

EVALIN

A CDC 6600 FORTRAN IV CODE
TO PERFORM AN
EXTENDED VARIATIONAL APPROXIMATION FOR LIGHT
AND INTERMEDIATE NUCLEI

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AECL-3801

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ABSTRACT

A computer code is described which performs an extended Hartree-Fock variational calculation for the intrinsic state of lighter nuclei having up to 82 protons and 82 neutrons. An exact treatment of the kinetic energy of the center-of-mass and the Coulomb two-body interaction is developed. The self-consistent orbitals can mix all the basis states including the time-reversed pairs but are restricted to having good parity; this results in an improved variational approximation which can be applied to odd nuclei. The neutron and proton wavefunctions are treated separately so as to exhibit the isospin violation due to the Coulomb force. The matrix elements of the nuclear interaction must be supplied as initial data. The initial trial wavefunction is taken to be that of the Nilsson model. Using the semi-realistic interaction No. 2 of Saunier & Pearson most calculated quantities are found to be within 10% of their experimental value, for nuclei with $4 \leq A \leq 40$.

Chalk River Nuclear Laboratories
Chalk River, Ontario
January, 1971

AECL-3801

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Code FORTRAN IV (CDC 6600) permettant
d'effectuer une approximation variationnelle étendue
pour les noyaux légers et intermédiaires

par

R.Y. Cusson et H.C. Lee

Résumé

Le code d'ordinateur décrit dans ce rapport effectue un calcul variationnel Hartree-Fock étendu pour l'état intrinsèque de noyaux légers ayant jusqu'à 82 protons et 82 neutrons. Le traitement exact de l'énergie synétique du centre de masse et de l'interaction Coulomb à deux corps est expliqué. Les orbitales harmonieuses peuvent mélanger tous les états de base y compris les paires à temps inversé mais elles doivent avoir une bonne parité; ce qui permet d'obtenir une approximation variationnelle améliorée pouvant être appliquée aux noyaux impairs. Les fonctions d'onde des protons et des neutrons sont traitées séparément ce qui facilite la détection de toute violation de l'isospin due à la force de Coulomb. Les éléments de la matrice de l'interaction nucléaire doivent être fournis comme données initiales. La fonction ondule de l'essai initial est considérée comme étant celle du modèle de Nilsson. En utilisant l'interaction semi-réaliste N^o2 de Saunier & Pearson, la plupart des quantités calculées sont cantonnées dans 10% de leur valeur expérimentale, pour les noyaux ayant $4 \leq A \leq 40$.

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Chalk River, Ontario
Janvier, 1971

AECL-3801

1. INTRODUCTION

It has become increasingly clear over the past few years that quantitative solutions of the nuclear many-body problem cannot be obtained reliably in restricted configuration spaces. If we let $H = T + V^{(2)}$ be the nuclear Hamiltonian consisting of the one-body kinetic energy operator T , and the two-body interaction potential $V^{(2)}$, we must solve the Schroedinger equation

$$H|\Psi\rangle = E|\Psi\rangle \quad (1.1)$$

in order to obtain the energy eigenvalues and eigenfunctions of the many-nucleon system. Since $|\Psi\rangle$ is antisymmetric in the A nucleon coordinates, it may be expanded in a basis consisting of single Slater determinants (SSD). The first sentence of this introduction refers to the fact that no single-particle basis has ever been found such that only one SSD will constitute a quantitatively accurate representation for the components of $|\Psi\rangle$ up to about 300 MeV.

The probable reason for this lack of convergence of SSD's to $|\Psi\rangle$ is that $|\Psi\rangle$ exhibits two-body correlations, over both large and small distances, which cannot be represented by SSD's. If we now think of the many-body Hilbert space of states of the $|\Psi\rangle$'s as being a direct product of one-particle spaces we can distinguish roughly three ingredients which must be present in order to obtain an accurate

representation for $|\Psi\rangle$: (i) the single particle basis should have a large dimension, (ii) highly excited 2-particle-2 hole (2p-2h) configurations must be included to account for short range effects, (iii) many coherent (Np-Nh) low energy configurations will be required to account for long range correlations. The first ingredient is required in order to pin down the single-particle properties and also to provide the underlying space for the 2nd and 3rd ingredients.

The number of SSD's required to obtain an accurate expansion of the solutions of (1.1) in a given orthonormal many-body basis remains out of the bound of even present day large, fast computers. However it is still possible to make quantitative predictions about the states, even when the basis is truncated heavily, if a different effective Hamiltonian $\tilde{H}$, appropriate for the particular truncation¹⁾ is used. In this case all other observables must also be represented by their effective counterpart²⁾ and often the burden of the problem is relegated to the operators instead of the states. For the purpose of low-energy nuclear spectroscopy it is believed that ingredient (ii) can be renormalised out of the wavefunctions and that a suitable K matrix^{3,4,5)} exists, which we will call $V^{(2)}$ from now on, such that only ingredients (i) and (iii) remain in $|\Psi\rangle$. It is further believed that, as long as short range effects are not involved, it will be possible to compute the matrix elements of any observables without renormalizing

them against effect (ii). But, if that last proviso holds, we need not have an exact mathematical prescription for the transition from the exact, highly singular interaction to our (smooth) $V^{(2)}$. Such a semi-realistic $V^{(2)}$ has been recently developed by Saunier & Pearson⁵⁾. Their potential #2 (SP2) has been found to give excellent results⁶⁻⁷⁾ in the code described here.

Still, additional truncations with respect to effects (i) and (iii) are needed in order to deal with a manageable problem. We can distinguish roughly two approaches to this question. In shell model calculations the single particle basis is first heavily truncated, the interaction is then renormalised once more ($V^{(2)} \rightarrow G$) and as many configurations of type (iii) are retained as the size of the matrix diagonalisation problem will allow. The usual net result of such calculations is that one obtains a rather large (perhaps 15-30, in the s-d shell) number of eigenstates, with moderate accuracy for any single one, and requiring a substantial amount of type (i) renormalisation to obtain transition matrix elements (presence of effective charges). The second approach is the object of this report, and consists in retaining the largest possible single particle basis (effect (i)). One then concentrates on obtaining type (iii) correction for a very limited number (1-5, say) of eigenstates, usually near the ground state: to do this, the unrestricted Hartree-Fock variational method should include projection to restore the

symmetries which may be violated by the variational mixing. Although a smaller number of states are described in this way, the accuracy of the wavefunctions is improved, with the result that little or no operation renormalisation is required (unrenormalised transition operators may be used).

Actually, there are many properties of the ground state and features of the nuclear systematics which can be described without performing the projection step, and so even though the present code does not project true eigenstates, but only obtains the so-called "intrinsic state", a detailed description of the methods used is warranted both for its own sake and as a step towards further elaboration of the present work.

The main new features of the code are i) extensive use of the "Wigner-Eckart theorem", although deformed states are considered throughout, ii) a flexible modular construction where each subroutine package performs a given physical or mathematical step, iii) liberal use of random-access mass storage facilities, iv) considerable flexibility including a complete Nilsson model code (ELMOS⁸) for the initialisation procedure which supplies the starting SSD trial wavefunction.

The first feature allows a several-fold increase in speed over the conventional methods, while the next two greatly facilitate extensions and modifications for special purposes. The last feature is of near vital

importance for such calculations because of the very large number of variational parameters involved.

The next section contains mostly a collection of the relevant mathematical equations involved in the Hartree-Fock approximation, while section 3 provides a guide to the structure of the program. Section 4 contains a brief discussion of the problems solved by this code. The appendices contain a listing of the code, a sample of the results, a list of error exit modes of termination, and finally, a short resume of the control card structure which is contained in a BLOCK DATA subprogram, instead of being read from cards.

An essential aspect of such a program is the preparation of the various two-body operator matrix elements which are required at the outset. A separate program EVAFME is also described here since it uses novel methods which considerably increase its speed and flexibility.

2. THE HARTREE-FOCK VARIATIONAL APPROXIMATION

2.1 THE BASIC EQUATIONS

The basis equations of the H.F. method are well known and we shall use mainly the notation and phase convention of Baranger¹⁰). Still, in order to completely define the numerical formalisms we shall review briefly the steps required to reduce the equations of the method to a computational algorithm.

We consider a nucleus composed of A nucleons (protons and neutrons of spin $\frac{1}{2}$) whose Hamiltonian is the following sums of one and two body terms

$$\begin{aligned}
 H &= \sum_{n=1}^A T(n) + \sum_{\substack{n=1 \\ m>n}}^A V(n,m) \\
 &= \sum_{n=1}^A T(n) + \frac{1}{2} \sum_{n \neq m=1}^A V(n,m) ,
 \end{aligned}
 \tag{2.1}$$

where $T(1)$ depends on the coordinates of the first particle only and $V(1,2)$ depends (symmetrically) on the coordinates of particles 1 and 2 only, etc. Typically $T(n)$ will be the kinetic energy of the n^{th} nucleon $\frac{1}{2m}|p_n|^2$, and $V(1,2)$ is a complicated interaction between the two nucleons which will be discussed later on.

The coordinate (or classical) expression (2.1) needs to be rewritten in the quantum mechanical second quantisation formalism. We let $c_{\alpha}^{\dagger}, c_{\alpha}$ be a set of fermion creation and destruction operators obeying the usual anticommutation relations and we define our single particle basis

$$\langle \underline{r} | \alpha \rangle = \langle \underline{r} | c_{\alpha}^{\dagger} | 0 \rangle = \phi_{\alpha}(\underline{r}), \quad \alpha = 1, \dots, B. \quad (2.2)$$

We now state the precise definition of $\phi_{\alpha}(\underline{r})$ which has been used throughout in this work. The index α stands for 4 labels: n_a , the radial label, j_a, m_a the total angular momentum and its projection along the z axis, and t_z , the isospin projection, which is $-\frac{1}{2}$ for neutrons and $+\frac{1}{2}$ for protons. This last label will be omitted because our basis will be the same for protons and neutrons. The structure of the basis used here is given in table 1. So we define

$$\langle \underline{r} | njm \rangle = R_{n\ell}(\frac{r}{b})(i)^{\ell} \sum_{\mu=-\frac{1}{2}}^{+\frac{1}{2}} Y_{\ell}^{m-\mu}(\theta, \phi) \chi_{\frac{1}{2}}^{\mu} \times C(\ell \frac{1}{2} j; m-\mu, \mu, m), \quad (2.3)$$

where $R_{n\ell}(r)$ is the normalised radial wavefunction for a particle in a 3-dimensional harmonic oscillator of frequency $\hbar\omega$, and oscillator parameter $b = \sqrt{\frac{\hbar}{m\omega}}$. Following Brody & Moshinsky¹¹⁾ we have for $R_{n\ell}(\rho)$, ($\rho = \frac{r}{b}$)

$$R_{nl}(\rho) = \left[\frac{(2n)!}{\Gamma(n+l+3/2)} \right]^{1/2} \rho^l e^{-1/2\rho^2} L_n^{l+1/2}(\rho^2), \quad (2.4)$$

where $L_n(z)$ is given as

$$L_n^a(z) = \frac{1}{n!} e^z z^{-a} \frac{\partial^n}{\partial z^n} (e^{-z} z^{n+a}). \quad (2.5)$$

The number n counts the number of sign changes of the radial wavefunction and R_{nl} is positive at the origin. The $Y^m(\theta, \phi)$ are the usual spherical harmonics of Condon & Shortley and $\chi_{1/2}^\mu$ is the appropriate spinor. Under the time reversal operator T we have

$$T(i^l Y_l^m) = (-1)^{l-m} (i^l Y_l^{-m}), \quad T|\chi_{1/2}^\mu\rangle = (-1)^{1/2-\mu} |\chi_{1/2}^{-\mu}\rangle. \quad (2.6)$$

The last symbol of (2.3) is the usual Clebsch-Gordan coefficient for recoupling of two angular momenta.

The wavefunctions defined by (2.3) agree in all respects but one with the usual definitions used in current shell model calculations. The factor i^l has been introduced in order to insure that under time reversal the states $|njm\rangle$ will transform as

$$T|njm\rangle = (-1)^{j-m} |nj-m\rangle. \quad (2.7)$$

This last equation is important in the present calculations where time-reversal properties are not conserved in the variational procedure.

Using c_α and $c_\alpha^\dagger$ it can be shown that eq. (2.1) can be rewritten as

$$H = \sum_{\alpha\beta} \langle \alpha | T(1) | \beta \rangle c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V(1,2) | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma, \quad (2.8)$$

where

$$\langle \alpha | T(1) | \beta \rangle = \int d^3 r_1 \phi_\alpha^*(r_1) T(r_1) \phi_\beta(r_1),$$

and

$$\langle \alpha\beta | V(1,2) | \gamma\delta \rangle = \int d^3 r_1 d^3 r_2 \phi_\alpha^*(r_1) \phi_\beta^*(r_2) V(r_1, r_2) \phi_\gamma(r_1) \phi_\delta(r_2). \quad (2.9)$$

We next defined the antisymmetrised, unnormalised matrix elements $V_{\alpha\beta\gamma\delta}$ as

$$\begin{aligned} V_{\alpha\beta\gamma\delta} &= \langle \alpha\beta | V(1,2) | \gamma\delta \rangle - \langle \alpha\beta | V(1,2) | \delta\gamma \rangle \\ &= -V_{\beta\alpha\gamma\delta} = -V_{\alpha\beta\delta\gamma} = V_{\beta\alpha\delta\gamma}, \end{aligned} \quad (2.10)$$

so that (2.8) takes the convenient and standard form

$$H = \sum_{\alpha\beta} T_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma. \quad (2.11)$$

The rotational invariance of H can be used to apply the Wigner-Eckart theorem to $V_{\alpha\beta\gamma\delta}$, giving the decompositions

$$\begin{aligned}
 V_{\alpha\beta\gamma\delta} &= \sum_{JM} F(acdbJ) s_{\beta} s_{\gamma} C(j_a j_c J; m_a, \bar{m}_c M) C(j_d j_b J; m_d, \bar{m}_b, M) \\
 &= \sum_{JM} G(abcdJ) C(j_a j_b J; m_a m_b M) C(j_c j_d J; m_c m_d M),
 \end{aligned} \tag{2.12}$$

where the second decomposition is the usual shell model one, apart from the normalisation, while the first one is more appropriate for our purpose. Note that $s_{\alpha} = (-1)^{j_{\alpha} - m_{\alpha}}$ and $\bar{m}_{\alpha} = -m_{\alpha}$. The F reduced matrix elements may be obtained from the G 's with the relation

$$F(acdbJ') = - \sum_J (2J+1) W(j_a j_b j_c j_d; JJ') G(bacdJ). \tag{2.13}$$

Let us now consider a single Slater determinant (SSD) trial wavefunction, for A particles, of the form

$$|\phi_A\rangle = \xi_{\lambda_1}^{\dagger} \xi_{\lambda_2}^{\dagger} \cdots \xi_{\lambda_A}^{\dagger} |0\rangle, \tag{2.14}$$

where

$$\xi_{\lambda}^{\dagger} = \sum_{\alpha} U_{\alpha\lambda} c_{\alpha}^{\dagger}, \quad \lambda = 1, \dots, A, \tag{2.15}$$

and $U_{\alpha\lambda}$ is a (complex) unitary transformation of the (fixed, laboratory, expansion) basis. The one-body density matrix $\hat{\rho}_{\alpha\beta} = c_{\beta}^{\dagger} c_{\alpha}$ has, on this state, the average value

$$\rho_{\alpha\beta} = \langle \phi_A | \hat{\rho}_{\alpha\beta} | \phi_A \rangle = \langle \phi_A | c_{\beta}^{\dagger} c_{\alpha} | \phi_A \rangle = \sum_{\lambda \text{ occupied}} U_{\alpha\lambda} U_{\beta\lambda}^*. \tag{2.16}$$

The average density defines the average potential energy matrix

$$\bar{v}_{\alpha\gamma} = \sum_{\beta\delta} V_{\alpha\beta\gamma\delta} \rho_{\delta\beta} . \quad (2.17)$$

This potential together with $T_{\alpha\gamma}$ defines the so-called Hartree-Fock Hamiltonian $h_{\alpha\gamma}$ as

$$h_{\alpha\gamma} = T_{\alpha\gamma} + \bar{v}_{\alpha\gamma} . \quad (2.17a)$$

The variational minimum to

$$\delta_U \langle \phi_A | H | \phi_A \rangle = 0 , \quad (2.18)$$

where one varies with respect to the parameters of the unitary transformation $U_{\alpha\lambda}$ can be shown to lead to the self-consistent eigenvalue equations

$$\sum_{\beta} h_{\alpha\beta} U_{\beta\lambda} = \epsilon_{\lambda} U_{\alpha\lambda} , \quad (2.19)$$

where the eigenvalues ϵ_{λ} are called the Hartree-Fock single particle energies. The equation (2.19) implies a self-consistency condition because the matrix $h_{\alpha\beta}$ to be diagonalised is itself a function of $U_{\alpha\lambda}$, through equations (2.17) and (2.16). The self consistent U is found by first selecting an initial U^0 then computing h from it and diagonalising it to get a new U^1 by populating the states of lowest ϵ_{λ} . This process is iterated until no further change in U is detected.

The eq. (2.17) is not practical to use when B is large because there are B^4 or, in this case, approximately 45 million matrix elements $V_{\alpha\beta\gamma\delta}$. We shall want to use only the F matrix elements of eq. (2.12). This can be accomplished by using a slight variation of the Wigner-Eckart theorem for $\rho_{\alpha\beta}$ and $\bar{v}_{\alpha\beta}$. We write

$$\langle j_a m_a | \bar{v} | j_b m_b \rangle = \bar{v}_{\alpha\beta} = s_{\alpha} \sum_J C(j_b j_a J; m_b, \bar{m}_a, M) (j_a \| \bar{v}_J^M \| j_b) \quad (2.21)$$

as the defining equation for the "reduced matrix elements" $(j_a \| \bar{v}_J^M \| j_b)$. A similar equation defines $(j_a \| \rho_J^M \| j_b)$. We substitute these in (2.17) and use (2.12) to obtain the new equation

$$(j_a \| \bar{v}_J^M \| d_c) = \sum_{bd} F(ca, db; J) (j_b \| \rho_J^M \| j_d) \quad (2.22)$$

This equation involves far fewer matrix elements of the potential (~ 15000 in the present case) and was used in the code. The inverse of eq. (2.21) is also required and comes out, using the orthogonality of the C.G. coefficients as

$$(j_a \| \bar{v}_J^M \| j_b) = \sum_{m_c} C(j_c j_a J; m_c, M-m_c) (-1)^{j_a+M-m_c} \langle j_a, -M+m_c | \bar{v} | j_c m_c \rangle. \quad (2.23)$$

The value of $\langle \phi_A | H | \phi_A \rangle$ can be computed and we obtain

$$E_{H.F.} = \langle \phi_A | H | \phi_A \rangle = \sum_{\alpha\beta} (T_{\alpha\beta} + \frac{1}{2} \bar{v}_{\alpha\beta}) \rho_{\beta\alpha} . \quad (2.24)$$

These, then, are the basic equations which were used in the code. The remainder of this section will be devoted to the symmetry properties and other matters which influence the structure of the code.

The F matrix elements have the symmetry $F(ab,cd;J) = F(cd,ab;J)$ and thus were stored as the lower triangular parts of symmetric matrices in the double index (a,b), for each J value.

The density matrix $\rho_{\alpha\beta}$ is hermitian, as can be seen from its definition (2.16). This implies the symmetry property for its reduced matrix element $(j_a || \rho_J^M || j_b)$

$$(j_c || \rho_J^{-M} || j_a) = \theta(j_c - j_a - M) (j_a || \rho_J^M || j_c)^*, \quad (2.25)$$

with $\theta(a+b+\dots) = (-1)^{a+b+\dots}$, so that only the matrix elements with $M \geq 0$ need be stored. This property is useful when computing the traces involved in eq. (2.24). In terms of reduced matrix elements we have

$$\text{Tr}[\rho \bar{v}] = \sum_{\alpha\beta} \rho_{\alpha\beta} \bar{v}_{\beta\alpha} = \sum_J \sum_{j_a j_b} (2-\delta_{M,0}) \text{Re}[(j_b || \rho_J^M || j_a) (j_b || \bar{v}_J^{-M} || j_a)^*] \quad (2.26)$$

This equation is used to define the partial components (J,M) of the trace sum. The equation (2.23) also serves as a natural definition of the spherical tensor parts of the deformed Hartree-Fock potential.

2.2 THE MATRIX ELEMENTS OF 1 AND 2-BODY OPERATORS

Apart from the matrix elements of the one-body kinetic energy and the two-body interaction discussed earlier, several other sets of matrix elements are used in the calculation.

The matrix elements of the following one-body operators are constructed:

i) the 21 symplectic operators of Lipkin¹²⁾:

$r_k r_\ell$ (6 operators), $p_k p_\ell$ (6 more), $r_k p_\ell$ (9) $k, \ell = 1, 2, 3$

ii) $r^L Y_L^M(\theta, \phi)$, $L = 0, 2, 4, 6$, $M = 0, 2, \dots, L$.

