	.10734E-01
.80	-.22981E-01	.22053E-01	-.92844E-03
.90	-.19818E-01	.77673E-02	-.12051E-01
1.00	-.16163E-01	-.50105E-02	-.21173E-01
1.10	-.12394E-01	-.14938E-01	-.27332E-01
1.20	-.88272E-02	-.21319E-01	-.30147E-01
1.30	-.56910E-02	-.24097E-01	-.29788E-01
1.40	-.31191E-02	-.23726E-01	-.26845E-01
1.50	-.11577E-02	-.20995E-01	-.22152E-01
1.60	.21737E-03	-.16822E-01	-.16604E-01
1.70	.10793E-02	-.12085E-01	-.11006E-01
1.80	.15280E-02	-.74983E-02	-.59703E-02
1.90	.16711E-02	-.35503E-02	-.18793E-02
2.00	.16094E-02	-.49891E-03	.11105E-02
2.10	.14280E-02	.15966E-02	.30246E-02
2.20	.11923E-02	.28200E-02	.40122E-02
2.30	.94762E-03	.33382E-02	.42858E-02
2.40	.72213E-03	.33487E-02	.40708E-02
2.50	.53009E-03	.30401E-02	.35702E-02
2.60	.37607E-03	.25694E-02	.29454E-02
2.70	.25847E-03	.20519E-02	.23104E-02
2.80	.17241E-03	.15623E-02	.17347E-02
2.90	.11176E-03	.11406E-02	.12624E-02
3.00	.70486E-04	.80175E-03	.87224E-03

3.10	.43289E-04	.54417E-03	.58746E-03
3.20	.25908E-04	.35742E-03	.38333E-03
3.30	.15119E-04	.22756E-03	.24268E-03
3.40	.86076E-05	.14063E-03	.14924E-03
3.50	.47828E-05	.84456E-04	.89238E-04
3.60	.25948E-05	.49329E-04	.51924E-04
3.70	.13749E-05	.28044E-04	.29419E-04
3.80	.71170E-06	.15529E-04	.16240E-04
3.90	.36001E-06	.83791E-05	.87391E-05
4.00	.17799E-06	.44061E-05	.45861E-05
4.10	.86031E-07	.22619E-05	.23479E-05
4.20	.40657E-07	.11324E-05	.11731E-05
4.30	.18790E-07	.55338E-06	.57217E-06
4.40	.84935E-08	.26401E-06	.27251E-06
4.50	.37555E-08	.12300E-06	.12676E-06
4.60	.16245E-08	.55977E-07	.57602E-07
4.70	.68752E-09	.24880E-07	.25576E-07

TEST CASE NO.2, 2+,P(0D5/2)-P(1S1/2),B=2.0(F) BORN APPROX ELECTRIC

Q(MEV/C)	Q(1/FM)	F(CHARGE)	FC.SQ	F(SPIN)	FS.SQ	FTOTAL.SQ
1.000	.005	-.16891E-08	-.13083E-06	-.62832E-08	-.48670E-08	0.
21.000	.106	-.15467E-04	-.11980E-04	-.57210E-04	-.44315E-04	0.
41.000	.208	-.11150E-03	-.86364E-04	-.40581E-03	-.31434E-03	0.
61.000	.309	-.34845E-03	-.26991E-03	-.12343E-02	-.95609E-03	0.
81.000	.410	-.75846E-03	-.58750E-03	-.25838E-02	-.20014E-02	0.
101.000	.512	-.13392E-02	-.10373E-02	-.43293E-02	-.33534E-02	0.
121.000	.613	-.20546E-02	-.15915E-02	-.62061E-02	-.48072E-02	0.
141.000	.715	-.28417E-02	-.22012E-02	-.78725E-02	-.60980E-02	0.
161.000	.816	-.36227E-02	-.28061E-02	-.89909E-02	-.69644E-02	0.
181.000	.917	-.43182E-02	-.33449E-02	-.93062E-02	-.72085E-02	0.
201.000	1.019	-.48601E-02	-.37646E-02	-.87004E-02	-.67393E-02	0.
221.000	1.120	-.52012E-02	-.40288E-02	-.72141E-02	-.55880E-02	0.
241.000	1.221	-.53201E-02	-.41209E-02	-.50310E-02	-.38970E-02	0.
261.000	1.323	-.52217E-02	-.40447E-02	-.24337E-02	-.18851E-02	0.
281.000	1.424	-.49330E-02	-.38211E-02	.25513E-03	.19762E-03	0.