The set i) is a general purpose one which is used to perform cranking operations and to obtain the free kinetic energy.

The second set ii) is used to evaluate the multipole moments of the intrinsic state $|\phi_A\rangle$. The set i) is obtained by relating r_i and p_i to harmonic oscillator creation and annihilation operators in the cartesian oscillator basis.

Linear combinations of the operators above were computed as follows, in units of b^2 ,

$$N_\lambda = \sum_{ij=1}^3 \Omega_{\lambda ij} \left(\frac{r_j p_i + p_j r_i}{2} \right) \quad \lambda = 1, \dots, 9, \quad (2.27a)$$

$$A^\pm = \sum_{ij=1}^3 \Omega_{\lambda ij} \left(\frac{p_j p_i \pm r_j r_i}{2} \right) \quad \lambda = 4, \dots, 9, \quad (2.27b)$$

where the 9 3×3 matrices Ω_λ are

$$\begin{aligned}\Omega_1 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, & \Omega_2 &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, & \Omega_3 &= \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\ \Omega_4 &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & \Omega_5 &= \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{bmatrix}, & \Omega_6 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \\ \Omega_7 &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, & \Omega_8 &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & \Omega_9 &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.\end{aligned}$$

The precise definition of the set ii) is

$$Q_L^M = r^L \sqrt{\frac{4\pi}{2L+1}} Y_L^M(\theta, \phi) = r^L C_L^M(\theta, \phi), \quad L \text{ even}$$

and its matrix elements are given by the formula

$$\begin{aligned}\langle n' \ell' j' m' | Q_L^M | n \ell j m \rangle &= (-1)^{\frac{\ell - \ell'}{2} + j - m} C(j' j k; m' \overline{m} M) \langle n' \ell' | r^L | n \ell \rangle \\ &\times \frac{(\ell' j' \| C(k) \| \ell j)}{\sqrt{2L+1}}\end{aligned}\tag{2.28}$$

The radial matrix element is evaluated in the usual manner while the angular reduced matrix element is given by Edmonds¹³⁾. The additional factor $(-1)^{\frac{\ell - \ell'}{2}}$ reflects the phase convention adopted here.

The computation of the matrix elements of the two-body operators used in the code is much more lengthy.

Apart from the nuclear potential the following operators are needed:

$$\begin{aligned}
 V_R^{(2)} &= \frac{1}{2} \sum_{n \neq m}^A |\tilde{r}^n - \tilde{r}^m|^2, \\
 V_P^{(2)} &= \frac{1}{2} \sum_{n \neq m}^A |\tilde{p}^n - \tilde{p}^m|^2, \\
 V_C^{(2)} &= \frac{1}{2} \sum_{n \neq m}^Z \frac{1}{|\tilde{r}^n - \tilde{r}^m|}.
 \end{aligned} \tag{2.29}$$

The first two operators are needed to treat the center of mass problem; their direct and exchange matrix elements must be calculated separately in the second quantisation formalism; thus two sets of V_R and V_P must be obtained. The last one is the Coulomb two-body potential. Since this distinction holds also for the nuclear interaction seven sets of two-body matrix elements, each of which contains ~ 15000 matrix elements in our basis, must be obtained. They are computed by a separate code EVAFME (EVALIN F-Matrix Element) in a suitable order for reading in as data by EVALIN. Section 2.5 discusses some of the important features of this calculation.

2.3 THE CENTER-OF-MASS PROBLEM

The initial trial wavefunction supplied by ELMOS very nearly puts the center-of-mass (CM) of the nucleus in the ground state (0s) of a harmonic oscillator of the same frequency as $\hbar\omega$, the basis frequency. Now the one-body kinetic energy

$$T_{\text{tot}} = \sum_n \frac{|p_n|^2}{2m}$$

contains T_{CM} , the kinetic energy of the CM. If we iterate using T_{tot} the final wavefunction will also tend to minimise T_{CM} , which means spreading the CM out over all the space allowed by the basis. This will confuse the interpretation of the single particle wavefunctions since they will then tend to smear out too. This effect can be corrected either by subtracting T_{CM} from T_{tot} or by adding to T_{tot} , V_{CM}

$$V_{\text{CM}} = \frac{1}{2} M \omega_{\text{CM}}^2 |\bar{R}|^2, \quad \bar{R} = \sum_{n=1}^A \bar{r}^{(n)} \frac{1}{A}, \quad (2.29)$$

which will bind the CM in a harmonic oscillator potential. The present code uses the first method; the second one is useful when it can not be established that the initial SSD has the desired CM wavefunction. The form of $T_{\text{rel}} = T_{\text{tot}} - T_{\text{CM}}$ can be obtained as

$$T_{rel} = \sum_n \frac{|\underline{p}^n|^2}{2m} - \frac{1}{2mA} \sum_{nm} \underline{p}^n \cdot \underline{p}^{m'} = \frac{1}{4mA} \sum_{n \neq m} |\underline{p}^n - \underline{p}^{m'}|^2 = \frac{1}{2mA} v_P^{(2)}. \quad (2.30)$$

This last equation shows that the Hamiltonian in the relative coordinate system has no one-body components but depends on the atomic number A.

The properties of the CM wavefunction enter again when computing the mean-square radius. One derives the identity

$$\overline{r_{rel}^2} = \frac{1}{A} \sum_{n=1}^A |\underline{r}^n - \underline{R}|^2 = \frac{1}{A^2} v_R^{(2)}. \quad (2.31)$$

The difference between (2.31) and the simplified expression $\frac{1}{A} \sum_n |\underline{r}^n|^2$ goes to zero for heavy nuclei but is appreciable for light nuclei, as can be seen in appendix II. A formula similar to eq. (2.31) has been worked out to compute the mean squared radius of the *protons only* with respect to the *total* CM, a quantity of interest in most experimental determinations of the charge radius of nuclei.

2.4 PROTON & NEUTRON DENSITY MATRICES & THE PARITY SELECTION RULES

The equations (2.15) and (2.16) for the density matrix did not differentiate between neutrons and protons whereas the equation (2.22) involves $F(ca,db;J)$ where a,b,c,d carry a proton or neutron label. Some detail about the actual procedure will now be given.

We can take, as a complete set of labels of our single particle states, the quantum numbers (n,j^π,m,t_z) . Next we restrict the U matrix of eq. (2.15) to be diagonal in the parity label and in the proton neutron label, that is to say the single particle Hartree-Fock states are either neutrons or protons of good parity. It is then clear from eq. (2.16) that the total density matrix breaks up into two submatrices ρ_p and ρ_n each of which breaks up further into two pieces, one density matrix for the positive parity states and one for the negative parity ones. The reduced matrix elements of ρ , ρ_p and ρ_n of a given J^π therefore contain only J^+ terms since $\pi_J = \pi_a \pi_b$. The complete set of reduced matrix elements of F in (2.22) has the labels $F(ct_c,at_a,dt_d,bt_b,J^\pi)$. From the properties of ρ and the eq. (2.22) we see that only the J^+ matrix elements with the pair db both protons or both neutrons are needed. By conservation of charge this means that the pairs ca are also both neutrons or both protons. Since we have the symmetry relation

$$F(ca,db;J) = F(db,ca;J), \quad (2.32)$$

the F matrix breaks up into the submatrices

$$F = \begin{bmatrix} F_{pp}^J & F_{pn}^J \\ F_{np}^J & F_{nn}^J \end{bmatrix}, \quad (2.33)$$

where the subscripts label the two particle hole pairs (ca and db).

Furthermore if we let ρ, σ stand for the two pairs ca,db it can be shown that

$$F_{pp}^J(\rho, \sigma) = F_{pp}^J(\sigma, \rho) = F_{nn}^J(\rho, \sigma) = F_{nn}^J(\sigma, \rho), \quad (2.34)$$

and

$$F_{pn}^J(\rho, \sigma) = F_{pn}^J(\sigma, \rho) = F_{np}^J(\rho, \sigma) = F_{np}^J(\sigma, \rho). \quad (2.34a)$$

Using the ρ, σ, η notation for pairs of labels, the equation (2.23) can now be rewritten as

$$\bar{v}_{Jp}^M(\sigma) = \sum_n (F_{pp}^J(\sigma, \eta) \rho_{Jp}^M(\eta) + F_{pn}^J(\sigma, \eta) \rho_{Jn}^M(\eta)), \quad (2.35)$$

$$\bar{v}_{Jn}^M(\sigma) = \sum_n (F_{pn}^J(\sigma, \eta) \rho_{Jp}^M(\eta) + F_{nn}^J(\sigma, \eta) \rho_{Jn}^M(\eta)).$$

This last equation was used in the code.

2.5 THE CONSTRUCTION OF TWO-BODY MATRIX ELEMENTS

Perhaps the most significant feature of the program EVAFME is its use of *exact* expressions for the construction of all the required two-body matrix elements of operators which do not involve tensor terms, namely the operators of eq. (2.29). The method of Talman¹⁴⁾ has been used with success.

For any two-body potential $V^{(1,2)}$, the anti-symmetrized F-matrix element can be written as

$$F(ab,cd;J) = f(abcdJ) - (-)^{j_a+j_d+J} \sum_{J'} (2J'+1)(-)^{J'} W(j_a j_b j_c j_d; JJ') f(acdbJ'), \quad (2.36)$$

where

$$f(abcdJ) = \sum_{\substack{m_a - m_b = M \\ m_c - m_d = M}} \langle \alpha \delta | V^{(1,2)} | \beta \gamma \rangle C(j_a j_b J; m_a \bar{m}_b M) \times C(j_c j_d J; m_c \bar{m}_d M) s_\beta s_\delta. \quad (2.37)$$

When $V(1,2)$ is a central force, i.e. $V(1,2) = V(|\underline{r}_1 - \underline{r}_2|)$, Talman's scheme yields the formula

$$f(abcdJ) = c_a c_b c_c c_d (-)^{j_a - j_c + (\ell_s + \ell_c - \ell_a - \ell_d)/2} \frac{\hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d}{(2J+1)} \times$$

$$W(\ell_a \ell_b j_a j_b; J \frac{1}{2}) W(\ell_c \ell_d j_c j_d; J \frac{1}{2}) \sum_{NMv} c_{NJ}^{ab} c_{MJ}^{cd} R(NMJv) I_v(v), \quad (2.38)$$

where $\hat{j}_a = \sqrt{2j_a + 1}$; we refer the reader to Talman's¹⁴⁾ equations (4), (14) and (15) for the computational definitions of the normalisation coefficients c_a , the transformation coefficients c_{NJ}^{ab} and $R(NMJv)$ respectively. Here I_v is the Talmi integral

$$I_v = 4\pi \int_0^\infty r^{2v+2} e^{-r^2} V(\sqrt{2} r) dr. \quad (2.39)$$

For example the case $V_C(1,2) = \frac{e^2}{|r_1 - r_2|}$ gives

$$I_v(V_C) = e^2 \frac{\pi}{\sqrt{2}} v!,$$

for the Talmi integrals of the Coulomb potential. The equation (2.38) implies the useful selection rules $J + \ell_a + \ell_b = \text{even}$, $\ell_c + \ell_d + J = \text{even}$, and the symmetry relations

$$f(abcdJ) = f(cdabJ) = -\theta(abJ)f(bacdJ).$$

3. CODING TECHNIQUES

3.1 GENERAL DESCRIPTION

The program EVALIN performs an Extended Variational Approximation for Light and Intermediate Nuclei. The size of the basis and the nuclear parameters are initial data, much of which is read in from magnetic tape at an early stage of execution. This tape must be prepared by EVAFME on a previous run. We first give the block structure of the tape.

The matrix elements of (2.29) are computed in dimensionless form and so are independent of $\hbar\omega$. They are first on the tape and require 6 blocks of data. There follows a variable number of sections consisting of 4 blocks each and pertaining to the various values of $\hbar\omega$ for which nuclear force matrix elements, in MeV, have been constructed. The first block of the dimensionless M.E. section is a 25 word control block containing the number of j shells to be considered (up to 16) and the corresponding lengths of the following 5 blocks. They in turn contain $V_{C_{pp}}^{(2)}$, $V_{R_{pp}}^{(2)}$, $V_{R_{pn}}^{(2)}$, $V_{P_{pp}}^{(2)}$, $V_{P_{pn}}^{(2)}$ of equation (2.29). The 4-block sections are composed of a control block, the G-matrix elements, F_{pp} , F_{pn} . We note that the G matrix elements are included for reference purposes only and are not used here. These matrix elements are *not* constructed by EVAFME either, EVAFME reads them in from magnetic tape or failing that the unsatisfied external PPME(I1,I2,I3,I4,J,KT,GGG,0) must be coded in as a supplier of the matrix elements of the two-body nuclear interaction.

After initialisation the overlay READIN is called and the initial data is transferred to a mass storage device (disk). Upon returning to the main overlay (EVALIN) the common block /BASIS/ is set up and contains detailed information related to the selected basis states (lengths of arrays etc....). Several nuclei (up to 40) may be processed in one run. This main loop begins at D0 11 etc. -- .

The processing of one nucleus begins with the generation of a trial wavefunction. It may be read from cards by calling READIN once more or constructed from the Nilsson model by calling the overlay ELMOSE⁸⁾. ELMOSE is called in any case in order to generate the one-body matrix elements defined in equations (2.27), and the printout character set.

The overlay NUHART is next called to perform the actual iterations. Several iterations are first performed using the relative coordinate total Hamiltonian. The results of this are considered to be the "best" wavefunction which may be saved permanently on punched cards. The wavefunction is also saved temporarily (until the next nucleus) on mass storage. After computing the relative coordinate rms radii a last iteration is performed with the sole purpose of obtaining the usual single particle energies (which include the K.E. of the center of mass). Finally, further iterations may be performed in the presence of a one-body external field (cranking).

The control is then transferred to the overlay MULTIP which computes the expectation values of the multipole moments defined by (2.28).

The final task is to produce a computer output plot of the density distribution defined by the saved wavefunctions BRPS,BIPS,BRNS,BINS through equation (2.16). The code is then ready for the next nucleus.

A listing of the codes EVALIN and EVAFME is given in appendix I. Most of the actual coding details can be obtained by studying this listing together with a sample of the output for ^4He , given in appendix II. Appendices III and IV pertain to the execution details while appendix V describes a magnetic tape containing the card images for the code. The following subsections provide some further relevant details for the computation.

3.2 WORKING ARRAYS & MASS STORAGE RETRIEVAL

The finite size of the central memory available restricts the code to having simultaneously in core only one set of two-body matrix elements and two sets of one-body matrix elements (we view the wavefunction $U_{\alpha\gamma}$ as a one-body array.) For this purpose one long (15000) array and two short ones (4000) are used as temporary storage only. All arrays of interest are stored on disk and transferred in and out by referring to their alphanumerical name with BUFFIN and BUFOUT. It is then practical to pass to subroutines only the names of the arrays of interest via the calling sequence.

The limitations on the size of the temporary storage are felt most severely when constructing the complete Hamiltonian including Coulomb interactions, since we must then take linear combinations of two (long) sets of two-body matrix elements. A subroutine ADLONG performs these operations piecemeal.

3.3 THE STRUCTURE OF F ARRAYS

Apart from containing the two-body matrix elements of some operator, an F array contains control data. These data are checked during processing to insure that garbage has not been read from mass storage.

We have

$F(1) = NV$ = number of levels in the basis

$F(I+1) = I$ = code number of the levels described in table I.

There follows $J_{\max}$ blocks for each positive parity J value occurring in (2.12) ($J_{\max} \leq 7$). The first element of each block is set to $64*J + DIMJ$, where $DIMJ$ = the number of different pairs (j_{α}, j_{γ}) which can couple to J^+ . Within a block the element $F^J(L, M)$ is located at the position $L + DIMJ*(M-1) - M(M-1)/2$, $L \geq M$. In the pair index $L \leftrightarrow (j_{\alpha}, j_{\gamma})$ the index α varies fastest in increasing order over the values of I which are allowed.

3.4 CONSTRUCTION OF REDUCED MATRIX ELEMENTS

Although most of the calculations are performed using the reduced matrix elements of $\bar{v}$ and ρ the diagonalisation involved in (2.19) must be performed using $\langle j_\alpha | \bar{v} | j_\beta \rangle$.

The coding for equations (2.21) and (2.23) is represented by the subroutines ROCONV, ROCONVP, ROCONIP, IDACSET, HISCLEB.

3.5 MISCELLANEOUS

The construction of the density matrix (eq. (2.16)) is coded in DENMAT and DENMATP. This pair of subroutines illustrates the technique of double calls to treat subblocks (in this case positive and negative parity blocks) of a matrix.

The selection of the orbits to be populated at each iteration is done by REORDER. The Z protons and N neutrons are simply put in the states with lowest $\epsilon_{\lambda p}$ and $\epsilon_{\lambda n}$.

The machine language code FTNUTIL is a general purpose debugging and tracing code of considerable usefulness when testing modifications to the program.

The overlay ELMOSE will not be discussed in this report since its coding techniques have been described elsewhere⁸⁾.

The subroutine HARFIT(ITE) performs ITE complete iterations including diagonalisations etc..., after which it extracts the single-particle r.m.s. radii, the deformation parameters and the expectation values of the 21 symplectic operators.

The subroutine TALMI in EVAFME constructs appropriately normalised talmi integrals instead of using the simpler expression (2.39), in order to improve the numerical stability of the sum defined by eq. (2.38).

The function TRVEROJ(R0,VB,---) returns the trace of $\rho^*\bar{v}$ and prints out the intermediate J sums multiplied by 0.5. This factor is not present in the total returned sum.

It will be seen that a judicious use of the routines VEEBAR and TRVEROJ allows the computation of the expectation value of *any* two-body operator whose reduced F matrix elements are in mass storage. For example this feature is used to compute the Coulomb energy and the relative coordinate rms radii.

4. RESULTS & DISCUSSION

The code has proved to be numerically quite stable and it has been found that 6-8 iterations would, in most cases, stabilise the wavefunction to about 1% or better. The most sensitive cases are those for a mid-shell odd-nucleus where the energy gap between the last occupied state and the unoccupied ones is small.

Results have been obtained using the K.L.S. G-matrix⁴⁾ in an $N = 0-2$, 3 major shells basis and using the Saunier-Pearson⁵⁾ potential No. 2 with $N = 0-2$ and $N = 0-4$. For both interactions the $N = 0-2$ results on s-d shell nuclei were in good agreement (4% or better) with those of Pal & Stamp³⁾, thus providing a check of the code.

Our best results have been obtained for nuclei in the range $4 \leq A \leq 40$, with $N = 0-4$ and using the S.P. No. 2 potential. For most of these nuclei the calculated total binding energy is within 10% of the experimental values (the calculated nuclei are *less* bound) and these nuclei have an experimental r.m.s. radius about 5% greater than the calculated ones. The computed values of the deformation parameters β and γ are in good agreement ($\pm 25\%$) with experiment when known. The position of the Fermi surface has been found to be usually within an MeV or two of the separation energy.

A striking feature of many of the density distributions determined here is that strong alpha clustering effects have been observed. In particular ^8Be , $^{12}\text{C}^*(7.67 \text{ MeV})$, $^{16}\text{O}^*(6.06 \text{ MeV})$ ^{20}Ne show promise of being quite good alpha cluster nuclei.

Perhaps the most severe limitation of the present method is that only the properties of the intrinsic state are obtained. It is probable that further improvements on the binding energies and r.m.s. radii can be obtained by using the generator coordinate method of Hill & Wheeler to project states of good angular momentum out of the intrinsic state obtained here. It is also probable that an increase in the maximum size of the basis up to $N = 6,7$ would improve the results on clustering effects and allow the study of much heavier nuclei, and higher multipole moments.

Another application of the code can be made to a detailed study of the **effects of the Coulomb** force, as a source of violation of isospin conservation. Preliminary results on its influence on the difference of the neutron and proton radii have proved interesting⁷⁾.

A detailed assessment of the usefulness of the code as a source of accurate nuclear wavefunctions will be published elsewhere⁶⁾.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge the active cooperation of Dr. D. McPherson and the entire staff of the Mathematics & Computation Branch of C.R.N.L. We have also benefited from many conversations with Dr. M. Harvey, Dr. F.C. Khanna and Dr. S.S.M. Wong.

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APPENDIX I

LISTING OF THE CODE

The following 56 pages contain a listing of EVALIN and EVAFME. A magnetic tape containing the card images of this listing is described in appendix V.

OVERLAY(EVALIN,0,0)
BLOCK DATA EVALI

EVALI ***MUST*** BE THE FIRST SUBR. OF THE (0,0) OVERLAY .
COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,ITER,ITCR,ATNO
1 ,NORBA(41),NOR8,BET,GAMD,NPTOT,NNTOT
COMMON/CONTRSN/ICON(2,40),RNU(5,40),IBLK,HBOW,TNAME,HBWA(30)
COMMON/EXFIN/EXFID(2,4,20)
COMMON/PRINLIM/EP5,IPR,QNO(82),IPUNCH
LOGICAL IPUNCH

DATA IPUNCH/.T./

DATA EPS,IPR/.003, 0/

DATA ICON/5,1,0,0/
DATA ICON/1,1,0,0/

DATA EXFID/0/

DATA IBLK/1/

DATA ITER,ITCR/6,2/
DATA ITER,ITCR/2,2/

DATA TNAME,HBWA/10H020SP2,16L,13.5,17.5,20.0,10.5,25.0,8.0,30.0,
DATA TNAME,HBWA/10H021SP2,6LV,13.5,17.5,20.0,10.5,25.0,8.0,30.0,
1 15.0,0.00/

DATA RNU/2.,2.,5LHE 4.,.001,0.,4.,4.,5LBE 8.,70,0.,	1,2
1 6.,6.,5LC 12.,5,180.,	3,4
2 10.,10.,5LNE 20.,45,0.,	5,6
3 14.,14.,5LSI 28.,50,180.,	7,8
4 18.,18.,5LAR 36.,18,180.,	9,10
5 20.,24.,5LCA 44.,15,0.,	11,12
6 40.,50.,5LZR 90.,001,0.,	13,14
7 6.,6.,5LC* 12,1,16,0.,	15,16
8 8.,12.,5LO 20.,25,10.,	17,18
8 8.,12.,5LO 20.,25,10.,	17,18
9 2.,8.,5LHE 10.,001,0.,	19,20
0 1.,1.,5LH 2.,001,0.,	21,22
1 8.,8.,5LO 16*,1,46,0.,	23,24
2 8.,9.,5LO 17.,05,0.,	25,26
3 2.,3.,5LHE 5.,32,0.,	27,28
4 5.,5.,5LB 10.,50,35.,	29,30
5 7.,8.,5LN 15.,05,180.,	31,32
6 8.,9.,5LO 17.,10,0.,	33,34
7 9.,8.,5LF 17.,05,0.,	35,36
8 10.,8.,5LNE 18.,25,0.,	37,38
8 5*0./	

END

PROGRAM EVALIN(OUTPUT,TAPE1,TAPE9=1,PUNCH=4008,INPUT=4008)

A CODE TO DO COMPLEX HARTREE-FOCK ITERATIONS.

TAPE1 MUST HAVE BEEN PRESET BY EVAFME .

LIMITATIONS. NOLV.LE.16,ICODE MUST CONTAIN BOTH + AND- PARITIES .

COMMON/OVERCUN/ FIRST,ISKP

COMMON/CONTRSN/ICON(2,40),RNU(5,40),IBLK,HBOW,TNAME,HBWA(30)

COMMON/HASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),

1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,TDSJ,JAR(14,2),IDAC(14,14),JMPO,

2 NBT,HBUM,OSPAZ

COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,ITER,ITCR,ATNO

```

1 ,NORBA(41),NORB,RET,GAMD,NPTOT,NNTOT
LOGICAL FIRST
COMMON/EXSYN/EXF(6,6),SYP(21),NOMM(20,3),COMM(20)

COMMON/CUDATPR/IBAQ(30)
REAL NAME$ DIMENSION CCCC(4)
COMMON/NAMEN/FPR,PTS,FPF,FNE,FNF,FDN,PTD,FDF,RONI,ROPI,SPE,SPEXF
1 ,RTS,RTD
COMMON/CLEHAT/ALOGF(30),SQRF(30)
COMMON/QUADSN/ QUADS(5,3)
DATA FPR,PTS,FPF,FNE,FNF,FDN,PTD,FDF,RONI,ROPI,SPE,SPEXF
1 ,RTS,RTD
1/3LFPR,3LPTS,3LFPF,3LFNE,3LFNF,3LFDN,3LPTD,3LDFD,4LRONI,4LROPI,
1 3LKEN,5LSPEXF,3LRTS,3LRTD/
DATA SYP/3LNL1,3LNL2,3LNL3,
1 3LNL4,3LNL5,3LNL6,3LNL7,3LNL8,3LNL9,
1 3LAP4,3LAP5,3LAP6,3LAP7,3LAP8,3LAP9,
1 3LAM4,3LAM5,3LAM6,3LAM7,3LAM8,3LAM9/
DATA COMM/ -1., 1., 1., -1., -1., 1., 1., -1., -1., -1., 2., 9*1./
DATA NOMM/1,1,2,2,3,3,4,4,5,5,5,6,6,7,7,8,8,9,9,9,
1 2,3,1,3,1,2,1,2,1,2,3,2,3,1,3,1,2,1,2,3,
2 3,2,3,1,2,1,1,2,1,2,3,3,2,3,1,2,1,1,2,3/
DATA IBAQ/
1 10100, 20201, 10201, 30302, 10300, 20302, 40403, 20401, 30403,
1 10401, 50504, 30502, 40504, 10500, 60605, 20502, 50605, 40603,
1 70706, 20601, 30603, 10601, 60706, 50704, 80807, 30702, 40704,
1 10700, 20702, 70807/
DATA EXF/4LR1R1,4LR2R1,4LR3R1,4LP1R1,4LP2R1,4LP3R1,
1 4LR2R1,4LR2R2,4LR3R2,4LP1R2,4LP2R2,4LP3R2,
2 4LR3R1,4LR3R2,4LR3R3,4LP1R3,4LP2R3,4LP3R3,
3 4LP1R1,4LP1R2,4LP1R3,4LP1P1,4LP2P1,4LP3P1,
4 4LP2R1,4LP2R2,4LP2R3,4LP2P1,4LP2P2,4LP3P2,
5 4LP3R1,4LP3R2,4LP3R3,4LP3P1,4LP3P2,4LP3P3/
DATA ELMOSE,NUHART,UENSITY,READIN,PROJECT,MULTIF/
1 6LELMOSE,6LNUHART,7LDENSITY,6LREADIN,7LPROJECT,6LMULTIF/
DATA MUD,FIRST/2.,T./,ISKP/-1/,CCCC/4*0/
CALL SFL(110V00B)
ALOGF(1)=0.$ SQRF(1)=1.$ DO 21 K = 2 , 30$ SQRF(K)= SQRT(FLOAT(K))
21 ALOGF(K)= ALOGF(K-1)+ ALOG(FLOAT(K-1))
PRINT 100
100 FORMAT(1HR)
PRINT 101
101 FORMAT(////40X10H***** * MULTI-SHELL H.F. CALC. *
1 10H***** ///)
CALL OVERLAY(READIN,3,0)
* RETURN 1
IF(IDF.LT.1) CALL ERREXIT(IDF)
OSPA2= 41.6/HBOM
PRINT 1006, HBOM
1006 FORMAT(/* OSC. ENERGY= *F10.2,* MEV.*/)
*
* INITIALISE THE HF PROCEDURE.
NB(1)=NB(2)=0$ DO 13 K = 1 , NOLV$ KP= ICODE(K)$ IQ= IBAQ(KP)
JPH= IQ/10000$ IT= MOD(IQ,10000)$ NT= IT/100$ LT= MOD(IT,100)
ISTA(K)= JPH$ IPAR(K)= 2-(LT.A.1)$ INPO(K)= NT$ ILC(K)= LT
IPT= 1+(LT.A.1)
13 NB(IPT)= NB(IPT)+ SHIFT(JPH,1) $ NBT= NB(1)+NB(2)
IDSC= NB(1)**2+NB(2)**2
*
DO 11 IN= 1 , 40$ IF(ICON(1,IN).EQ.0) GO TO 99
ISKP= ICON(2,IN)$ ILA= ICON(1,IN)$ IF(ILA.LT.1) CALL ERREXIT(ILA)
NPTOT= RNU(1,ILA)$ NNTOT= RNU(2,ILA)$ NAME= RNU(3,ILA)

```

```

COCO(1)= NAMES$ CALL REMARK(COCO)
GAMD= RNU(5,ILA)$ ATNO= NPTOT+NNTOT$ BET= RNU(4,ILA)
NP(1)= NPTOT$ NN(1)= NNTOT$ NP(2)=NN(2)=0
NORR= (MAX0(NPTOT,NNTOT)+1)/2$ DO 1 K = 1 , NORB
1 NORR(K)= K $ IF(ISKP.EQ.0.A..N.FIRST) GO TO 5
CALL OVERLAY(ELMOSE,1,0)
5 IF(ISKP.EQ.0) CALL OVERLAY(READIN,3,0)

CALL OVERLAY(NUHART,2,0)
CALL OVERLAY(MULTIP,6,0)
CALL OVERLAY(DENSITY,4,0)
FIRST= .F.
11 CONTINUE
99 CONTINUE
END
SUBROUTINE ADLONG(FL1,C1,FL2,C2,FLT,AS1,AL1)
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
DIMENSION AS1(1),AL1(1)
DATA FLD/3LFTD/
IDS= MIN0(IDF,8000)$ IF(SHIFT(IDS,1).LT.IDF) CALL ERREXIT(IDS,IDF)
CALL BUFIN(FL1,AL1,IDF)$ CALL BUFIN(FL2,AS1,IDS)
DO 1 K = 1 , IDS
1 AS1(K)= C1*AL1(K)+ C2*AS1(K)$ IF(IDF.EQ.IDS) GO TO 7
CALL BUFOUT(FLD,AS1,IDS)$ IDP1= IDS+1$ DO 3 K = IDP1,IDF
3 AS1(K-IDS)= AL1(K)$ CALL BUFIN(FL2,AL1,IDF)$ DO 5 K = IDP1 , IDF
5 AL1(K)= C2*AL1(K)+ C1*AS1(K-IDS)$ CALL BUFIN(FLD,AL1,IDS)
CALL BUFOUT(FLT,AL1,IDF)$ RETURN
7 CALL BUFOUT(FLT,AS1,IDS)$ RETURN
END
SUBROUTINE REORDER(VAL,NP)
*
* TO SUPPLY A NEW SET OF NP(MUD) .
COMMON/DUMPN/TA(100),ITAG(100),TAP(100)
DIMENSION VAL(1),NP(1)
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
NPT=0$ ILA=1$ DO 3 K = 1 , MUD$NPT=NPT+NP(K)
ND= NB(K)$ DO 3 L = 1 . ND$ TA(ILA)= VAL(ILA)$ITAG(ILA)= K
3 ILA= ILA+1$ CALL SORTAG(TA,1,NBT,ITAG)$ IF(NPT.EQ.0) RETURN
NP(1)=NP(2)=0$ DO 7 L = 1 , NPT
7 NP(ITAG(L))= NP(ITAG(L))+1$ RETURN
END
SUBROUTINE ROCONV(RO,ROJ,IDIR)
*
* WHEN IDIR.GT.0 ,
* TO CONVERT FROM RO IN (JC,MC,/RO/JA,MA) BASIS TO ROJ IN
* (JC,JA,J,M) BASIS, NOTE JA VARIES MOST RAPIDLY
* WHEN IDIR .LE.0 DO THE INVERSE TRANSFORMATION .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
DIMENSION RO(1), ROJ(1)
IC= 1$ CALL IDACSET(0)$ DO 1-K = 1 , 2$ IF(IDIR.GT.0) GO TO 3
CALL ROCONIP(RO(IC),ROJ,K-1,NB(K))$ GO TO 1
3 CALL ROCONVP(RO(IC),ROJ,K-1,NB(K))
1 IC= IC+ NB(K)*2$ RETURN
END
SUBROUTINE IDACSET(IPR)
*

```

```

*   TO GENERATE THE BASE ADDRESSES OF ROJ(J,M,PI) IN IDAC(M,J),
*   IPI= 1 IF PI= -, IPI= 2 IF PI= + .
*   JAR(J,3-IPIT) IS ALSO CONSTRUCTED = DIM OF A J , IPIT SUBSPACF .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
DO 21 K = 1 , 28
21 JAR(K,1)= 0.$ JM= 1$ DO 1 K1= 1 , NOLV$ J1PH= ISTA(K1)
IPI= IPAR(K1)$ JM= MAX0(JM,J1PH)$ DO 1 K2= 1 , NOLV
J2PH= ISTA(K2)$ IPI= 1+ MOD(IPI+IPAR(K2),2)
JMIN= IABS(J1PH-J2PH)+1$ JMAX= J1PH+J2PH$ DO 1 JL= JMIN, JMAX
1 JAR(JL,IPI)= JAR(JL,IPI)+1$ JMPO= JM+JM$ ILAB= 1$DO 7 K = 1 , 196
7 IDAC(K,1)= 0.$ DO 11 JPO= 1 , 14
DO 11 MPO= 1 , JPO$ IDAC(MPO,JPO)= ILAB
11 ILAB= ILAB+ 2*JAR(JPO,1)$ IDSJ= ILAB-1
IF(IPR.LT.3) RETURN$ PRINT 101,(ISTA(1),IPAR(1),I=1,NOLV)
PRINT 103, JAR,IDAC$ RETURN
101 FORMAT(//* ISTA AND IPAREXP, PAR=(-1)*2H**IPAREXP*/(1X16(I6,I2)))
103 FORMAT(//* DIM. FOR EACH J*//1X14I6/1X14I6/* BASE ADDRESSES FOR R
10J*//1X14I6))
END
SUBROUTINE ROCONVP(R0,ROJ,IPAC,NB)

*
*   TO CONVERT RO= (JC,MC/R0/JA,MA) OF PARITY IPAC TO
*   ROJ= R0(JC,JA/J,M)
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,DD(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
COMMON/HISCLE/N00,N1,N21,N31,N12,N2,N4,N13,N3,N5,CLEB
DIMENSION RO(NB,NB),ROJ(1)$ INTEGER TJPC,TJPA
IRAC= 0$ DO 3 KC= 1 , NOLV$ JPHC= ISTA(KC)
IF(MOD(IPAC+IPAR(KC),2).NE.0) GO TO 3$ TJPC= SHIFT(JPHC,1)-1
IRAA= 0$ DO 5 KA = 1 , NOLV$ JPHA= ISTA(KA)
IF(MOD(IPAC+IPAR(KA),2).NE.0)GOTO5$JACPO=JPHC+JPHA$TJPA=2*JPHA-1
JAMCPO= IABS(JPHC-JPHA)+1$ DO 7 JPO= 1 , JAMCPO , JACPO
N1$= JPHA+JPHC-JPO$ DO 7 MPO= 1 , JPO $ MINT= JPHA-JPHC-MPO+1
NAMIN= MAX0(0,MINT)+1$ NAMAX= MIN0(TJPA,JACPO-MPO)+1
ROR=ROI=0.$ IPHAS= 1-SHIFT(MOD(1+NAMIN+IABS(MINT),2),1)
DO 11 NAL= NAMIN , NAMAX$ NCL= NAL- MINT$ N1= N1$ N2= NAL-1
N4= TJPA-N2$ N5= NCL-1$ N3= TJPC-N5$ CALL HISCLEB$ IC= IRAC+NCL
IA= IRAA+ NAL$ CLET= CLEB*IPHAS$ IF(IC-IA) 17,15,13
13 ROR=ROR+CLET*RO(IC,IA)$ ROI=ROI-CLET*RO(IA,IC)$ GO TO 11
15 ROR= ROR+ CLET*RO(IC,IC)$ GO TO 11
17 ROR= ROR+CLET*RO(IA,IC)$ ROI= ROI+ CLET*RO(IC,IA)
11 IPHAS= -IPHAS
ILAB= IDAC(MPO,JPO)$ ROJ(ILAB)= ROR$ ROJ(ILAB+1)= ROI
IDAC(MPO,JPO)= ILAB+2$ IRAA= IRAA+ TJPA+1
5 CONTINUE $ IRAC= IRAC+ TJPC+1
3 CONTINUE$ RETURN
END
SUBROUTINE ROCONTIP(R0,ROJ,IPAC,NB)

*
*   TO DO THE INVERSE OF ROCONVP AND RETURN TO (JC,MC/R0/JA,MA) BASIS
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,DD(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
COMMON/HISCLE/N00,N1,N21,N31,N12,N2,N4,N13,N3,N5,CLEB
DIMENSION RO(NB,NB),ROJ(1),RJT(2,14)$ INTEGER TJPC,TJPA
IRAC= 0$ DO 3 KC= 1 , NOLV$ JPHC= ISTA(KC)
IF(MOD(IPAC+IPAR(KC),2).NE.0) GO TO 3$ TJPC= SHIFT(JPHC,1)-1
IRAA= 0$ DO 5 KA = 1 , NOLV$ JPHA= ISTA(KA)
IF(MOD(IPAC+IPAR(KA),2).NE.0)GOTO5$JACPO=JPHC+JPHA$TJPA=2*JPHA-1