TEST CASE NO.2, 2+,P(0D5/2)-P(1S1/2),B=2.0(F)
ELECTRIC J=2 L=3, X=R/B, DENSITY TIMES B-CUBED IS PRINTED

X	CHARGE	SPIN	TOTAL
.10	-.23677E-04	.10966E-03	.85982E-04
.20	-.18382E-03	.84109E-03	.65727E-03
.30	-.59014E-03	.26453E-02	.20552E-02
.40	-.13043E-02	.56767E-02	.43724E-02
.50	-.23281E-02	.97433E-02	.74152E-02
.60	-.36040E-02	.14345E-01	.10741E-01
.70	-.50253E-02	.18788E-01	.13762E-01
.80	-.64565E-02	.22337E-01	.15880E-01
.90	-.77557E-02	.24379E-01	.16624E-01
1.00	-.87979E-02	.24546E-01	.15748E-01

1.10	-.94920E-02	.22775E-01	.13283E-01
1.20	-.97912E-02	.19304E-01	.95131E-02
1.30	-.96950E-02	.14606E-01	.49115E-02
1.40	-.92436E-02	.92843E-02	.40672E-04
1.50	-.85072E-02	.39558E-02	-.45513E-02
1.60	-.75725E-02	-.84509E-03	-.84178E-02
1.70	-.65300E-02	-.47368E-02	-.11267E-01
1.80	-.54623E-02	-.75183E-02	-.12981E-01
1.90	-.44374E-02	-.91615E-02	-.13599E-01
2.00	-.35042E-02	-.97767E-02	-.13281E-01
2.10	-.26921E-02	-.95640E-02	-.12256E-01
2.20	-.20135E-02	-.87637E-02	-.10777E-01
2.30	-.14670E-02	-.76130E-02	-.90801E-02
2.40	-.10418E-02	-.63169E-02	-.73588E-02
2.50	-.72136E-03	-.50315E-02	-.57529E-02
2.60	-.48726E-03	-.38609E-02	-.43481E-02
2.70	-.32119E-03	-.28616E-02	-.31828E-02
2.80	-.20667E-03	-.20527E-02	-.22594E-02
2.90	-.12985E-03	-.14274E-02	-.15573E-02
3.00	-.79687E-04	-.96342E-03	-.10431E-02
3.10	-.47774E-04	-.63179E-03	-.67956E-03
3.20	-.27987E-04	-.40291E-03	-.43089E-03
3.30	-.16023E-04	-.25005E-03	-.26607E-03
3.40	-.89674E-05	-.15112E-03	-.16008E-03
3.50	-.49065E-05	-.88979E-04	-.93888E-04
3.60	-.26250E-05	-.51070E-04	-.53695E-04
3.70	-.13734E-05	-.28585E-04	-.29958E-04
3.80	-.70277E-06	-.15607E-04	-.16310E-04
3.90	-.35176E-06	-.83159E-05	-.86676E-05
4.00	-.17224E-06	-.43250E-05	-.44973E-05
4.10	-.82516E-07	-.21963E-05	-.22788E-05
4.20	-.38676E-07	-.10892E-05	-.11279E-05
4.30	-.17741E-07	-.52764E-06	-.54536E-06
4.40	-.79633E-08	-.24972E-06	-.25769E-06
4.50	-.34982E-08	-.11549E-06	-.11899E-06
4.60	-.15041E-08	-.52204E-07	-.53708E-07
4.70	-.63300E-09	-.23065E-07	-.23698E-07