```

```
JAMCPO= IABS(JPHC-JPHA)+1$ DO 7 MPO= 1 , JACPO
MINT= JPHA-JPHC-MPO+1$ JPOMIN= MAX0(MPO,JAMCPO)
DO 8 JPO= JPOMIN , JACPO$ ILAB= IDAC(MPO,JPO)
RJT(1,JPO)= ROJ(ILAB)$ RJT(2,JPO)= ROJ(ILAB+1)
```

```
*
* TEST TO MAKE SURE THAT ROJ IS A HERMITIAN OPERATOR .
IF(KC.EQ.KA.AND.MPO.EQ.1.AND.RJT(2,JPO).GT.1.E-12) CALL ERREXIT
1 (JPO,KC,RJT,2HFL,28)
```

```
8 IDAC(MPO,JPO)= ILAB+2$ NAMIN= MAX0(0,MINT)+1
NAMAX=MIN0(TJPA,JACPO-MPO)+1 $ DO 7 NAL= NAMIN , NAMAX
NCL= NAL-MINT$ ROTR=ROTI=0.$ IPHAS= 1-2*MUD(NCL-1,2)
DO 11 JPO= JPOMIN , JACPO$ N1= JACPO-JPO$ N2= NAL-1$ N4= TJPA-N2
N5= NCL-1$ N3= TJPC-N5$ CALL HISCLB
ROTR= ROTR+ CLEB*RJT(1,JPO)$ ROTI= ROTI+CLEB*RJT(2,JPO)
11 CONTINUE$ IC= IRAC+NCL$ IA= IPAA+NAL$ IF(IC-IA)17,15,13
13 RO(IC,IA)= ROTR*IPHAS$ RO(IA,IC)= -ROTI*IPHAS$ GO TO 7
15 RO(IC,IC)= ROTR*IPHAS$ GO TO 7
17 RO(IA,IC)= ROTR*IPHAS$ RO(IC,IA)= ROTI*IPHAS
7 CONTINUE$ IRAA= IRAA+ TJPA+1
5 CONTINUE$ IRAC= IRAC+ TJPC+1
3 CONTINUE $ RETURN
END
SUBROUTINE HISCLB
```

```
*
* TO DO A HIGH SPEED COMPUTATION OF CLEBSCH(J1,M1,J2,M2/J3) .
* USING THE FORMULA OF SCHWINGER(REF. QUANTUM THEORY OF ANG. MOM.,
* BY RIEDENHARN,P246), AND THE REGGE SYMMETRIES(REF.1B1D,P.296) .
* PAR. ARE IN /HISCLE/N1=J1+J2-J3,N2=J1-M1,N3=J2-M2,N4=J1+M1,N5=J2+
* M2. NO TESTING IS DONE, ANSWER IS IN CLEB IF ALL NIJ ARE NON-NEG.
* INTEGERS . .....WARNING.....ALL 5 NIS MAY BE CHANGED .
* COMMON/HISCLE/N00,N1,N21,N31,N12,N2,N4,N13,N3,N5,CLEB
COMMON /HISCLE/NR(1),N11,N21,N31,N12,N22,N32,N13,N23,N33,CLEB
COMMON/CLEBDAT/ALOGF(30),SQRF(30)
```

```
*
* PREPARE THE REGGE Q-NOS IN NIJ .
N21= N32+N33-N11$ N31= N22+N23-N11$ JT= N21+N22+N23$ IFSE=0
N12= N23+N33-N11$ N13= N22+N32-N11$ JJP= JT-N11+1
```

```
*
* FIND NZE THE SMALLEST NIJ AND BRING IT TO N11 POSITION .
NZE= MIN0(N11,N12,N13,N21,N22,N23,N31,N32,N33)
IF(NZE.EQ.N11) GO TO 7$ IF(NZE.EQ.N31) GO TO 43
IF(NZE.EQ.N12) GO TO 44$ IF(NZE.EQ.N22) GO TO 45
IF(NZE.EQ.N32) GO TO 46$ IF(NZE.EQ.N13) GO TO 47
IF(NZE.EQ.N23) GO TO 48$ IF(NZE.EQ.N33) GO TO 49
42 IFSE= N33$ NW= N21$ N21= N11$ N11= NW$ NU= N12$ N12= N22$ N22= NU
NV= N13$ N13= N23$ N23= NV$ GO TO 7
43 IFSE= N22$ NW= N31$ N31= N11$ N11= NW$ NU= N12$ N12= N32$ N32= NU
NV= N13$ N13= N33$ N33= NV$ GO TO 7
44 IFSE= N33$ NW= N12$ N12= N11$ N11= NW$ NU= N21$ N21= N22$ N22= NU
NV= N31$ N31= N32$ N32= NV$ GO TO 7
45 NW= N22$ N22= N11$ N11= NW$ NT= N21$ N21= N12$ N12= NT
NU= N13$ N13= N23$ N23= NU$ NV= N31$ N31= N32$ N32= NV$ GO TO 7
46 IFSE= N11+N32$ NW= N32$ N32= N11$ N11= NW$ NT= N31$ N31= N12$ N12= NT
NU= N13$ N13= N33$ N33= NU$ NV= N21$ N21= N22$ N22= NV$ GO TO 7
47 IFSE= N22$ NW= N13$ N13= N11$ N11= NW$ NT= N21$ N21= N23$ N23= NT
NU= N31$ N31= N33$ N33= NU$ GO TO 7
48 IFSE= N11+N23$ NW= N23$ N23= N11$ N11= NW$ NU= N31$ N31= N33$ N33= NU
NT= N21$ N21= N13$ N13= NT$ NV= N12$ N12= N22$ N22= NV$ GO TO 7
49 NW= N33$ N33= N11$ N11= NW$ NT= N31$ N31= N13$ N13= NT
NU= N21$ N21= N23$ N23= NU$ NV= N12$ N12= N32$ N32= NV
```

```
*
* CONSTRUCT DELTA*NORMALISATION AND DO THE SUM .
```

```

7   SUM= .5*(-ALOGF(N11+1)+ALOGF(N12+1)+ALOGF(N13+1)+ALOGF(N21+1)-
1   ALOGF(N22+1)+ALOGF(N23+1)+ALOGF(N31+1)+ALOGF(N32+1)-ALOGF(N33+1)
2   -ALOGF(JT+2))-ALOGF(N32-N11+1)-ALOGF(N23-N11+1)
   SUP= 1.$ IF(N11.LT.1) GO TO 13$ DO 15 K = 1 , N11
15  SUP=1.-SUP*K*(N22-N11+K)*(N33-N11+K)/((N11+1-K)*(N23+1-K)*(N32+1-K
1  ))
13  CLEB= SUP*EXP(SUM)*(1-SHIFT(MOD(IFSE,2),1))*SQRF(JJP)$ RETURN
   END
   SUBROUTINE BUFOUT(NAME,DUA,LNGT)
*
*   TO USE MASS STORAGE FACILITIES
*   UP TO 100 RECORDS WITH ALPHA NAMES .
   COMMON/BUFFIN/INDX(201),OPEN
   LOGICAL OPEN
   DATA OPEN/.FALSE./, INDL/201/
   IF(OPEN) GO TO 1$ OPEN= .TRUE.
   CALL OPENMS(9,INDX,INDL,1)
1   CALL WRITMS(9,DUA,LNGT,NAME)
   RETURN
   END
   SUBROUTINE DENMAT(RO,BR,BI,NO)
*
*   TO CONSTRUCT RO FROM BR,BI, ALL IN CARTESIAN BASIS .
   COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPU(16),INUC(16),
1   ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2   NBT,HBOM,OSPA2
   DIMENSION RO(1),BR(1),BI(1),NO(2)
   M= 1$ DO 1 K = 1 , MUD$ ND= NB(K)
   CALL DENMATP(RO(M),BR(M),BI(M),NO(K),ND,NO,ND)
1   M= M+ NO**2$ RETURN
   END
   SUBROUTINE DENMATP(RO,BR,BI,NPA,NBA,IB,IR)
*
*   TO CONSTRUCT RO(I,J)= SUM(K OCC.)R(I,K)*B(J,K)**CC .
   DIMENSION RO(IR,IR),BR(IB,IR),BI(IB,IB)
   NP= NPA$ NB= NBA$ DO 1 I = 1 , NB$ DO 1 J = 1 , 1$ T=U=0.
   IF(NP.LI.1) GO TO 41$ DO 5 K = 1 , NP
   T= T+ BR(I,K)*BR(J,K)+ BI(I,K)*BI(J,K)
5   U= U-BR(I,K)*BI(J,K)+BI(I,K)*BR(J,K)
41  RO(I,J)= TS IF(I.EQ.J) GO TO 1$ RO(J,I)= -U
1   CONTINUE$ RETURN
   END
   SUBROUTINE BUFFIN(NAME,DUA,LNGT)
   CALL READMS(9,DUA,LNGT,NAME)
   RETURN
   END
   SUBROUTINE SORTAG(A,II,JJ,TAG)
C   SORTS ARRAY A INTO INCREASING ORDER, FROM A(II) TO A(JJ)
C   ARRAY TAG IS PERMUTED THE SAME AS ARRAY A
C   ORDERING IS BY INTEGER SUBTRACTION, THUS FLOATING POINT
C   NUMBERS MUST BE IN NORMALIZED FORM.
C   ARRAYS IU(K) AND IL(K) PERMIT SORTING UP TO I*(K+1)-1 ELEMENTS
   DIMENSION A(1),IU(16),IL(16),TAG(1)
   INTEGER A,T,TT
   M= 1$ I= II$ J= JJ
5   IF(I .GE. J) GO TO 70
10  K= 1$ IJ= (J+ I)/2$ T= A(IJ)$ IF(A(I).LE.T) GO TO 20
   A(IJ)= A(I)$ A(I)= TS T= A(IJ)$ TG= TAG(IJ)$ TAG(IJ)= TAG(I)
   TAG(I)= TG
20  L= JS IF(A(J).GE.T) GO TO 40 $ A(IJ)= A(J)$ A(J)= TS T= A(IJ)
   TG= TAG(IJ)$ TAG(IJ)= TAG(J)$ TAG(J)= TG$ IF(A(I).LE.T) GOTO 40
   A(IJ)= A(I)$ A(I)= TS T= A(IJ)$ TG= TAG(IJ)$ TAG(IJ)= TAG(I)

```

```

TAG(I)= TG$ GO TO 40
30  A(L)= A(K)$ A(K)= TT$ TG= TAG(L)$ TAG(L)= TAG(K)$ TAG(K)= TG
40  L= L- 1$ IF(A(L).GT.T) GO TO 40 $ TT= A(L)
50  K= K+ 1$ IF(A(K).LT.T) GO TO 50$ IF(K.LE.L) GO TO 30
    IF(L-I.LE.J-K) GO TO 60$ IL(M)= I$ IU(M)= L$ I= K$ M= M+ 1
    GO TO 80
60  IL(M)= K$ IU(M)= J$ J= L$ M= M+ 1$ GO TO 80
70  M= M- 1$ IF(M.EQ.0) RETURN$ I= IL(M)$ J= IU(M)
80  IF(J-I.GE.11) GO TO 10$ IF(I.EQ.I1) GO TO 5$ I= I- 1
90  I= I+ 1$ IF(I.EQ.J) GO TO 70$ T= A(I+1)$ IF(A(I).LE.T) GO TO 90
    TG= TAG(I+1)$ K= I
100 A(K+1)= A(K)$ TAG(K+1)= TAG(K)$ K= K- 1$ IF(T.LT.A(K)) GO TO 100
    A(K+1)= T$ TAG(K+1)= TG$ GO TO 90
END

```

IDENT FTNUTIL

LIST

USE START.

TRACE. VFD 42/7LFTNUTIL,18/FTNUTIL

TEMPA0. BSS 18

ENTRY. BSS 08

FTNUTIL BSS 18

SX6 A0

SA0 A1

SA6 TEMPA0.

FTNNOP. DATA 46000460004600046000B

USE CODE.

USE DATA.

NAM VFD 60/7LCALINGP

LIN DATA 00000000000000007777B

S BSS 18

T BSS 18

PARNO DATA 0000000000000000001B

ADDR DATA 0000000000000000777777B

DFL DATA 000000000000000000777B

X BSS 3H

FL. DIS 1,FL

TRCEBCK EQU ENTRY.

ENTRY TRCEBCK

NOPS. DATA 46000460004600046000B

ENTR. MACRO NAME

LOCAL X,Z,T

EQ T

NAME BSS 1

ENTRY NAME

SA2 X

BX6 X2

SA6 FTNNOP.

EQ ENTRY.+1

X EQ Z

Z SA1 NOPS.

SA2 NAME

BX6 X1

LX7 H0,X2

SA6 FTNNOP.

SA7 ENTRY.

T BSS 0

ENDM

.201 VFD 60/6C 201

DIS 5. (/* TRCEBCK CALLED BY *A7.* AT LINE *14)

.202 VFD 60/6C 202

DIS 6. (/* TRCEDMP CALLED BY *A7.* AT LINE *14.16X*REAL*19X*DECIN

DIS 2,T*20X*OCTAL*)

```

.203      VFD 60/6C 203
DIS 6,(/* TIMEPRT CALLED BY *A7,* AT LINE *I4,*, CP TIME=*F9.3,*
DIS 3,SEC, SYSTEM TIME *A10)
.204      VFD 60/6C 204
DIS 6,(/* ERREXIT CALLED BY *A7,* AT LINE *I4,16X*REAL*19X*DECINT
DIS 2,*20X*OCTAL*)
.211      VFD 60/6C 211
DIS 4,(10X*CALLED BY *A7,* AT LINE *I4)
J01      VFD 60/6C 301
DIS 6,(/* PAR. NO. *12,* AT OCTALL *06,*, DFL= *I3,6X1PE22.14.5X1
DIS 1,16,8X020)
.302      VFD 60/6C 302
DIS 3,(46X1PE22.14.5X116,8X020)
.401      VFD 60/6C 401
DIS 4,(//* SYSTEM COMM. AREA OCTAL DUMP*/)
.403      VFD 60/6C 403
DIS 6,(//* WORKING AREA DUMP. 4000R AROUND ERREXIT CALL*/)
IEN      BSS 1R
EXT      OUTPUT$
EXT      OPUIC1.
EXT      OUTPTC.
EXT      SECONDS$
EXT      TIME$
EXT      PDUMPS$
IS       BSS 1R
IF       BSS 1R
IADR     BSS 1R
CALLA    BSS 1R
EXT      EXIT$
CON. HSS 0B
DATA 000000000000000000000000H
DATA 000000000000000000000100R
DATA 000000000000000000000004H
USE CODE.
* SX6 1R
SA6 IEN
EQ .100
ENTR. TRCEDMP
* SX6 2R
SA6 IEN
EQ .100
ENTR. TIMEPRT
* SX6 3R
SA6 IEN
EQ .100
ENTR. ERREXIT
* SX6 4R
SA6 IEN
.100 HSS 0B
SA5      ENTRY.
AX5      30
HX6      X5
SA6      CALLA
SA4      X5-1B
SA3      X4
BX6      X3
SA6      NAM
AX4      1R
MX7      4R
HX6      -A7*X4
SA6      LIN
MX7      42

SAVE      X5=RET.ADDR.
CALL ADDRESS
X4=-VFD12/LIN,18/TRACE.
X3=VFD42/7LCALPNAM,18/CALPNAM

```

```

      RX6      -X7*X3
      SA6      IADR
SA4 IEN
SX0 X4-4B
SH1 X4-2B
PL X0,.104
LT R1,R0,.101
JP R1+EGL1
EGL1 BSS 0B
EQ .102
EQ .103
.101 HSS 0B
+ SR2 OUTPUT=
  SR3 .201
+ RJ OUTPUT1.
- VFD 12/14B,1B/TRACE.
+ SH1 NAM
      SH2      2B
  RJ OUTPTC.
+ SH1 -1B
  RJ OUTPTC.
  EQ .200
.102 HSS 0B
+ SH2 OUTPUT=
  SR3 .202
+ RJ OUTPUT1.
- VFD 12/17B,1B/TRACE.
+ SR1 NAM
      SH2      2B
  RJ OUTPTC.
+ SR1 -1B
  RJ OUTPTC.
  EQ .300
.103 HSS 0B
+ SA1 IAP1
+ RJ SECONDS
- VFD 12/23B,1B/TRACE.
+ SA5 S
  SA4 A0
  BX7 X5
  SA1 IAP2
  SA7 X4
  NO
+ RJ TIME$
- VFD 12/23B,1B/TRACE.
+ SH2 OUTPUT=
  SR3 .203
+ RJ OUTPUT1.
- VFD 12/24B,1B/TRACE.
+ SR1 NAM
      SH2      4B
  RJ OUTPTC.
+ SR1 -1B
  RJ OUTPTC.
  EQ .99
.104 HSS 0B
+ SH2 OUTPUT=
  SR3 .204
+ RJ OUTPUT1.
- VFD 12/30B,1B/TRACE.
+ SR1 NAM
      SH2      2B

```

STORE PREVIOUS ENTRY

DO BOTH NAM AND LIN

PRINT NAM,LIN,S,T

PRINT , NAMJ,LIN

RJ OUTPTC.

+ SB1 -1B

RJ OUTPTC.

.200 HSS 0B
 SA4 IADR
 ZR X4,.299
 SA5 X4
 AX5 30
 SA4 X5-1B
 SA3 X4
 HX6 X3
 SA6 NAM
 AX4 1B
 MX7 4B
 HX6 -X7*X4
 SA6 LIN
 MX7 42
 HX6 -X7*X3
 SA6 IADR

SB2 OUTPUT

SB3 .211

+ RJ OPUTCI.

- VFD 12/7B,1B/TRACE.

+ SB1 NAM

SB2 2B

RJ OUTPTC.

+ SB1 -1B

RJ OUTPTC.

EQ .200

.299 HSS 0B

SA5 IEN

SX0 4B

IX7 X5-X0

NO

NZ X7,.99

.300 HSS 0B

SX6 1B

SA6 PARNO

SA5 40

AA

HSS 0B

SA4 X5

SB2 OUTPUT

SB3 .301

HX7 X4

SA7 X

SA7 X+1B

SA7 X+2B

HX6 X5

SA6 ADDR

SA5 40+1B

SA4 X5

SA3 FL.

IX0 X3-X4

ZR X0,.21

SX6 1B

SA6 OFL

EQ .23

.21 HSS 0B

SA0 40+2B

SA5 40

ZR X5,.25

SA4 X5

FULL TRACE ENTRY .

JMP,TRACE ENDS.

X5=-ET.ADD-

X4=-VFD12/L+N,1B/T-ACE.

X3=VFD42/7LCALPNAM,1B/CALPNAM

STORE PREVIOUS ENTRY

BRING FIRST PAR. AD.

FETCH FIRST PAR.

	SX0	X4-1B	
	NG	X0..25	IF DFL LT 1 RETURN
	SX7	X4-777B	
	NG	X7..27	
	SX4	777B	DFL LE 777B
.27	HSS	0B	
	HX6	X4	
	SA6	DFL	
.23	HSS	0B	
+	RJ	OUTPUTC.	
-	VFD	12/12B,18/TRACE.	
+	SB1	PARNO	
	SB2	6B	
	RJ	OUTPTC.	
+	SB1	-1B	
	RJ	OUTPTC.	
	SA5	DFL	
	SX6	2B	
	IX0	X5-X6	
	HX7	X0	
	SA7	DFL	
	NG	X0..29	IF DFL LT 2 GO FOR NEXT PAR.
+	SR2 OUTPUTC		
	SB3	.302	
+	RJ OUTPUTC.		
-	VFD	12/6B,18/TRACE.	
AB	HSS	0B	
	SA5	ADDR	
	SX4	X5+1B	
	SA3	X4	
	HX7	X4	
	SA7	ADDR	
	HX6	X3	
	SA6	X	
	SA6	X+1B	
	SA6	X+2B	
+	SH1	X	
	SH2	3B	
	RJ	OUTPTC.	
	SA5	DFL	
	SX7	X5-1B	
	SA7	A5	
	PL	X7,AB	
+	SB1	-1B	
	RJ	OUTPTC.	
.29	HSS	0B	
	SA0	40+1B	LOOK AT NEXT PAR.
	SA5	A0	X5= AD. OF NEXT PAR.
	ZR	X5..25	IF NO MORE END IT ALL.
	SA4	PARNO	
	SX7	X4+1B	
	SX0	X7-25B	
	SA7	A4	
	NG	X0,AA	
.25	HSS	0B	
	SA5 IEN		
	SX0 4B		
	IX7 X5-X0		
	NO		
	NZ X7..99		
	SR2 OUTPUTC		
	SR3 .401		

PARNO= 1 , 20

```

+ RJ OUTPUTI.
- VFD 12/53B,1B/TRACE.
+ SR1 -1R
  RJ OUTPUTC.
+ SA1 [AP3
+ RJ PDUMPS
- VFD 12/55B,1B/TRACE.
+ SR2 OUTPUTI
  SR3 .403
+ RJ OUTPUTI.
- VFD 12/56B,1B/TRACE.
+ SR1 -1R
  RJ OUTPUTC.
+ SA1 [AP4
      SA5      CALLA
      SX7      X5-2000B
      PL       X7,.9H
      SX7      0B
.98    RSS     0B
      SX6      X5+1777B
      SA7 IS
      SA6 IF
+      RJ      PDUMPS
- VFD 12/60B,1B/TRACE.
+      RJ      EXIT$
-      VFD     12/61B,1B/TRACE.
.99 BSS 0B
+ SA5 TEMP00.
  SA0 X5
  NO
  EQ ENTRY.
[AP1      BSS 0B
  VFD 60/S
  DATA 0B
[AP2      BSS 0B
  VFD 60/T
  DATA 0B
[AP3      BSS 0B
      VFD     60/CON.
  VFD 60/CON.+1R
  VFD 60/CON.+2H
  DATA 0B
[AP4      BSS 0B
  VFD 60/IS
  VFD 60/IF
  VFD 60/CON.+2B
  DATA 0B
      END
      OVERLAY(READIN,3,0)
      PROGRAM READIN
*
*   TO READ IN THE TWO-BODY MATRIX ELEMENTS .
*   ALL WILL BE OVERWRITTEN TO LENGTH 15000 .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
COMMON/CONTRSN/ICON(2,40),RNU(5,40),ISLK,HBOW,TNAME,HBWA(30)
COMMON/OVERCON/ FIRST,ISKP
COMMON AS1(8000),AL1(1)
DIMENSION NA(2),IPOS(8),COA(8),BTA(2)
DATA BTA/4LR0N1,4LR0P1/
CALL TIMEPRT(YT)$ IF(ISKP.EQ.0) GO TO 1

```

```

CALL REUFAT1(TNAME,IDG,IBLK,AL1)$ REWIND 1
*
* FLD CONTAINS THE DIMENSIONLESS COULOMB ANTIS. MATRIX ELEMENTS .
E2B= SQRT(.0241145*HBOM)*1.44
CALL ADLONG(3LFNE,1.,3LFLD,E2B,3LFPR,AS1,AL1)
CALL BUFIN(3LFLD,AL1,IDF)$ DO 15 K = 1 , IDF
15 AL1(K)= E2B*AL1(K)$ CALL BUFOUT(3LFCO,AL1,IDF)$ GO TO 99
1 DO 9 KIN= 1 , 2
READ 103,CNAME,NA,KIND,CTNAME,IBLKC,CHROM,CWHEN,CNOW
PRINT 105,CNAME,NA,KIND,CTNAME,IBLKC,CHBOM,CWHEN,CNOW
103 FORMAT(A10,2I4,2X2A10,15,F10.2,2A10)
105 FORMAT(1XA10,2I4,2X2A10,15,F10.2,2A10)
101 FORMAT(8(I4,F6.4))
102 FORMAT(1X8(I4,F6.4))
IS= ICNT=0$ IDSC= 2*IDSC$ DO 11 I = 1 , IDSC
11 AS1(I)= 0.$ DO 3 KC= 1 , 1340
READ 101,(IPOS(J),COA(J),J=1,8)
PRINT 102,(IPOS(J),COA(J),J=1,8)
IREIM= 1$ DO 3 JC= 1 , 8$ IF(COA(JC).NE.0) GO TO 7
IF(IPOS(JC).NE.ICNT) CALL ERREXIT(IPOS(JC),ICNT)$ IS= IDSC$ICNT=0
IREIM= IREIM+1$ ICNT=0$ IF(IREIM.LE.2) 3,13
7 IF(IPOS(JC).GT.IDSC) CALL ERREXIT(IDSC,IPOS(JC))
AS1(IS+IPOS(JC))= COA(JC)$ ICNT= ICNT+1
3 CONTINUE$ CALL ERREXIT(KKIN,CNAME)
13 CALL DENMAT(AL1,AS1,AS1(IS+1),NA)$ CALL ROCONV(AL1,AS1,1)
CALL BUFOUT(BTA(KKIN),AS1,IDSJ)
9 CONTINUE
99 CONTINUE
END
SUBROUTINE REDFAT1(FLNAME,IDG,IBLK,AL1)
*
* FLD= FCS
* READ FROM TAPE1 INTO DISC THE 7 ARRAYS .
* NOLV= F(1)= NUMBER OF LEVELS .
* ICODE(NOLV)= CODENUMBER ARRAY= F(2,...,NOLV+2) .
* IDF= NUMBER OF F ELEMENTS READ .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPU,
2 NBT,HBOM,OSPA2
DIMENSION TA(25),NAA(7),AL1(1)
DATA NAA/3LFNE,3LFDN,3LFLD,3LRTS,3LRTO,3LPTS,3LPTD/
REWIND 1
IBLP= IBLK+1$ DO 11 IBL= 1 , IBLP,IBLK$IB=IBL-1
IF(IB-1.LT.1) GOTO5$IRS= IB-1$ DO 3 ISK= 1 , IRS$ DO 3 K = 1 , 4
3 READ(1)
5 READ(1) TA $ TITLE= TA(1)$ IF(TITLE.NE.FLNAME) GO TO 101
NOLV= TA(2)$ DO 7 K = 1 , NOLV
7 ICODE(K)= TA(K+2)
IDF= TA(21)$ IDG= TA(22)$ HBOM= TA(23)$ IF(IB.LT.1) GO TO 13
READ(1) (AL1(I),I=1,IDG)$ CALL BUFOUT(5LGMATR,AL1,IDG)
13 DO 1 L = 1 , 7$ IF((IB.LT.1.A.L.LT.3).OR.(IB.GT.0.A.L.GT.2))GOTO1
READ(1) (AL1(I),I=1,IDF)$ CALL BUFOUT(NAA(L),AL1,IDF)
1 CONTINUE
11 CONTINUE
105 RETURN
101 PRINT 103
103 FORMAT (/* F ARRAY NOT ON TAPE */)
GO TO 105
END
OVERLAY(ELMOSE,1,0)
PROGRAM ELMOSE