TEST CASE NO.2, 2+,P(0D5/2)-P(1S1/2),B=2.0(F)

BORN APPROX ELECTRIC

Q(MEV/C)	Q(1/FM)	F(CHARGE)	FC.SQ	F(SPIN)	FS.SQ	FTOTAL.SQ
1.000	.005	-.13791E-08	.74689E-18	-.51302E-08	.10336E-16	.16639E-16
21.000	.106	-.12628E-04	.62627E-10	-.46712E-04	.85686E-09	.13828E-08
41.000	.208	-.91036E-04	.32545E-08	-.33134E-03	.43114E-07	.70059E-07
61.000	.309	-.28451E-03	.31786E-07	-.10078E-02	.39886E-06	.65584E-06
81.000	.410	-.61928E-03	.15060E-06	-.21097E-02	.17478E-05	.29245E-05
101.000	.512	-.10935E-02	.46953E-06	-.35348E-02	.49068E-05	.84121E-05
121.000	.613	-.16775E-02	.11051E-05	-.50673E-02	.10083E-04	.17865E-04
141.000	.715	-.23202E-02	.21141E-05	-.64278E-02	.16225E-04	.30053E-04
161.000	.816	-.29579E-02	.34358E-05	-.73411E-02	.21163E-04	.41653E-04
181.000	.917	-.35258E-02	.48817E-05	-.75985E-02	.22673E-04	.48596E-04
201.000	1.019	-.39683E-02	.61838E-05	-.71038E-02	.19817E-04	.48142E-04
221.000	1.120	-.42467E-02	.70822E-05	-.58903E-02	.13625E-04	.40354E-04
241.000	1.221	-.43438E-02	.74098E-05	-.41078E-02	.66263E-05	.28050E-04
261.000	1.323	-.42635E-02	.71383E-05	-.19871E-02	.15506E-05	.15343E-04
281.000	1.424	-.40278E-02	.63707E-05	.20831E-03	.17041E-07	.57288E-05

Case No. 3: $|f\rangle = |(0p_{1/2})(0p_{3/2})^{-1}; 1^+, T=1\rangle$; Magnetic transition

```
 2 2.000 .100    48 20.0300.0 -0.0 -0.0 20.0 -0.0 -0.0 -0.0 -0.0 1 1-0-0


TEST CASE NO.3, 1+,T=1, (0P3/2)*(0P1/2), B=2.0(F)                    MAGNETIC
 2  31  .70710  2  30 -.70710
   6000000002060212066      0000000002060212066


TEST CASE NO.3, 1+,T=1, (0P3/2)*(0P1/2), B=2.0(F)
    MAGNETIC    J=1 L=1,  X=R/B, DENSITY TIMES B-CUBED IS PRINTED
```

X	CHARGE	SPIN	TOTAL
.10	-.25472E-02	-.58663E-02	-.84135E-02
.20	-.49439E-02	-.10689E-01	-.15633E-01
.30	-.70542E-02	-.13593E-01	-.20648E-01
.40	-.87697E-02	-.14014E-01	-.22784E-01
.50	-.10019E-01	-.11772E-01	-.21791E-01
.60	-.10770E-01	-.70867E-02	-.17857E-01
.70	-.11033E-01	-.51857E-03	-.11552E-01
.80	-.10853E-01	.71414E-02	-.37118E-02
.90	-.10301E-01	.15008E-01	.47075E-02
1.00	-.94650E-02	.22243E-01	.12778E-01
1.10	-.84394E-02	.28162E-01	.19723E-01
1.20	-.73149E-02	.32317E-01	.25002E-01
1.30	-.61716E-02	.34518E-01	.28346E-01
1.40	-.50737E-02	.34816E-01	.29742E-01
1.50	-.40676E-02	.33456E-01	.29389E-01
1.60	-.31823E-02	.30811E-01	.27629E-01
1.70	-.24308E-02	.27305E-01	.24874E-01
1.80	-.18137E-02	.23357E-01	.21543E-01
1.90	-.13224E-02	.19330E-01	.18007E-01
2.00	-.94247E-03	.15504E-01	.14561E-01
2.10	-.65674E-03	.12069E-01	.11412E-01
2.20	-.44756E-03	.91293E-02	.86818E-02
2.30	-.29835E-03	.67167E-02	.64184E-02
2.40	-.19458E-03	.48103E-02	.46157E-02
2.50	-.12417E-03	.33557E-02	.32315E-02
2.60	-.77545E-04	.22815E-02	.22040E-02
2.70	-.47399E-04	.15126E-02	.14652E-02
2.80	-.28360E-04	.97836E-03	.95000E-03
2.90	-.16611E-04	.61755E-03	.60093E-03
3.00	-.95254E-05	.38054E-03	.37102E-03