```

```

* ELMOSE PROVIDES THE FOLLOWING SERVICES FOR EVALIN.
* IT SETS QNO(NHT), THE CHARACTER ARRAY, THE SINGLE PART. MES.
* IT PROVIDES THE INITIAL GUESS FOR THE NUCLEAR WAVEFUNCTION TO BE
* USED IN NUHART, IF ISKP.NE.0 .
COMMON/HASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUJ,IOF,IOJC,IOJ,JAR(14,2),IDAC(14,14),JMPO,
2 NHT,HRUM,OSPA2
COMMON/OVERCUN/FIRST,ISKP
COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,ITER,ITCR,ATNO
1 ,NORHA(41),NORB,BET,GAMD,NPTOT,NNTOT
COMMON/NAMEN/FPR,PTS,FPF,FNE,FNF,FON,PTD,FDF,RONI,ROPI,SPE,SPEXF
1 ,RTS,RID
COMMON AS1(4000),AS3(4000)
COMMON/PRINLIM/EPS,IPR,QNO(82)
COMMON /SPINORH/ CHI(7),RD(7)/EXSYPN/EXF(6,6),SYP(21),NOMM(20,3),
1 COMM(20)/CARTEMP/AS2(5726)
LOGICAL FIRST
EQUIVALENCE (KTMP,IOJ)
DATA CHI,RD/4*.07,3*.05,3*.1,.35,3*.45/
CALL TIMEPRT(Y)$ CALL CARTOJ(0)$ IF (ISKP.EQ.0) GO TO 20
PRINT 103,NAME$ CALL ELTRIAL(AS1,IPR)
103 FORMAT(*1 TRIAL WAVE FUNCTION COMPUTATION FOR *A10)
DO 11 K = 1 , IOJC
11 AS2(K)= 0.$ CALL REORDER(VALP,NP)$ CALL DENMAT(AS3,AS1,AS2,NP)
CALL ROCONV(AS3,AS2,1)$ CALL BUFOUT(ROPI,AS2,IOJ)$ DO 13 K=1,IOJC
13 AS2(K)= 0.$ CALL REORDER(VALP,NN)$ CALL DENMAT(AS3,AS1,AS2,NN)
CALL ROCONV(AS3,AS2,1)$ CALL BUFOUT(ROPI,AS2,IOJ)
*
* FIRST TIME AROUND COMPUTE THE 21 EXTERNAL FIELD OPS. XI*XJ,PI*PJ,
* RI*PJ,I,J=1,2,3,IN DIMENSIONLESS FORM .
20 IF(.NOT.FIRST) GO TO 22$ DO 21 K1= 1 , 6$ DO 21 K2= 1 , K1
CALL EXF1H(AS3,K1,K2)
IF(IPR.GT.4) PRINT 101,EXF(K1,K2),(AS3(I),I=1,IOJC)
CALL ROCONV(AS3,AS1,1)$ CALL BUFOUT(EXF(K1,K2),AS1,KTMP)
101 FORMAT(// * EXT FIELD NAME *A10/(1X10F12.5))
21 CONTINUE
*
* NOW PUT THE 21 OPERATORS IN THE SYMPLECTIC BASIS .
ICO=1$ DO 201 IS= 1 , 9$ DO 203 K = 1 , KTMP
203 AS1(K)= 0.
207 CALL BUFFIN(EXF(NOMM(ICO,3),NOMM(ICO,2)+3),AS2,KTMP)
CONS= COMM(ICO)$ DO 205 K = 1 , KTMP
205 AS1(K)= AS1(K)+ AS2(K)*CONS
ICO= ICO+1$ IF(NOMM(ICO,1).EQ.IS) GO TO 207
201 CALL BUFOUT(SYP(IS),AS1,KTMP)
ICO= 7$ DO 211 IS= 4 , 9$ DO 213 K = 1 , KTMP$ AS3(K)= 0
213 AS1(K)= 0
217 CALL BUFFIN(EXF(NOMM(ICO,3),NOMM(ICO,2)),AS2,KTMP)
CONS= COMM(ICO)$ DO 215 K = 1 , KTMP
215 AS1(K)= AS1(K)+ AS2(K)*CONS
CALL BUFFIN(EXF(NOMM(ICO,3)+3,NOMM(ICO,2)+3),AS2,KTMP)
DO 225 K = 1 , KTMP
225 AS3(K)= AS3(K)+AS2(K)*CONS$ ICO=ICO+1$IF(NOMM(ICO,1).EQ.IS)GOTO217
*
* SAVE THE KIN ENERGY .
IF(IS.NE.9) GO TO 226$ RKEN= .5*HRUM/CONS$ DO 227 K = 1 , KTMP
227 AS2(K)= RKEN*AS3(K)$ CALL BUFOUT(SPE,AS2,KTMP)
226 DO 233 K = 1 , KTMP$ AS2(K)= .5*(AS3(K)+AS1(K))
233 AS1(K)= .5*(AS3(K)-AS1(K))
CALL BUFOUT(SYP(IS+6),AS2,KTMP)$CALL BUFOUT(SYP(IS+12),AS1,KTMP)
SYP(10,,15)= .5*(PI*PJ+RI*RJ),SYP(16,,21)= .5*(PI*PJ-RI*RJ)
*
211 CONTINUE$ CALL CARSET(QNO)
22 CONTINUE

```


END

SUBROUTINE ELTRIAL(BR,IPR)

```

*
* BR(ND,ND)= REAL PART OF EIG. VECT MATRIX TO BE FILLED.
* NB= RETURNED VALUE OF BASIS DIM.
* NORBA(NORB)= ARRAY OF NILSSON ORBITS TO BE FILLED,
* AT VALUES OF BET= BETA GAMD= GAMMA IN DEGREES .
* CODA(NOLV)= CODENUMBER ARRAY TO DESCRIBE THE BASIS .
* IPR= PRINT INDEX VARIES FROM -1 TO +6 .
  COMMON/BASIS/ ICODE(16),ISTA(16),IPAA(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NRT,HBOM,OSPA2
  COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,ITER,ITCR,ATNO
1 ,NORBA(41),NORB,BET,GAMD,NPTOT,NNTOT
  DIMENSION HR(1),MLAM(2),ITE(2),IFL(2),IBSAD(7,7)
  COMMON/SPINORB/CHI(7),RD(7)
  COMMON /WAVN/ ARRAYS(4116),TAU(3),SR(3)
  COMMON /DISTRU/ FNNP(7,4,3) /DUMPN/C1(75,2),C2(75,2)
  DO 1 K = 1, 75 DO 1 L = 1, 7
1   IBSAD(K,L)=0$ IFL(1)=1$ IFL(2)= 1
  DO 3 K = 1, NOLV$ JPH= ISTA(K)$ NPO= INPO(K)$ IPAR= 3-IPAA(K)
  IBSAD(NPO,JPH)= IFL(IPAR)$ IFL(IPAR)= IFL(IPAR)+ 2*JPH
3  CONTINUE
  CALL WAVSET(BET,GAMD,CHI,RD,IPR)
  DO 45 K = 1, 3
45  CALL DISTR(TAU(K),FNNP(1,1,K),7,4)
  KMA= IDSC$ DO 5 I = 1, NRT
5   VALP(I)= 100.$ DO 35 I = 1, KMA
35  BR(I)=0.$ MLAM(1)=0$ MLAM(2)= NB(1)**2$ ITE(1)=1$ ITE(2)=I+NB(1)
  ENLA= 1.$ DO 49 INP= 1, NORB$ JNIL= NORBA(INP)
  DO 49 KTR= 1, 2 $ IF(KTR.GT.1) GO TO 53
  CALL OBCFP(JNIL,C1,N1,75,1)$ GO TO 51
53  CALL TIMEREV(C1,N1,75)$ CALL SPRNTC(C1,N1,C1(1,2))
51  DO 55 N= 1, N1$ IQN= C1(N,1)$ NSHELL= IQN/10000
  IPAR= 1+ MOD(NSHELL,2)
  NREM= IQN- 10000*NSHELL$ JPK= NREM/100$ JMK= NREM-100*JPK
  JPH= (JPK+JMK+1)/2$ IADR= IBSAD(NSHELL+1,JPH)
  IF(IADR.EQ.0) GO TO 55
  IALAM= IADR+ JMK+ MLAM(IPAR)
  BR(IALAM)= C1(N,2)
55  CONTINUE $ MLAM(IPAR)= MLAM(IPAR)+ NB(IPAR)
  VALP(ITE(IPAR))= ENLA$ ENLA= ENLA+1.
  ITE(IPAR)= ITE(IPAR)+1
49  CONTINUE$ IF(IPR.GT.5) PRINT 103,(BR(I),I=1,IDSC)$ RETURN
103  FORMAT(/** THE TRIAL WF*//(1X10F12.5))
  END
SUBROUTINE CARTOJ(IPR)
*
* TO GENERATE THE ARRAYS STUCO(1260,2) AND CSS(300,2) WITH THEIR
* DICTIONARY IQN(34,6), ICSD(49) .
* STUCO CONTAINS THE COMPONENTS IN THE SPIN-CART. BASIS OF THE
* SPHERICAL EIGENSTATES/N,J,K), WITH K=.5= EVEN, WITH THE
* BRODY-MOSHINSKY PHASE . CSS CONTAINS THE COMPONENTS OF THE
* SOLID SPHERICAL HARMONICS IN THE S-C OPERATOR BASIS.
* THE METHOD USED IS BASICALLY THAT OF MOSHINSKY IN THE NOTES.
* GROUP THEORY AND COLLECTIVE MOTION,1962, LATIN AM. SCHOOL OF PHYS.
  COMMON /CARJN/ STUCO(1260,2),IQN(34,6),CSS(300,2),ICSD(49)
  COMMON /CARTEMP/ CS(25,2,13),CU(15,2,13),CJA(30,2,49),IAD(7,14,14)
1 ,NPA(13),SFAC(7),USFAC(7),IJA(49),ITQN(49,2),C(50,2),CP(50,2)
  DATA PI/3.14 159 265 358 98/
  DSFAC(1)= SFAC(1)= 1.$ NX= 1$ DO 21 I = 1, 6
  DSFAC(I+1)= USFAC(I)*SQRT(FLOAT(2*I+1))

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```

21 SFAC(I+1)= SFAC(I)*SQRT(FLOAT(I))
*
* FOR N = 0-6 SHELLS, L= 0-6
* ICL= 1$ DO 1 IL= 1 , 7$ L= IL-1$ RIL= L$ RLH= 1./SQRT(2.*RIL+1.)
*
* FIRST CONSTRUCT YLL IN THE A,B,C BASIS AS  $(4*\pi/(2*L+1))^{.5}*R^{.5}*L*Y(L,L)$ 
N= 1$ C(1,1)= FLOAT(10000*L)
503 C(1,2)= DSFAC(IL)/SFAC(IL)*RLH*(1-2*MOD(L,2))
505 KMM= 2*L+1$ M= L$ DO 3 KM= 1 , KMM
CALL POLTRA(CS(1,1,KM),NPA(KM),25,C,N,50)
CALL TRIMUP(CS(1,1,KM),NPA(KM),25,1.E-8)
ICM= NPA(KM)$ ITE= 10000*ICL+ ICM
DO 511 IC= 1 , ICM$ DO 513 J = 1 , 2
513 CSS(ICL,J)= CS(IC,J,KM)
511 ICL= ICL+ 1$ IF (KM.EQ.KMM) GO TO 3
CALL NOLMIN(CP,NP,50,L,M, C,N,50)
DO 7 J = 1 , NP$ DO 7 I = 1 , 2
7 C(J,I)= CP(J,I)$ N= NP
3 CONTINUE
5 IF(IPR.LT.2) GO TO 10$ PRINT 101, L
101 FORMAT(///' SPHER. HARM. OF ORDER *12,* IN SPIN-CART. OP. BASIS*
1 //)
*
* NOW USE CS THE OPERATOR TO CONSTRUCT CU THE STATE VECTOR .
10 DO 9 KM= 1 , KMM$ M= L+ 1- KMS ISWI= MOD(IABS(M),2)+ 1
JM= NPA(KM)$ DO 23 J = 1 , JMS NTE= IFIX(CS(J,1,KM))
N1= NTE/10000$ NTE= NTE- 10000*N1$ N2= NTEP/100$ N3= NTEP-100*N2
N12= MOD(N1*N2,2)$ GO TO (25,27) ISWI
25 IPHAS= 1- 2*MOD(N2/2+N12,2) $ GO TO 29
27 IPHAS= 1-2*MOD((N2+1)/2+N12,2)
29 CNOR= SFAC(N1+1)*SFAC(N2+1)*SFAC(N3+1)*IPHAS$CU(J,1,KM)=CS(J,1,KM)
23 CU(J,2,KM)= CS(J,2,KM)*CNOR$ IF(IPR.LT.2) GO TO 9
PRINT 119, M
119 FORMAT(4HOM= I3)
CALL SPRNTC(CS(1,1,KM),NPA(KM),CS(1,2,KM))
9 CONTINUE
*
* NEXT CONSTRUCT STATES OF GOOD J,K IN CJA , WITH K-.5= EVEN.
DO 31 IPH= 1 , 2$ JPH= IL+ IPH- 2$ IF(JPH.LT.1) GO TO 31
ISWI= IPH$ DO 33 IAK= 1 , JPH
IAKM= MOD(IAK-1,2)$ RK= (FLOAT(IAK)-.5)*(1-2*IAKM)
IKPH= IAK*(1-2*IAKM)+ IAKM $ C01= SQRT(RIL+ .5*RK)*RLH
C02= SQRT(RIL-.5-RK)*RLH$ GO TO (35,37) ISWI
35 A1= -C02$ A2= + C01$ GO TO 39
37 A1= C01$ A2= C02
39 KM1= IL- IKPH+ 1$ KM2= KM1-1$ N1= 0
IF(KM1.LT.1.OR.KM1.GT.2*IL-1) GO TO 41$ N1= NPA(KM1)
41 N2= 0$ IF(KM2.LT.1.OR.KM2.GT.2*IL-1) GO TO 43$ N2= NPA(KM2)
43 CALL LINCOM(A1,CU(1,1,KM1),N1,15,A2,CU(1,1,KM2),N2,15,
1 CJA(1,1,NX),IJA(NX),30)
IN1= JPH+ IKPH$ IN2= JPH- IKPH+1$ IAD(IL,IN1,IN2)= NX
ITON(NX,1)= IN1- 1$ ITON(NX,2)= IN2- 1$ NX= NX+ 1
33 CONTINUE
31 CONTINUE
1 CONTINUE
*
* START COPYING INTO MAIN ARRAY STUCO .
ILAH= NY= 1$ DO 51 IN= 1 , 7 $ NSH= IN- 1$ ILU= NSH/2+ 1
IREM= MOD(NSH,2)$ IL= IREM+ 1$ DO 53 ILT= 1 , ILU$ L= IL- 1
NEX= (NSH- L)/2$ IN1= MAX0(IL,2)$ IN2= IN1- 1$ KMM= 2*IL- 1
NAST= IAD(IL,IN1,IN2)$ DO 55 KM= 1 , KMM
TFAC= SQRT(FLOAT(2*IL-1))/DSFAC(IL)$ BNOR= 1.

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```

IF(NEX.EQ.0) BNOR= TFAC$ INEM= IJA(NAST)$ DO 59 INE= 1 , INEM
C(INE,1)= CJA(INE,1,NAST)
59 C(INE,2)= CJA(INE,2,NAST)$ IF(NEX.EQ.0) GO TO 71
*
* HERE PUT IN THE REQUIRED POWERS OF (ABS(ACROSS))**2 .
DO 57 JNE= 1 , NEX $ A= 1.
TFAC= -TFAC/SQRT(FLOAT((2*JNE+2*IL-1)*2*JNE))
IF(JNE.EQ.NEX) A= TFAC$ CALL SCALN2(A,CP,NP,50,C,INEM,50)
CALL TRIMUP(CP,NP,50,1,E-8)$ DO 61 INE= 1 , NP$ C(INE,1)=CP(INE,1)
61 C(INE,2)= CP(INE,2)$ INEM= NP
57 CONTINUE
71 IQN(NY,5)= ILAB$ DO 62 INE= 1 , INEM$ STUCO(ILAB,1)= C(INE,1)
STUCO(ILAB,2)= C(INE,2)*BNOR
62 ILAB= ILAB+ 1$ IQN(NY,6)= ILAB- 1$ IQN(NY,1)= NY
IQN(NY,2)= NSH$ IQN(NY,3)= ITQN(NAST,1)+ ITQN(NAST,2)
IQN(NY,4)= ITQN(NAST,1)- ITQN(NAST,2)
STUCO(ILAB,1)= 999900+ NY+ 1 $ STUCO(ILAB,2)= 0.$ ILAB= ILAB+ 1
NAST= NAST+ 1$ NY= NY+ 1
55 CONTINUE $ IL= IL+ 2
53 CONTINUE
51 CONTINUE
ILABT= ILAB- 1$ IF(ILABT.GT.1260) CALL EXIT
*
* ORDER STUCO FOR FUTURE USE IN SCALP .
DO 81 I= 1 , 8$ II= IQN(I,5)$ JJ= IQN(I,6)
81 CALL SORTAG(STUCO(1,1),II,JJ,STUCO(1,2))$ IF(IPR.LT.1) RETURN
PRINT 213
213 FORMAT(//*1 XPANS. COEF. OF SPHER. STATES IN S-C. BASIS*//)
CALL SPRNTC(STUCO(1,1),ILABT,STUCO(1,2))$ PRINT 217
217 FORMAT(//*1QUANTUM NUMBER DICTIONARY*/)
ITPR= 1$ DO 69 K= 1 , 7$ ITPM= ITPR+11
PRINT 219, ((IQN(I,J),I=ITPR,ITPM),J=1,6)
219 FORMAT (5H I= 12(3XI4,3X)/5H NH= 12(3XI4,3X)/5H 2*J=
1 12(3XI4,3X)/5H 2*K= 12( 3XI4,3X)/5H IAS= 12(3XI4,3X)/5H IAF=
2 12(3XI4,3X)/)
69 ITPR= ITPR+ 12$ RETURN
END
SUBROUTINE POLTRA(CP,NP,NDP,C,N,ND)
C
C CP(N,1)= 10000*NP1+ 100*NP2+ NP3 .
C CP(N,2)= COEFFICIENT .
C THIS SUBR. DOES POLYNOMIAL MANIPULATIONS.
C CP = CP+ C*(X-Y)**N1*(X+Y)**N2*Z**N3/2**((N1+N2)/2) .
C
DIMENSION CP(NDP,2),C(ND,2)
DATA SQA/.70710 67811 86548/
NP= 0$ IF(N.EQ.0) RETURN$ DO 1 NC= 1 , N$ BN= C(NC,2)
INT= IFIX(C(NC,1))$ N1= INT/10000$ INR= INT- 10000*N1$N2=INR/100
N3= INR- 100*N2$ SQ= SQA**((N1+N2)*BN$ CT1= 1.$ N1F= N1+1
DO 1 NR= 1 , N1F$ CT2= 1.$ N2F= N2+ 1$ DO 3 NS= 1 , N2F
CST= 10000*(N1F-NR+N2F-NS)+ 100*(NR+NS-2)+ N3
COE= SQ*CT1*CT2$ IF(NP.EQ.0) GO TO 7 $ DO 5 NPP= 1 , NP
IF(CST.NE.CP(NPP,1)) GO TO 5$ CP(NPP,2)= CP(NPP,2)+ COE$GOTO9
5 CONTINUE
7 NP= NP+ 1$ IF(NP.GT.NDP) CALL EXIT$ CP(NP,1)= CST$ CP(NP,2)=COE
9 CT2= CT2*(N2F-NS)/FLOAT(NS)
3 CONTINUE
CT1= -CT1*(N1F-NR)/FLOAT(NR)
1 CONTINUE$ RETURN
END
SUBROUTINE TRIMUP (C,N,ND,EPS)
C EPS= SMALLEST TERM TO BE RETAINED .

```

```

C      N WILL BE CHANGED .
C
      DIMENSION C(ND,2)
      IF (N.EQ. 0) RETURN$ NP= 0$ DO 1 NT= 1 , N
      IF (ABS(C(NT,2)).LT.EPS) GO TO 1$ NP= NP+ 1
      IF (NP.GT.ND) CALL EXIT$ C(NP,1)= C(NT,1)$ C(NP,2)= C(NT,2)
1 CONTINUE$ N= NP$ RETURN
      END
      SUBROUTINE NULMIN(CP,NP,NDP,L,M,C,N,ND)
C
C      COMPUTE THE ACTION OF THE NORMALISED LOWERING OPERATOR.
C
      DIMENSION CP(NDP,2),C(ND,2),IN(2),TEC(2),SIG(2)
      DATA TEC/99.,-9999./, SIG/1.,-1./
      NP = 0$ IF(N.EQ.0) RETURN $ IF(M.LE.-L) GO TO 17
      CNOR= SQRT(2./FLOAT((L+M)*(L-M+1)))$ DO 1 NT= 1 , N
      INT = IFIX(C(NT,1))$ INTP= INT/100$ IN(1)= INT- 100*INTP
      IN(2)= INT/10000$ DO 1 J = 1 , 2$ IF(IN(J).LT.1) GO TO 1
      QNT = C(NT,1)+ TEC(J)$ CT= SIG(J)*IN(J)*C(NT,2)*CNOR
      IF(NP.EQ.0) GO TO 7$ DO 5 NPT= 1 , NP$ IF(QNT.NE.CP(NPT,1))GOTO 5
      CP(NPT,2)= CP(NPT,2)+ CT$ GO TO 1
5 CONTINUE
7 NP = NP + 1$ IF(NP.GT.NDP) CALL EXIT $ CP(NP,1)= QNT$CP(NP,2)= CT
1 CONTINUE
17 M = M-1$ RETURN
      END
      SUBROUTINE SPRNTC(RQN,LGT,COE)
*
*      TO PRINT THE LGT QUANTUM NUMBERS IN RQN AND UNDER THEM THE LGT
*      CORRESPONDING COEFFICIENTS .
      DIMENSION RQN(1),COE(1),IQD(12)
      DATA LEFSQB,RITSQB/1L(.1L)/
      ITPR= 1$ KTOT= (LGT+ 11)/12$ DO 67 K = 1 , KTOT
      ITPM= MIN0(LGT,ITPR+11)$ IMX= ITPM- ITPR+ 1
      DO 1 I = ITPR, ITPM$ IT= I- ITPR+ 1
1      IQD(IT)= RQN(I)
      PRINT 215,(LEFSQB,IQD(I),RITSQB,I=1,IMX)
215 FORMAT(* QN=*12(2X1,I7,A1))
      PRINT 217,(COE(I),I=ITPR,ITPM)
217 FORMAT(* CI=* 12F11.7)
67 ITPR= ITPR+ 12$ RETURN
      END
      SUBROUTINE LINCOM(A1,C1,N1,ND1,A2,C2,N2,ND2,C,N,ND)
C
      DOES C = A1*C1+ A2*C2 .
      DIMENSION C1(ND1,2),C2(ND2,2),C(ND,2)
      N = 0$ IF(N1.EQ.0) GO TO 1$ IF(N1.GT.ND) CALL EXIT
      DO 3 IT= 1 , N1$ C(IT,1)= C1(IT,1)
3 C(IT,2)= A1*C1(IT,2)
      N = N1
1 IF (N2.NE.0) RETURN$ DO 5 IT= 1 , N2$ IF(N.EQ.0) GO TO 9
      DO 7 JT= 1 , N$ IF(C(JT,1).NE.C2(IT,1)) GO TO 7
      C(JT,2)= C(JT,2)+ A2*C2(IT,2)$ GO TO 5
7 CONTINUE
9 N = N+ 1$ IF(N.GT.ND) CALL EXIT$ C(N,1)= C2(IT,1)
      C(N,2)= A2*C2(IT,2)
5 CONTINUE$ RETURN
      END
      SUBROUTINE SCALN2(A,CP,NP,NDP,C,N,ND)
*
*      COMPUTES (ABS(ACROSS))**2 ON THE SPIN-CART. STATE IN C AND PUTS
*      THE RESULTING (UNNORMALISED) STATE IN CP .
      DIMENSION CP(NDP,2),C(ND,2),RINC(3),IAN(3)

```

```

DATA RINC/20000.,200.,2./
NP = 0$ IF(N.EQ.0) RETURN$ DO 1 IN= 1 , N$ CT= C(IN,1)
NIN = IFIX(CT)$ CT2= C(IN,2)$ N1= NIN/10000$ NTE= NIN-10000*N1
N2 = NTE/100$ N3= NTE- 100*N2$ IAN(1)= N1$ IAN(2)=N2$ IAN(3)=N3
IPHAS= 1$ DO 1 JK= 1 , 3$ IF(JK.EQ.2) IPHAS= 1- 2*MOD(N1,2)
IF(JK.EQ.3) IPHAS= 1- 2*MOD(N1+N2,2)
FAC= SQRT(FLOAT((IAN(JK)+1)*(IAN(JK)+2)))$ CTP= CT+ RINC(JK)
IF(NP.EQ.0) GO TO 7$ DO 5 INP= 1 , NP
IF(CTP.NE.CP(INP,1)) GO TO 5
CP(INP,2)= CP(INP,2)+ A*FAC*CT2$ GO TO 1
5 CONTINUE
7 NP = NP+ 1$ IF(NP.GT.NDP) CALL EXIT$ CP(NP,1)= CTP
CP(NP,2)= A*FAC*CT2
1 CONTINUE$ RETURN
END
SUBROUTINE WAVSETE(BET,GAMD,CHI,RD,IPR)

```

```

*
* TO COMPUTE THE WAVEFUNCTIONS OF A SINGLE NUCLEON IN AN ELLIP-
* SOIDAL MODIFIED OSCILLATOR, FOR N= 0-6. SEE REF. S.G. NILSSON,
* DAN.MAT.FYS.MEDD.29,NO.16(1955), FOR INTERPRETATION AS A DEF.
* BASIS OR AS A SPHERICAL BASIS.
* BET,GAMD,CHI(7), RD(7), ARE INPUT PARAMETERS OF THE MODEL.
* IPR= -1 ELIMINATES PRINTOUT, 0.LE.IPR.LE.6 SPECIFIES PRINT
* DETAILING.
* THE BLOCK/WAVN/ CONTAINS ALL COMPUTED RESULTS.
* NOTE THAT THE NATURAL ORDER IS THE ONE IN WHICH THE STATES ARE
* OBTAINED WHILE THE INCREASING ORDER IS THE ONE FOR WHICH THE
* ENERGY EIGENVALUES ARE INCREASING. ALL ARRAY SUBSCRIPTS WITH 1.LE.I.LE.
* 84 REFER TO THE NATURAL ORDER EXCEPT THOSE OF EAV(J) AND ITAG(J,1)
* EAV(J)= AVER. ENERGY, T+.5*V, OF THE STATE WHICH HAS THE JTH
* LOWEST EIGENVALUE, ITAG(J,1)=I=NATURAL ORDER OF THIS JTH LOWEST
* STATE. ENE,EAV, ARE IN UNITS OF H BAR OMEGA.
* ITAG(I,2)= STARTING POSITION IN WAVSET WHERE THE COMPONENTS AND
* Q.N. OF STATE I ARE STORED. THE END OF THE STATE I IS SIGNIFIED
* BY STORING 9999XX,(XX=1) IN WAVF(IEND,1) .
* RJZ(I), QUAD(I,3)= AVERAGES OF JZ,X**2,Y**2,Z**2,DIMENSIONLESS.
* NHA(I)= MAJOR SHELL QUANTUM NUMBER .
* TAUP(K)= NON-AXIAL DEFORMATION PARAMETERS .
* SR(K)= OMEGK/OMEG0.
* ALL INITIAL SPINS ARE + .
* THE Q.N. OF THE STATES +000 IS STORED AS +.1.
COMMON /WAVN/WAVF(1680,2),EAV(84),ENE(84),QUAD(84,3),ITAG(84,2),
1 RJZ(84),NHA(84),TAUP(3),SR(3)
COMMON /CARTEMP/ HAM(28,28),VEC(28,28),XHTQ(28,3),JLAB(84),
1 XHTL(28),RESTA(3962)
DIMENSION CHI(7),RD(7),TOU(3),SUMA(3),BSQ(3),INS(7),BOBO(3)
DATA PI,INS,TT/3.1415926535897,0,1,2,3,4,5,6,.6666666666666666/
ND= 28$ GAM= PI*GAMD/180.$ C1= .5*SQRT(1.25/PI)*BET
DO 1 K = 1 , 3$ TOU(K)= TAUP(K)= C1*COS(GAM- TT*K*PI)
BOBO(K)= EXP(TOU(K))$ BSQ(K)= BOBO(K)**2
1 SR(K)= 1./BSQ(K)$ ILAB= IWL= 1
DO 3 NZ= 1 , 7$ IRET= 0$ NH= NZ-1$ NST= (NH+1)*(NH+2)/2
CALL MOSDI(NH,TOU,CHI(NZ),RD(NZ),ENE(ILAB),RJZ(ILAB),IPR,IRET,
1 HAM,VEC,XHTL,XHTQ,ND)

```

```

*
* GENERATE/WAVN/BLOCK
DO 4 II = 1 , NST$ SUMA(1)= SUMA(2)= SUMA(3)= SUM1= 0.
ITAG(ILAB,2)= IWL$ DO 5 JJ = 1 , NST$ WAVF(IWL,1)= XHTL(JJ)
WAVF(IWL,2)= ETA= VEC(JJ,II)$ ETA= ETA**2$ HAMD= 0.
DO 104 K = 1 , 3$ HAMD= HAMD+ XHTQ(JJ,K)*SR(K)
104 SUMA(K)= SUMA(K)+ XHTQ(JJ,K)*ETAS$ SUM1= SUM1+ HAMD*ETAS
5 IWL= IWL+ 1$ EAV(ILAB)= .5*ENE(ILAB)+ .25*SUM1

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ITAG(ILAB,1)= ILAB$ NHA(ILAB)= NH
WAVF(IWL,1)= 999900.+ FLOAT(ILAB)$ WAVF(IWL,2)=0.$IWL= IWL+ 1
DO 4 K = 1 , 3
*9 QUAD(ILAB,K)= SUMA(K) SPHE.BA.
9 QUAD(ILAB,K)= HSQ(K)*SUMA(K) DEFO.BA.
4 ILAR= ILAB+ 1
3 CONTINUE$ ILAB= ILAB- 1
*
* ORDER EAV ACCORDING TO INCREASING ENE .
DO 21 K = 1 , 84$ JLAB(K)= K
21 XHTQ(K,1)= ENE(K)$ CALL SORTAG(XHTQ,1,84,ITAG)$ DO 23 K = 1,84
23 XHTQ(K,1)= EAV(ITAG(K,1))$ DO 25 K = 1 , 84
25 EAV(K)= XHTQ(K,1)$ IF(IPR.LT.0) RETURN
PRINT 101, HET,GAMD,(INS(J),CHI(J),RD(J),J=1,7)
101 FORMAT(/4X*ELLIPSOIDAL MODIFIED HARMONIC OSCILLATOR COMPUTATION*
1 //36X* DEF. PAR. OF POTENTIAL ARE, BETA=*F9.6,*, GAMMA=*F9.3//
2 33X*MAJOR SHELL N*6X*SPIN-ORBIT STRENGTH CHI*5X*LSQR STRENGT D*
3 //(38X12,19XF7.4,17XF7.4 ))
PRINT 103
103 FORMAT(/25X* STATE ORDERING ACCORDING TO INCREASING ENERGY EIG.
1VAL., FOR SUMMING PURPOSES*/)
ITPR= 1$ KMX= (ILAB+ 11)/12$ DO 12 K = 1 , KMX$ ITPM= ITPR+ 11
PRINT 105,(JLAB(I),I= ITPR,ITPM),(ITAG(I,1),I=ITPR,ITPM)
1 ,(EAV(I),I=ITPR,ITPM)
105 FORMAT(16H INCR. ORD.NO. J12(4X12,4X)/16H NATU. ORD.NO. I
2 12(4X12,4X)/ 16H EAV. OF JTH ST.12(1XF9.6)/)
12 ITPR= ITPR+ 12$ PRINT 107
107 FORMAT(/21X*ENERGY EIG.VAL., JZ AVER. AND MAJOR SHELL Q.N. IN THE
1 NATURAL ORDER(ORDER OF COMPUTATION)*/)
ITPR= 1$ DO 14 K = 1 , KMX$ ITPM= ITPR+ 11
PRINT 109, (JLAB(I),I=ITPR,ITPM),(ENE(I),I=ITPR,ITPM),
1 (RJZ(I) , I= ITPR, ITPM), (NHA(I),I=ITPR,ITPM)
109 FORMAT(/16H NATU. ORD.NO. I12(4X12,4X)/16H ENE. OF ITH ST.
1 12(1XF9.6)/16H JZA. OF ITH ST.12(1XF9.5)/16H NMSH OF ITH ST.
3 12(4X12,4X))
14 ITPR= ITPR+ 12$ IF(IPR.LT.1) RETURN$ PRINT 111
111 FORMAT(/31X*THE EIGENFUNCTIONS IN THE S-C. BASIS FOR INIT. SPIN=
1+, NAT. ORD.*//)
CALL SPRNTC(WAVF(1,1),IWL-1,WAVF(1,2))$ RETURN
END
SUBROUTINE MOSDI(NH,TOU,CHI,D,ENE,RJZ,IPR,IRET,HAM,VEC,XHTL,
1XHTQ,ND)
C
C NH = MAJOR SHELL
C TOU(K)= SQRT(5/4PI)/2*COS(GAM-2/3K*PI)*BETA .
C CHI=-L.SIG STRENGTH
C D= L**2 STRENGTH .
* IF IRET= 0 SET VEC TO 1 IF IRET= 1 USE CURRENT VALUE OF VEC .
* RJZ= AVERAGE VALUE OF JZ . VEC= EIGENVECTORS BY COLUMNS.
* ENE= EIGENVALUES , XHTL(N)= Q. NOS. OF THE BASIS STATES.
* XHTQ(N,K)=NK*.5 .
DIMENSION TOU(3),ROMG(3),SR(3),ENE(1),RJZ(1),XHTL(1),XHTQ(ND*3),
1 HAM(ND,ND),VEC(ND,ND)
NST= ((NH+1)*(NH+2))/2$ DO 1 K = 1 , 3$ ROMG(K)= EXP(-TOU(K))
1 SR(K)= ROMG(K)**2$ ITM= NH+1$ DO 3 I = 1 , NST$ DO 3 J = 1 , NST
3 HAM(I,J)= VEC(I,J)=0.$ C= -CHI*D
*
* IN HAM PUT H0= X*D*L*SIG*ROMG . IN VEC PUT L*SIG*ROMG .
N= 1$ DO 7 IT= 1 , ITM$ DO 7 IMU= 1 , ITS$ INU= IT- IMU+ 1
RINU= FLOAT(INU)$ RIMU= FLOAT(IMU)$ RITU= FLOAT(ITM-IT)
XHTQ(N,1)= RINU- .5$ XHTQ(N,2)= RIMU- .5$ XHTQ(N,3)= RITU+ .5
XHTL(N)= 10000.*(RINU-1.)+ 100.*(RIMU-1.)+ RITU

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IF(XHTL(N).LT.1.E-5) XHTL(N)= .1
HAMT= 0.$ DO 501 K= 1 , 3
501 HAMT= HAMT+ SR(K)*XHTQ(N,K)$ HAM(N,N)= HAMT$ IF(INU.LE.1) GO TO 5
T= (1- 2*MOD(INU+1,2))*SQRT((RINU-1.)*(FLOAT(IT)-RINU+1.))
HAM(N+1,N)= T*ROMG(3)*C$ VEC(N+1,N)= T/ROMG(3)
5 IF(IT.GE.ITM) GO TO 7
T= (1-2*MOD(IMU,2))*SQRT(RITD*RIMU)
HAM(N+IT+1,N)= T*ROMG(1)*C$ VEC(N+IT+1,N)= T/ROMG(1)
T= (1-2*MOD(IT,2))*SQRT(RITD*RINU)
HAM(N+IT,N)= T*ROMG(2)*C$ VEC(N+IT,N)= T/ROMG(2)
7 N= N+1
* NEXT DO HAM= HAM-X*(VEC+ D*(VEC)**2) AS MATRICES
DO 23 I = 1 , NST$ DO 23 J = 1 , 1$ TPP= 0.
DO 21 K = 1 , NST$ IF(J-K) 11,13,13
11 IF(I-K) 17,19,19
13 TPP= TPP+ VEC(I,K)*VEC(J,K)$ GO TO 21
19 TPP= TPP+ VEC(I,K)*VEC(K,J)$ GO TO 21
17 TPP= TPP+ VEC(K,I)*VEC(K,J)
21 CONTINUE
23 HAM(I,J)= HAM(I,J)- CHI*(VEC(I,J)+ D*TPP)
67 CALL DIAGTVN(NST,28,VEC,HAM,IRET)
*
* COMPUTE JZ AVERAGE, SELEC. RULE IS N-NP= 0,+1,-1 .
DO 120 I = 1 , N
120 ENE(I)= HAM(I,I)$ N= 1$ DO 27 IT= 1 , ITM
DO 27 IMU= 1 , ITS INU= IT-IMU+1$ IF(N.LT.NST) HAM(N+1,N)= 0.
HAM(N,N)= .5*(1- 2*MOD(IT-1,2))$ IF(INU.LE.1) GO TO 27
HAM(N+1,N)= (1- 2*MOD(IT+INU,2))*SQRT(FLOAT((INU-1)*IMU))
27 N= N+1
DO 31 L = 1 , NST$ T= 0.$ DO 33 N = 1 , NST
T= T+ HAM(N,N)*VEC(N,L)**2$ IF(N.EQ.NST) GO TO 31
33 T= T+ 2*HAM(N+1,N)*VEC(N+1,L)*VEC(N,L)
31 RJZ(L)= T$ IF(IPR.LT.6) RETURN$ PRINT 10
10 FORMAT(/# EIGENVALUES*20X*EIGENVECTORS*)
DO 39 I = 1 , NST
39 PRINT 61, ENE(I), (VEC(J,I),J=1,NST)
61 FORMAT(1PE14.6,7E16.6/(14X,7E16.6))
RETURN
END
SUBROUTINE DIAGTFC(N,ND,B,E,IT)
H(I,K) CONTAINS THE KTH EIGENVECTOR STORED BY COLUMNS.
C E(I,J) 1.GE.J CONTAINS THE LOWER TRIANGULAR PART OF THE MATRIX
C TO BE DIAGONALISED . E IS DESTROYED. WHEN RETURNING E(K,K) CON
C TAINS THE KTH EIGENVALUE .
C N= DIMENSION OF MATRIX TO BE DIAGONALISED . 1.LE.N.LE.100.
C ND=DIM.OF ARRAY IN WHICH B AND E ARE STORED,N.LE.ND.
C DIMENSION H(ND,ND),E(ND,ND)
C IF IT=0 WHEN ENTERING SET B TO 1 INITIALLY.
C IF IT.GT.0 WHEN ENTERING USE CURRENT VALUE OF B,
C THIS OPTION CAN BE USEFUL FOR ITERATIONS.
C IF DIAGONALISATION FAILS IT IS RETURNED AS -1.
* ACCURACY, 1 IN 10 TO THE 6.
DIMENSION H(1),E(1)
DIMENSION XMS(100),JS(100)
10 FORMAT(/5X*DIAG FAILS*E11.2/)
ENTRY DIAGTVN
IF (N.LT.2) GO TO 501$ IF(IT.GT.0) GO TO 55
DO 57 I = 1 , N$ IJ= 1$ DO 57 J = 1 , N$ B(IJ)= 0.
IF(I.EQ.J) B(IJ)= 1.
57 IJ= IJ+ ND
55 TEST = 0.$ DO 20 I = 1 , N$ IJ= 1$ DO 20 J = 1 , 1$ EPSP= 2.
IF(I.EQ.J) EPSP= 1.$ T= E(IJ)$ TEST= TEST+ EPSP*T

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20  IJ= IJ+ ND $ IF(TEST.EQ.0.) GO TO 502$ XNOM= (N*N-N)/TEST
    NMAX= 5*N*N$ KT= 0$ DO 123 K = 2 , N$ XM= 0.$ J= 1$ KK= K- 1
    KL= K$ DO 22 L = 1 , KK$ Q= ABS(E(KL))$ KL= KL+ ND
    IF(Q.LE.XM) GO TO 22$ XM= Q$ J= L
22  CONTINUE$ XMS(K)= XM
123 JS(K)= J
*
*  LOOP ENTRY POINT FOR 1 JACOBI ITERATION .
27  XM= 0.$ DO 222 K = 2 , N$ Q= XMS(K)$ IF(Q.LE.XM) GO TO 222$ XM= Q
    I= K
222 CONTINUE
    R= XNOM*XM*XM$ IF(R.LT.1.E-12) GO TO 502$ KT= KT+ 1
    IF(KT.GT.NMAX) GO TO 26$ J= JS(I)$ JT= MAX(2,J)$ MJ= ND*(J- 1)
    IJ= MJ+ 1$ P= E(IJ)$ E(IJ)= 0.$ MI= ND*(I- 1)$ JJ= MJ+ JS(I)=MI+ 1
    Y= .5*(E(JJ)- E(II))$ X= P/SIGN(ABS(Y)+ SQRT(Y*Y+ P*P),Y)$ P= P*X
    E(JJ)= E(JJ)+ P$ E(II)= E(II)- P$ C= 1./SQRT(1.+ X*X)$ S= X*C
    KJ= MJ+ 1$ KI= MI+ 1$ JK= JS(IK)= I$ DO 25 K = 1 , N$ Y= B(KJ)
    Z= B(KI)$ B(KJ)= C*Y+ S*Z$ B(KI)= C*Z- S*Y$ IF(K-I) 29,24,28
28  IZJZ=KI
30  IYJY= KJ$ GO TO 290
29  IZJZ= IK$ IF(K-J) 31,24,30
31  IYJY= JK
290 Y= E(IYJY)$ Z= E(IZJZ)$ E(IYJY)= Y*C+ S*Z$ E(IZJZ)= C*Z- S*Y
24  KJ= KJ+ 1$ KI= KI+ 1$ JK= JK+ ND$ IK= IK+ ND
25  CONTINUE$ DO 301 K = JT , N$ IF(K-I) 308,309,310
310 JSK= JS(K)$ IF(J.EQ.JSK.OR.I.EQ.JSK) 309,301
308 IF(J.NE.JS(K).AND.J.NE.K) GO TO 301
309 KK= K-1$ XM= 0.$ JJ= 1$ KL= K$ DO 305 L = 1 , KK$ Q= ABS(E(KL))
    IF (Q .LE. XM) GO TO 305$ XM= Q$ JJ= L
305 KL= KL+ND$ XMS(K)= XM$ JS(K)= JJ
301 CONTINUE$ GO TO 27
26  IT= -1$ PRINT 10, R $ GO TO 502
C  ASSUME N= 1
501 H(1)= 1.
502 RETURN
    END
    SUBROUTINE D1STOR (TAU1,FNNP,ND,NOD)
*
*  COMPUTE THE XFORMATION FROM THE DEFORMED BASIS TO THE ISOTROPIC
*  ONE ALONG ONE OF THE AXIS, AS A XFORM. ON A 1-DIM. OSCILLATOR.
    DIMENSION FNNP(ND,NOD),TSQR(60)
    EXT= EXP(TAU1)$ EXTI= 1./EXT$ CHT= .5*(EXT+ EXTI)
    SHT = (EXT- EXTI)*.5$ THT= SHT/CHT$ FNNP(1,1)= 1./SQRT(CHT)
    FNNP(2,1)= FNNP(1,1)/CHT$ DO 1 I = 1 , 60
1  TSQR(I)= SQRT(FLOAT(I))$ DO 3 IDL= 2 , NOD$ IN= 1
    NP = 2*IDL- 3+ IN
    FNNP(1,IDL) = +TSQR(NP-1)/TSQR(NP)*THT*FNNP(1,IDL-1)$ NP= NP+ 1
3  FNNP(2,IDL)= TSQR(NP)*FNNP(1,IDL)/CHT
    DO 5 IDL= 1 , NOD$ DO 5 IN= 3 , NOD$ N= IN- 1$ NP= 2*IDL- 3+ IN
5  FNNP(IN,IDL)= ((N+NP-1)*FNNP(IN-1,IDL)- TSQR(N-1)*TSQR(NP-1)*CHT*
1  FNNP(IN-2,IDL))/(TSQR(N)*TSQR(NP)*CHT)$ RETURN
    END
    SUBROUTINE OBCFPE(NTN,CP,NP,ND,IPR)
*
*  COMPUTES COMP. OF NTH LOWEST NILSSON STATE IN N,J+K,J-K, BASIS .
    COMMON /WAVN/WAVF(1680,2),EAV(84),ENE(84),QUAD(84,3),ITAG(84,2),
1  RJZ(84),NHA(84),TAUP(3),SR(3)
    DIMENSION CP(ND,2),C(84,2)
    ENTRY OBCFP
    J= ITAG(NTN,1)$ ILAB= ITAG(J,2)$ NJ= ITAG(J+1,2)-ILAB-1
    DO 3 I = 1 , NJ$ ILT= ILAB-1+I$ CP(I,1)= WAVF(ILT,1)
3  CP(I,2)= WAVF(ILT,2)$ CALL TRIMUP(CP,NJ,ND,1.E-5)

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IF(,PR.LT.0) GO TO 5$ PRINT 101, NTH
101 FORMAT(*UOMP, OF*I3,*TH L, ORB IN SPIN-CART. DEFORM. BASIS,{MU,NX
1,NY,NZ} .*)
CALL SPRNTC(CP,NJ,CP(1,2))
5 CALL DISTRA(C,N,84,CP,NJ,ND)$ CALL TRIMUP(C,N,84,1,E-5)
CALL CNNJK(CP,NP,ND,C,N,84)$ CALL TRIMUP(CP,NP,ND,1,E-4)
IF(IPR.LT.0) RETURNS$ PRINT 103
103 FORMAT(* EXPANSION COEF. IN [NT,J+K,J-K] SPHERICAL BASIS*)
CALL SPRNTC(CP,NP,CP(1,2)) $ RETURN
END
SUBROUTINE DISTRAE(CP,NP,NDP,C,N,ND)

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*
* HERE COMPUTE THE 3-DIM. DEFORMATION XFORMATION USING PRODUCTS OF
* THE COEFS IN FNNP .
* C AND CP MUST BE IN THE SPIN-CART. BASIS.
* C HAS THE COMP. IN THE DEF. BASIS , CP WIL HAVE THE COMP. IN THE
* ISOTROPIC BASIS .
C THE MES OF THE TRANSF. FROM THE DEF BASIS TO THE ISOTROPIC ONE
C ARE CONTAINED IN FNNP(ND,NOD,K), K=1,2,3.

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DIMENSION CP(NDP,2),C(ND,2)
COMMON/DISTORA/ FNNP(7,4,3)
ENTRY DISTRA
NP = 0$ IF(N.LT.1) RETURNS$ DO 1 IN= 1 , N$ IQN= IFIX(C(IN,1))
N1= IQN/10000$ NTE= IQN- 10000*N1$ N2= NTE/100$ N3= NTE- 100*N2
IR1= MOD(N1,2)$ IR2= MOD(N2,2)$ IR3= MOD(N3,2)
DO 3 J1= 1 , 7 , 2$ NP1= J1- 1+ IR1$ IF(NP1.GT.6) GO TO 1
IQNP1= 10000*NP1$ K1= MIN0(N1,NP1)+ 1$ L1= IABS((NP1-N1)/2)+ 1
F1= (1-2*MOD(IDIM((N1-NP1)/2,0),2))*FNNP(K1,L1,1)
DO 5 J2= 1 , 7 , 2$ NP2= J2- 1+ IR2$ IF(NP1+ NP2.GT.6) GO TO 3
IQNP2= IQNP1+ 100*NP2$ K= MIN0(N2,NP2)+ 1$ L= IABS((NP2-N2)/2)+ 1
F2= (1-2*MOD(IDIM((N2-NP2)/2,0),2))*FNNP(K,L,2)
DO 7 J3= 1 , 7 , 2$ NP3= J3- 1+ IR3$ IF(NP1+NP2+NP3.GT.6) GO TO 5
IQNP3= IQNP2+ NP3$ K= MIN0(N3,NP3)+ 1$ L= IABS((NP3-N3)/2)+ 1
F3= (1-2*MOD(IDIM((N3-NP3)/2,0),2))*FNNP(K,L,3)
COET= C(IN,2)*F1*F2*F3$ IF(NP.EQ.0) GO TO 9
DO 11 INP= 1 , NP$ IF(CP(INP,1).NE.IQNP3) GO TO 11
CP(INP,2)= COET+ CP(INP,2)$ GO TO 7
11 CONTINUE
9 NP = NP+ 1$ IF(NP.GT.NDP) CALL EXIT$ CP(NP,1)= IQNP3
CP(NP,2)= COET
7 CONTINUE
5 CONTINUE
3 CONTINUE
1 CONTINUE$ RETURN
END
SUBROUTINE CNNJKTE(CP,NP,NDP,C,N,ND)