3.10	-.53482E-05	.22899E-03	.22364E-03
3.20	-.29403E-05	.13460E-03	.13166E-03
3.30	-.15829E-05	.77299E-04	.75716E-04
3.40	-.83454E-06	.43381E-04	.42547E-04
3.50	-.43090E-06	.23796E-04	.23365E-04
3.60	-.21790E-06	.12761E-04	.12543E-04
3.70	-.10793E-06	.66906E-05	.65827E-05
3.80	-.52358E-07	.34304E-05	.33780E-05
3.90	-.24880E-07	.17202E-05	.16953E-05
4.00	-.11581E-07	.84371E-06	.83212E-06
4.10	-.52809E-08	.40482E-06	.39954E-06
4.20	-.23589E-08	.19003E-06	.18767E-06
4.30	-.10322E-08	.87278E-07	.86246E-07
4.40	-.44251E-09	.39225E-07	.38783E-07
4.50	-.18585E-09	.17252E-07	.17066E-07
4.60	-.76472E-10	.74255E-08	.73491E-08
4.70	-.30828E-10	.31282E-08	.30974E-08

TEST CASE NO.3, 14,T=1, (0P3/2)*(0P1/2), B=2.0(F) BORN APPROX MAGNETIC

Q(MEV/C)	Q(1/FM)	F(CHARGE)	FC.SQ	F(SPIN)	FS.SQ	FTOTAL.SQ
1.000	.005	-.57773E-04	.31457E-09	.54306E-03	.27795E-07	.22196E-07
21.000	.106	-.11996E-02	.13563E-06	.11212E-01	.11849E-04	.94489E-05
41.000	.208	-.22687E-02	.48508E-06	.20865E-01	.41031E-04	.32594E-04
61.000	.309	-.32031E-02	.96694E-06	.28670E-01	.77469E-04	.61126E-04
81.000	.410	-.39541E-02	.14735E-05	.34037E-01	.10919E-03	.85292E-04
101.000	.512	-.44904E-02	.19004E-05	.36681E-01	.12681E-03	.97661E-04
121.000	.613	-.47998E-02	.21713E-05	.36636E-01	.12650E-03	.95526E-04
141.000	.715	-.48890E-02	.22527E-05	.34225E-01	.11039E-03	.81107E-04
161.000	.816	-.47804E-02	.21537E-05	.29979E-01	.84705E-04	.59845E-04
181.000	.917	-.45084E-02	.19157E-05	.24552E-01	.56811E-04	.37862E-04
201.000	1.019	-.41146E-02	.15956E-05	.18613E-01	.32651E-04	.19811E-04
221.000	1.120	-.36425E-02	.12504E-05	.12766E-01	.15360E-04	.78455E-05
241.000	1.221	-.31330E-02	.92513E-06	.74866E-02	.52824E-05	.17863E-05
261.000	1.323	-.26219E-02	.64788E-06	.30878E-02	.89861E-06	.20461E-07
281.000	1.424	-.21369E-02	.43035E-06	-.27926E-03	.73502E-08	.55019E-06

C.3 SPECIAL RELATIONS FOR CHECKING THE RESULTS

There are some special properties of the densities and form factors which are useful to know. Using the "form factors" given in equations (C.1,2)

$$\langle \vec{\mathcal{L}}_\lambda \cdot \vec{J} \rangle = \sqrt{4\pi}\ (\sqrt{\lambda}\ f_{\lambda,\lambda-1}(q) - \sqrt{\lambda+1}\ f_{\lambda,\lambda+1}(q)). \qquad (C.4)$$

Here $\langle\ \rangle$ means the reduced matrix element between the initial and final states.