```

```

*
* WHEREAS STUCO GIVES THE SPIN-CART. COMPONENTS OF THE SPHERICAL
* STATES THIS ROUTINE STARTS FROM A STATE C IN THE SPIN-CART. BASIS
* AND PUTS IN CP ITS COMPONENTS IN THE SPHERICAL BASIS .
C CP(NP,1)= 10000*NT+100*(J+K)+(J-K)
C CP(NP,2)= COEFFICIENTS .
* THIS VERSION HAS CORRECT TIME REV. PHASE.
DIMENSION CP(NDP,2),C(ND,2),CT(30,2)
COMMON /CARJN/ STUCO(1260,2),IQN(84,6),CSS(300,2),ICSD(49)
ENTRY CNNJK
CALL SORTAG(C(1,1) , 1,N,C(1,2))$ NP= 0$ IF(N.EQ.0) RETURN
DO 1 NY= 1 , 84$ I1= IQN(NY,5)$ J1= IQN(NY,6)- IQN(NY,5)+ 1
DO 3 I= 1 , J1$ IT= I1+ I- 1$ CT(I,1)= STUCO(IT,1)
3 CT(I,2)= STUCO(IT,2)$ SCT= SCALP(CT,J1,30,C,N,ND)
IF(ABS(SCT).LT.1.E-4) GO TO 1 $ NP= NP+ 1$ IF(NP.GT.NDP) CALL EXIT
CP(NP,1)= 10000*IQN(NY,2)+50*(IQN(NY,3)+IQN(NY,4))

```

```

1 (IGN(NY,3)-IGN(NY,4))/2
*   MODIFY PHASE FROM MUSHINSKY DEF.
    ICH= MOD(IGN(NY,3),8)-2*MOD(IGN(NY,2),2)
    IF(ICH.EQ.3.OR.ICH.EQ.5) SCT= -SCT$ CP(NP,2)= SCT
1 CONTINUE$ RETURN
END
FUNCTION SCALP(CH,NB,NDB,CA,NA,NDA)
C   EACH CI(I,1) MUST BE UNIQUE .
*   CA AND CB MUST BE ORDERED .
    DIMENSION CA(NDA,2), CH(NDB,2)
    SCT= 0.$ IA= IB= 1$ IF(NA.LT.1.OR.NB.LT.1) GO TO 101
    IT= MAX0(NA,NB)$ DO 1 J = 1 , IT
9   IF (CB(IR,1)- CA(IA,1)) 3, 5, 7
7   IA = IA+ 1$ IF(IA.GT.NA) 101,9
3   IB = IB + 1$ IF(IB.GT.NB) 101,9
5   SCT = SCT+ CB(IB,2)*CA(IA,2) $ IA= IA+ 1$ IB= IB+ 1
    IF(IA.GT.NA.OR.IB.GT.NB) GO TO 101
1   CONTINUE
101 SCALP= SCT$ RETURN
END
SUBROUTINE TIMEREV(C,NC,ND)
*
*   THE STATE C(ND,2) IS TIME REVERSED.
*
    DIMENSION C(1)
    IQ=1$ IC= ND+1
    DO 1 N = 1 , NC
    IQN= C(IQ)
    JMK= MOD(IQN,100)$ JPK= MOD(IQN/100,100)
    C(IC)= C(IC)*(1-2*MOD(JMK,2))
    IQN= IQN+100*(JMK-JPK)+JPK-JMK$ C(IQ)= IQN
    IC= IC+1$ IQ= IQ+1
1 CONTINUE $ RETURN
END
SUBROUTINE EXFI1B(EXM,K1,K2)
*
*   TO GENERATE MUD CALLS TO EXFI1BP
    COMMON/HASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMP0,
2 NBT,HBOM,OSPA2
    DIMENSION EXM(1),ICO(16)
    M=1$ DO 1 K = 1 , MUD$ NLP=0$ DO 3 L = 1 , NOLV$ IPR= 3-IPAR(L)
    IF(IPR.NE.K) GO TO 3$ NLP= NLP+1$ ICO(NLP)= ICODE(L)
3   CONTINUE
    CALL EXFI1BP(EXM(M),ICO,NLP,K1,K2)
1   M= M+ NB(K)**2
    RETURN
END
SUBROUTINE EXFI1HP(EXM,CODA,NOLV,K1,K2)
*   KI= 1,2,3, DO X,Y,Z, KI=4,5,6, DO PX,PY,PZ
*   USING THE STUCO ARRAYS OF J,M STATES IN CARTESIAN BASIS .
*   EXM(NB,NB)= HERMITIAN MATRIX EL. OF K1*K2 .
*   CODA(NOLV)= CODE NUMBER ARRAY .
*   IKIN= +1, REAL SYMM. , IKIN=-1, IM. ANTIS.
    COMMON/HASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLT,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMP0,
2 NBT,HBOM,OSPA2
    INTEGER CODA
    DIMENSION EXM(1),CODA(1),IFAS(6)
    COMMON /CARJN/ STUCO(1260,2),IQN(84,6),CSS(300,2),ICSD(49)
    COMMON/CARTEMP/C(100,2),CP(100,2),CT(100,2),IBSI(50),IFIGN(50),
1 ITAG(50),ITP(50),LAR(50),RESTA(4876)

```

```

DATA IFAS/0,1,0,3,0,3/
*
* NEXT STATEMENT TO TELL SPIN UP FROM SPIN DOWN.
STUCO(1,1)=.1
IFT= MOD(IFAS(K1)+IFAS(K2),4)
IKIN= 1-2*MOD(IFT,2)$ IPH= 1-2*(IFT/2)
IC1= 1+MOD(K1-1,3)$ IP1= 1-2*((K1-1)/3)
IC2= 1+MOD(K2-1,3)$ IP2= 1-2*((K2-1)/3)
ASSIGN 11 TO IHER$ IF (IP1+IP2.EQ.0) ASSIGN 13 TO IHER
*
* NOW FILLIN IBSI WITH NILSSON NUMBERS IN IQN .
ILA= 1$ DO 3 K = 1 , NOLV$ KP= CODA(K)$ LAM= ILC(KP)
JPH= ISTA(KP)$ NPO= INPO(KP)$ JPHD= SHIFT(JPH,1)
DO 3 M = 1 , JPHD$ JMK= M-1$ JPK= JPHD-M
ISIGN(ILA)= SHIFT(NPO-1,12)+ SHIFT(JPK,6)+JMK
ITAG(ILA)= ILA$ LAR(ILA)= LAM
3 ILA= ILA+1$ IDIM= ILA-1
CALL SORTAG(ISIGN,1,IDIM,ITAG)
DO 1 L = 1 , IDIM
1 IBSI(L)=0
DO 5 IL= 1 , 84 $ NH= IQN(IL,2)$ NILN= IQN(IL,1)
TOJ= IQN(IL,3)$ TOK= IQN(IL,4)$ JPK= (TOJ+TOK)/2
JMK= (TOJ-TOK)/2
ISIGP= SHIFT(NH,12)+ SHIFT(JPK,6)+JMK
IR= INBINS(ISIGN,1,IDIM,ISIGP)
IF (IR.LT.1) GO TO 5$ IBSI(ITAG(IR))=IL$ ITP(ITAG(IR))=JMK
ISIGP= SHIFT(NH,12)+ SHIFT(JMK,6)+ JPK
IR= INBINS(ISIGN,1,IDIM,ISIGP)$ IF (IR.LT.1) CALL EXIT
IBSI(ITAG(IR))= -IL$ ITP(ITAG(IR))= JPK
5 CONTINUE
KAREA= IDIM**2$ DO 25 K = 1 , KAREA
25 EXM(K)= 0.
*
* IL LOOP STARTS HERE
DO 7 IL= 1 , IDIM
NILNO= IBSI(IL)$ IF (NILNO.EQ.0) GO TO 101
NILN= IABS(NILNO)$ LAL= LAR(IL)
IAS= IQN(NILN,5)$ IAF= IQN(NILN,6)$ ILA= 1
DO 9 K = IAS,IAF
C(ILA,1)= STUCO(K,1)$ C(ILA,2)= STUCO(K,2)
9 ILA= ILA+1$ ILA= ILA-1
IF (NILNO.LT.0) CALL TIMEREK(C,ILA,100,ITP(IL))
GO TO IHER,(11,13)
11 NT=0$ CALL DIPSTAE(CT,NT,100,IC2,C,ILA,100,1.,IP2)
NP= 0$ CALL DIPSTAE(CP,NP,100,IC1,CT,NT,100,1.,IP1)$ GO TO 15
13 NT=0$ CALL DIPSTAE(CT,NT,100,IC2,C,ILA,100,1.,IP2)
NP=0$ CALL DIPSTAE(CP,NP,100,IC1,CT,NT,100,.5,IP1)
NT=0$ CALL DIPSTAE(CT,NT,100,IC1,C,ILA,100,1.,IP1)
CALL DIPSTAE(CP,NP,100,IC2,CT,NT,100,.5,IP2)
15 CALL SORTAG(CP,1,NP,CP(1,2))
*
* IM LOOP STARTS HERE
DO 17 IM= 1 , IL$ LAM= LAR(IM)
* IF (MOD(LAM+LAL,2).NE.0) GO TO 17
* THIS PUTS IN THE TIME-REVERSAL PHASE .
TRPH= (-1)**((LAM-LAL)/2)
NILNM= IBSI(IM)$ NILNM=IABS(NILNM)
IASM= IQN(NILNM,5)$ IAFM= IQN(NILNM,6)$ ILM=1
DO 19 KM= IASM,IAFM$ CT(ILM,1)= STUCO(KM,1)$ CT(ILM,2)=STUCO(KM
19 ILM= ILM+1$ ILM= ILM-1
IF (NILNM.GT.0) GO TO 27$ CALL TIMEREK(CT,ILM,100,ITP(IM))
CALL SORTAG(CT,1,ILM,CT(1,2))