For the magnetization current

$$\langle \vec{\mathcal{L}}_\lambda \cdot (\vec{\nabla}\times\vec{\mu}) \rangle \propto \langle \phi_\lambda \vec{\nabla}\cdot(\vec{\nabla}\times\vec{\mu})\rangle \equiv 0.$$

Therefore we have the first general relation

$$\text{(i)} \quad \sqrt{\lambda}\ f^m_{\lambda,\lambda-1} - \sqrt{\lambda+1}\ f^m_{\lambda,\lambda+1} \equiv 0; \quad \underline{\text{general}}. \qquad (C.5)$$

If the <u>convection current</u> is conserved we have

$$\langle \vec{\mathcal{L}}_\lambda \cdot \vec{J}^c \rangle = \frac{k}{q} \langle \phi_\lambda \rho \rangle,$$

where k is the wave-number of the energy transfer. This leads to the second relation

$$\text{(ii)} \quad \sqrt{\lambda}\ f^c_{\lambda,\lambda-1} - \sqrt{\lambda+1}\ f^c_{\lambda,\lambda+1} = \frac{k}{q}\ \hat{\lambda} f_\lambda; \ \underline{\text{if } \vec{J}^c \text{ conserved}}. \qquad (C.6)$$

This relation must be used with discretion since in a microscopic, many-body calculation $\vec{J}^c$ is almost never conserved. However in the single-particle model, where the one-body potential is momentum-independent, (ii) is satisfied. In the special case of harmonic oscillator, the energy difference in the transition $|b\rangle \to |a\rangle$ is

$$\Delta N\hbar\omega = (2n_a+\ell_a - 2n_b-\ell_b)\hbar\omega$$

and

$$k = \Delta N\cdot\hbar c/(Md^2)$$

where M is the nucleon mass and d is the oscillator length parameter. For such cases

$$\text{(iii)}\quad \sqrt{\lambda}\, f^c_{\lambda,\lambda-1} - \sqrt{\lambda+1}\, f^c_{\lambda,\lambda+1} = \frac{\Delta N\cdot\hbar c}{qMd^2}\,\hat{\lambda} f_\lambda ;$$

harm. osc. s.p. transition (C.7)

A special case for (iii) is when $|a\rangle$ and $|b\rangle$ are orbitals in the same shell, in which case $\Delta N = 0$; therefore the LHS of (C.7) must vanish.

We recall (see section 2.8) that $\vec{J}^c$ vanishes in an elastic transition. This can be extended to transitions between two s.p. states split by a simple spin-orbit interaction (constant $\times \vec{L}\cdot\vec{\sigma}$), since this

interaction does not affect the spatial wavefunctions. The harmonic oscillator model provides such an example. Therefore we have

$$\text{(iv)} \quad \rho^{C}_{\lambda,\lambda\pm1} = f^{C}_{\lambda,\lambda\pm1} \equiv 0; \quad \text{s.p. transition, } n_a=n_b, \ell_a=\ell_b. \tag{C.8}$$

Equations (C.4,6,7) can be used to check the results of MICRØDENS. Equation (C.8) has been incorporated into the coding of the program.

As was mentioned earlier, the form factors in MICRØDENS are calculated analytically rather than by Bessel transforming the computed densities. In particular the magnetic form factor is calculated using (the first line of) (A.27c') which involves formulas significantly different from those used in computing the magnetic density. Therefore an additional consistency check can be made by performing the integrations in (C.1,2).

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