```

```

27 PE= SCALP(CT,ILM,100,CP,NP,100)*TRPH
*
* WE HAVE (M/K1*K2/L) UPPER TRIAN PART
IF(IKIN.LT.0) GO TO 21 $ EXM(IL+IDIM*(IM-1))= IPH*PE$ GO TO 17
21 IF(IL.NE.IM) GO TO 23 $ IF(ABS(PE).GT.1.E-10)103,17
23 EXM(IM+IDIM*(IL-1))= IPH*PE
17 CONTINUE
7 CONTINUE$ RETURN
101 PRINT 105,IL$ GO TO 109
105 FORMAT (/ * FOR IL= *I5,* WE HAVE NO SPHERICAL STATE, EXIT...*)
103 PRINT 107, IL,IM ,PE
107 FORMAT (/ *XXXXXXXXXXXXX FOR IL AND IM = *2I5,*WE HAVE A ME=*E10.3 )
109 CALL EXIT
END
SUBROUTINE TIMEREK(C,N,ND,MPS)
*
* C(ND,2) CONTAINS N COMP. IN SPIN-CART. BASIS .
* ON RETURNING C CONTAINS THE TIME REV. STATE*(-1)**MPS.
* NOTE THAT /J,-M)= (-1)**(J-M)*T*C WHEN C HAS GOOD J,M .
* FORMULA IS T*/N1,N2,N3,MU)= MU*/N1,N2,N3,-MU)
*
DIMENSION C(1)
IFAS= (-1)**MPS$ IF(N.GT.0) GO TO 1
3 RETURN
1 DO 5 K1= 1 , N$ K2= K1+ND
RQ= C(K1)$ C(K1)= -RQ
5 C(K2)= C(K2)*SIGN(1.,RQ)*IFAS
GO TO 3
END
SUBROUTINE DIPSTAE(CP,NP,NDP,K,C,N,ND,CBT,IPH)
*
* DIM CP(NDP,2), C(ND,2)
* IF IPH= 1, DO XK, IF IPH=-1, DO PK ON THE STATE C.
* CP= OK*C.
DIMENSION CP(1),C(1),CT(2),M(3)
IF (N.LT.1) RETURN$ DO 1 L = 1 , N$ L2= L+ ND$ IT= IFIX(ABS(C(L)))
M(1) = IT/10000$ NR= IT- 10000*M(1)$ M(2)= NR/100
M(3)= NR- 100*M(2)$ PHI= 1$ IF(K.LT.3) PHI= 1- 2*MOD(M(3),2)
IF(K.LT.2) PHI= PHI*(1- 2*MOD(M(2),2))$ SGZ= 1.
SGZ= SIGN(SGZ,C(L))$ CT(2)= PHI*C(L2)$ IF(K.GT.1)CT(2)= SGZ*CT(2)
IF(K.LT.3) SGZ= -SGZ$ CT(1)= SGZ*ABS(C(L))$ MT= M(K)
DO 3 J = 1 , 2$ CTT= SQRT(FLOAT(MT+2-J)/2)
IF (CTT.LT.1.E-4) GO TO 3$ IF(J.EQ.1) CTT= CTT*IPH
M(K)= MT+3-2*J$ CT(1)= SGZ*(10000*M(1)+ 100*M(2)+ M(3))
IF (CT(1).EQ.0.) CT(1)= .1*SGZ$ IF(NP.LT.1) GO TO 8
DO 7 LP = 1 , NP $ LP2= LP+NDP$ IF(CT(1).NE.CP(LP)) GO TO 7
CP(LP2) = CP(LP2) + CTT*CT(2)*CBT$ GO TO 3
7 CONTINUE
8 IF (NP.LT.0) NP = 0$ CP(NP+1)= CT(1)$ CP(NP+1+NDP)= CTT*CT(2)*CBT
NP= NP+ 1
3 CONTINUE
1 CONTINUE$ RETURN
END
SUBROUTINE CARSET(CARA)
COMMON/BASIS/ ICOD(16),ISTA(16),IPAR(16),INPU(16),INUC(16),
1 ILC(16),NOLV,N8(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBUM,OSPA2
DIMENSION ICOD(16),CARA(1)
INTEGER CARA
M=1$ DO 1 K = 1 , 2$ NV=0$ DO 3 NT= 1 , NOLV
IF(IPAR(NT).NE.3-K) GO TO 3$ NV= NV+1$ ICOD(NV)= ICOD(NT)
3 CONTINUE$ CALL CARSETP(ICOD,NV,CARA(M),IDM)

```

```

1  M= M+ IIMS$ RETURN
   END
   SUBROUTINE CARSETP(CODA,NOLP,CARA,IDM)
   COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1  ILC(16),NOLV,NB(2),MUD,IDF,IUSC,IUSJ,JAR(14,2),IDAC(14,14),JMPO,
2  NBT,HBOM,OSPA2
   DIMENSION C:RA(1), CODA(1)$ INTEGER CODA,CARA
   DIMENSION ISHC(8),ITJC(8),ITKC(16)
   DATA ISHC/3356B,3456B,3556B,3656B,3756B,4056B,4156B,4256B/,
1  ITJC/3456B,3656B,4056B,4256B,4456B,343456B,343656B,344056B/,
2  ITKC/3440B,3436B,3434B,44B,42B,40B,36B,34B,
3  4634B,4636B,4640B,4642B,4644B,463434B,463436B,463440B/
   ILA=1$ DO 3 K = 1 , NOLP$ KC= CODA(K)$ JPH= ISTA(KC)
   NPO= INPO(KC)$ LTL= SHIFT(JPH,1)$ DO 3 L = 1 , LTL$ LK= L+8-JPH
   CARA(ILA)= SHIFT(ISHC(NPO),42)+ SHIFT(ITJC(JPH),24)
1 + SHIFT(ITKC(LK),06)+ 61000000000000000062B
3  ILA= ILA+1$ IDM= ILA-1$ RETURN
   END

```

IDENT INBINS

LIST L,R

```

* FUNCTION INBINS(A,II,JJ,X)
* THE ARRAY A MUST BE IN INCREASING ORDER.
* A BINARY SEARCH IS DONE IN ARRAY A FROM ELEMENT II TO JJ,
* FOR THE VALUE X. THE VALUE IX OF THE LOCATION WHERE X IS STORED IN
* A IS RETURNED AS A FUNCTIONAL VALUE IF THE SEARCH IS SUCCESSFUL.
* THE VALUE 0 IS RETURNED IF X IS NOT FOUND. THE VALUE -1 IS
* RETURNED IF THE SEARCH FAILS BECAUSE OF IMPROPER CALLING.
* A AND X MUST BE NORMALISED IF THEY ARE REAL.. IF X IS CONTAINED IN
* SEVERAL LOCATIONS THE RETURNED VALUE WILL BE ONE OF THOSE.
* THE FOLLOWING IS A FORTRAN CODE WHICH COULD BE USED.
* INTEGER A,X
* DIMENSION A(1)
* IX= II
* IF(A(IX)-X) 1 , 3 , 5
* 3 INBINS= IX
* 7 RETURN
* 5 INBINS= 0
* GO TO 7
* 1 IL= IX
* IX= JJ
* IF(A(IX)-X) 5,3,9
* 9 IU= IX
* DO 11 K = 1 , 20
* IR= IU- IL
* IF(IR- 1) 5, 5, 13
* 13 IX= IL+ IR/2
* IF(A(IX)-X) 17 , 3 , 15
* 15 IU= IX
* GO TO 11
* 17 IL= IX
* 11 CONTINUE
* INBINS= -1
* GO TO 7
* END

```

	USE	START.
TRACE.	VFD	42/7LINBINS +18/INBINS
TEMPAO.	BSS	1B
ENTRY.	BSS	0B
	ENTRY	INBINS
INBINS	BSS	1B
	SX6	A0
	SA0	A1

A0= PAR. LIST FIRST ADDRESS

```

SA6      TEMPA0.
USE      CODE.
*        X6=IX,R1=IL,B2=IU,B3=AD(A)-1B,X1=IR,B4=K-1,B5=19,X2=X.
SA5      A0+1B      GET AD(II)
SA4      A0+3B      GET AD(X)
SA3      X5
RX6      X3      IX= II
SA2      X4      GET X
SA1      A0      GET AD(A)
SB3      X1-1B      R3= AD(A)-1B
SA4      X6+B3      X4= A(IX)
IX0      X4-X2      X0= A(IX)-X
ZR      X0,.7      IF(A(IX)-X) 1,7,5
NG      X0,.1      IF(A(IX)-X).LT.0) GO TO 1
EQ      .5
.7      HSS      QB
SA4      TEMPA0.      R
SA0      X4      E
EQ      ENTRY.      TURN
.5      HSS      QB
MX6      0      IX= 0
EQ      .7
.1      HSS      QB
SB1      X6      IL= IX
SA5      A0+2B      GET AD(JJ)
SA3      X5      X3= JJ
RX6      X3      IX= JJ
SA4      X6+B3      X4= A(IX)
IX0      X4-X2
ZR      X0,.7
NG      X0,.5
SB2      X6      IU= IX
SB4      QB      K-1= 0
SB5      23B      H5= 19
JAA      HSS      QB      DO 11 K= 1 , 20
SX1      H2-B1      IR= IU-IL
SB6      X1-1B
LE      R6,.5      IF(IR.LT.2) GO TO 5
AX1      1B      IR= IR/2
SX6      X1+B1      IX= IL+ IR
SA4      X6+B3      X4= A(IX)
IX0      X4-X2
ZR      X0,.7
NG      X0,.17
SB2      X6      IU= IX
EQ      .11
.17      HSS      QB
SB1      X6      IL= IX
.11      HSS      QB
SB4      B4+1B      K= K+1
LE      B4,B5.)AA      CONTINUE
SX6      -1B      IX= -1
EQ      .7
END

```

OVERLAY(NUHART,2,0)
PROGRAM NUHART

```

*
* FIRST DO ITER ITERATIONS WITH NO C.M. KINETIC ENERGY THEN SAVE
* THIS WAVEFUNCTION IN RS AND ROS AND DO 1 ITERATION WITH K.E. OF
* C.M. INCLUDED TO GET THE USUAL SINGLE-PARTICLE ENERGIES. FINALLY
* DO ITER ITERATIONS FOR EACH EXTERNAL FIELD EXFID, USING THE
* SAVED WAVEFUNCTION .

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COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
COMMON/NAMES/ROP,RON,ROPS,RONS,BRPS,BIPS,BRNS,BINS,VPP,VNP,VPN
1 , PROT,NEUT,NUCL
COMMON AS1(4000),AS2(4000),AL1(15000)
COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,ITER,ITCR,ATNO
1 ,NORBA(41),NORB,BET,GAMD,NPTOT,NNTOT
COMMON/EXFIN/EXFID(2,4,20)
COMMON/NAMEN/FPR,PTS,FPF,FNE,FNF,FDN,PTD,FDF,RONI,ROPI,SPE,SPEXF
1 , RTS,RTD
DATA ROP,RON,ROPS,RONS,BRPS,BIPS,BRNS,BINS,VPP,VNP,VPN
1 , PROT,NEUT,NUCL/3LROP,3LRON,4LROPS,4LRONS,4LBRPS,4LBIPS,4LBRNS,
1 4LBINS,3LVPP,3LVNP,3LVPN,9LPROTON(S),10LNEUTRON(S),10LNUCLEON(S)/
PRINT 103$ CALL TIMEPRT(Y)$ FACF= .5*HBOM/ATNO
CALL ADLONG(FPR,1.,PTS,FACF,FPF,AS1,AL1)
CALL ADLONG(FNE,1.,PTS,FACF,FNF,AS1,AL1)
CALL ADLONG(FDN,1.,PTD,FACF,FDF,AS1,AL1)
CALL HARFIT(RONI,ROPI,FPF,FNF,FDF,0,ITER,.T.)
*
* NOW COMPUTE THE R.M.S. RADIUS W.R.T. THE C.M.
CALL BUFFIN(ROP,AS1,IDSJ)$ CALL BUFFIN(RTS,AL1,IDF)
CALL VEEBAF(AS2,AL1,AS1,0)$ TE1= TRVEROJ(AS1,AS2,0)
CALL BUFFIN( RON,AS1,IDSJ)$ CALL VEEBAF(AS2,AL1,AS1,0)
TE2= TRVEROJ(AS1,AS2,0)$ CALL BUFFIN(RTD,AL1,IDF)
CALL VEEBAF(AS2,AL1,AS1,0)$ CALL BUFFIN(ROP,AS1,IDSJ)
TE3= TRVEROJ(AS1,AS2,0)$ FAMU= OSPA2*.5/ATNO**2
CALL BUFFIN(3LFCO,AL1,IDF)$ CALL VEEBAF(AS2,AL1,AS1,0)
TMS= FAMU*(TE1+TE2+2.*TE3) $ RMS= SQRT(TMS)
ECOUL= .5*TRVEROJ(AS1,AS2,0)$ IF(NPTOT) 703,701
703 PFACF= OSPA2*.5/(NPTOT*ATNO**2)
TPMS= PFACF*(TE1*(ATNO+NNTOT)- NPTOT*TE2+ 2.*NNTOT*TE3)
PRMS= SQRT(TPMS)$ GO TO 705
701 PRMS= 0.
705 PRINT 101, RMS, PRMS,ECOUL
*
* DO 1 MORE ITERATION TO GET S.P. ENERGIES. WITH K.E. ,THEN
* PROCEED WITH THE EXTERNAL FIELDS IF ANY .
PRINT 103$ CALL HARFIT,RON,ROP,FPR,FNE,FDN,SPE,1.,.F.)
DO 120 K = 1 , 20$ IF(EXFID(1,1,K).EQ.0) GO TO 99
PRINT 103$ PRINT 105,((EXFID(I,J,K),I=1,2),J=1,4)
CALL BUFFIN(EXFID(1,1,K),AS1,IDSJ)$ DO 121 M = 1 , IDSJ
121 AS1(M)= AS1(M)*EXFID(2,1,K)$ DO 123 J = 2 , 4
IF(EXFID(1,J,K).EQ.0.OR.EXFID(2,J,K).EQ.0) GO TO 123
CALL BUFFIN(EXFID(1,J,K),AS2,IDSJ)$ DO 125 M = 1 , IDSJ
125 AS1(M)= AS1(M)+ AS2(M)*EXFID(2,J,K)
123 CONTINUE$ CALL BUFOUT(SPEXF,AS1,IDSJ)
120 CALL HARFIT(RONS,ROPS,FPF,FNF,FDF,SPEXF,ITCR,.F.)
101 FORMAT(/10H ***** * TOTAL R.M.S. RADIUS W.R.T. C.M.= *F9.5,
1 * F., PROTON R.M.S. RADIUS W.R.T. TOTAL C.M.=*F10.5,* F. *
110H*****//10X*COULOMB ENERGY=*F12.5,* MEV.*)
103 FORMAT(1HR)
105 FORMAT(/** THE STRUCTURE OF SPEXF IS: NAME*10X*AMPLITUDE(MEV)*/(
115X10,10XF12.5))
99 CONTINUE
END
SUBROUTINE HARFIT(RONI,ROPI,FPR,FNE,FDN,SPE,ITER,ISAV)
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,DD(2),ATNO
1 ,NORBA(41),NORB,BET,GAMD,NPTOT,NNTOT

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COMMON/EXSYN/EXF(36),SYP(21)
LOGICAL NOSPE,NOSAV,IPRS,ISAV,IPUNCH          $REAL NEUT,NUCL,IXX
COMMON/NAMES/ROP,RON,ROPS,RONS,BRPS,BIPS,BRNS,BINS,VPP,VNP,VPN
1  , PROT,NEUT,NUCL
COMMON/DUMPN/RMES(25,3),STD(3,5),QUADN(5),NPQUAD(5),BETD(5),
1  GAMP(5),QZDB(5),DDO(185)
COMMON/PRINLM/EPS,IPR,QNO(82),IPUNCH
COMMON/QUADSN/ QUADS(5,3)
COMMON AS1(4000),AS2(4000),AL1(15000)
CALL HUFFIN(ROI,AS1,IDSJ)$ CALL HUFFIN(ROI,AS2,IDSJ)
CALL BUFOUT(ROI,AS1,IDSJ)$ CALL BUFOUT(ROI,AS2,IDSJ)
PRINT 209,ROI,ROI,FPR,FNE,FON,SPE$ ES=0.
NOSPE= SPE.EQ.0$ DO 3 IL= 1 , ITER$NOSAV=.N.(ISAV.A.IL.EQ.ITER)
PRINT 201, IL,NPTOT,NNTOT,NAMES$ IPRS=IPR,LT.1.A.IL.NE.ITER
CALL BUFFIN(ROP,AS1,IDSJ)$ RTP=TRVEROJ(AS1,AS1,0)$ IF(NOSPE)GOTO11
CALL BUFFIN(SPE,AL1,IDSJ)$ ES= TRVEROJ(AS1,AL1,0)
11 CALL BUFFIN(FPR,AL1,IDSJ)$ CALL VEEBAR(AS2,AL1,AS1,IPR)
CALL BUFOUT(VPP,AS2,IDSJ)$ CALL BUFFIN(FON,AL1,IDSJ)
CALL VEEBAR(AS2,AL1,AS1,IPR)$ CALL BUFOUT(VNP,AS2,IDSJ)
CALL BUFFIN(ROI,AS1,IDSJ)$ CALL VEEBAR(AS2,AL1,AS1,IPR)
CALL BUFOUT(VPN,AS2,IDSJ)$ RTN= TRVEROJ(AS1,AS1,0)$IF(NOSPE)GOTO12
CALL BUFFIN(SPE,AL1,IDSJ)$ ES= ES+ TRVEROJ(AL1,AS1,0)
12 CALL BUFFIN(FNE,AL1,IDSJ)$ CALL VEEBAR(AS2,AL1,AS1,IPR)
CALL BUFFIN(VNP,AL1,IDSJ)$ DO 21 K = 1 , IDSJ
21 AS2(K)= AS2(K)+ AL1(K)$ IXX=0$ IF(IL.EQ.ITER) IXX= NEUT
IF(IL.EQ.1) GO TO 7$ IF((RTP-NPTOT)**2+(RTN-NNTOT)**2.GT.1.E-20)
1 CALL ERREXIT(RTP,RTN,NPTOT,NNTOT,IL)
7 ETN= .5*TRVEROJ(AS2,AS1,IXX)$ IF(NOSPE) GO TO 13
CALL BUFFIN(SPE,AL1,IDSJ)$ DO 23 K = 1 , IDSJ
23 AS2(K)= AS2(K)+ AL1(K)
13 CALL DIAGON(AS2,AS1,AL1,VALN,NN)
CALL WAVPRT(AS1,AL1,VALN,NNTOT,NEUT,IPRS)
CALL DENMAT(AS2,AS1,AL1,NN)$ IF(NOSAV) GO TO 30
CALL BUFOUT(BRNS,AS1,IDSJ)$ CALL BUFOUT(BINS,AL1,IDSJ)
IF(IPUNCH) CALL WAVPUN(AS1,AL1,NN,NEUT,NAME)
30 CALL ROCONV(AS2,AL1,1)$IF(.N.NOSAV)CALLBUFOUT(RONS,AL1,IDSJ)
CALL BUFOUT(ROI,AL1,IDSJ)
,
,
NOW REPEAT FOR PROTONS .
CALL BUFFIN(VPN,AS2,IDSJ)$ CALL BUFFIN(VPP,AL1,IDSJ)$DO25K=1,IDSJ
25 AS2(K)= AS2(K)+AL1(K)$ IXX=0$ IF(IL.EQ.ITER) IXX= PROT
CALL BUFFIN(ROP,AS1,IDSJ)$ ETP= .5*TRVEROJ(AS2,AS1,IXX)
IF(NOSPE) GO TO 15$ CALL BUFFIN(SPE,AL1,IDSJ)$ DO 27 K = 1 , IDSJ
27 AS2(K)= AS2(K)+ AL1(K)
15 CALL DIAGON(AS2,AS1,AL1,VALP,NP)
CALL WAVPRT(AS1,AL1,VALP,NPTOT,PROT,IPRS)
CALL DENMAT(AS2,AS1,AL1,NP)$ IF(NOSAV) GO TO 32
CALL BUFOUT(BRPS,AS1,IDSJ)$ CALL BUFOUT(BIPS,AL1,IDSJ)
IF(IPUNCH) CALL WAVPUN(AS1,AL1,NP,PROT,NAME)
32 CALL ROCONV(AS2,AS1,1)$IF(.N.NOSAV)CALLBUFOUT(ROPS,AS1,IDSJ)
CALL BUFOUT(ROP,AS1,IDSJ)$ ETOT= ETP+ETN+ES
ECOUL= ETP-ETN$ PRINT 203,ETOT,ETP,ETN,ECOUL,ES
3 CONTINUE$ CALL BUFFIN(ROI,AS2,IDSJ)$PRINT 205,OSPA2,PROT,NEUT,NUCL
DO 117 ISY = 1 , 21$ CALL BUFFIN(SYP(ISY),AL1,IDSJ)
RMES(ISY,1)= TRVEROJ(AS1,AL1,0)$ RMES(ISY,2)= TRVEROJ(AS2,AL1,0)
RMES(ISY,3)= RMES(ISY,1)+ RMES(ISY,2)
117 PRINT 207,SYP(ISY),(RMES(ISY,J),J=1,3)$ QUADN(1)= PROT
QUADN(2)= NEUT$ QUADN(3)= NUCL$ NPQUAD(1)= NPTOT$ NPQUAD(2)=NNTOT
NPQUAD(3)= NPTOT+NNTOT$ DO 119 J = 1 , 3
STD(3,J)= OSPA2*(RMES(15,J)-RMES(21,J)+RMES(11,J)-RMES(17,J))/3
STD(1,J)= OSPA2*(-RMES(11,J)+RMES(17,J)+RMES(10,J)-RMES(16,J))/2+
1 STD(3,J)$ STD(2,J)= STD(1,J)-OSPA2*(RMES(10,J)-RMES(16,J))

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119 CALL GAMEXT(STD(1,J),BETD(J),GAMP(J),QZOB(J),NPQUAD(J),QUADN(J);
    IF(NOSAV) RETURN$ DO 121 J = 1 , 3$ QUADS(4,J)= QUADN(J)
    QUADS(5,J)= NPQUAD(J)$ DO 121 K = 1 , 3
121 QUADS(K,J)= SQRT(STD(K,J)/QUADS(5,J))$ RETURN
201 FORMAT(/// * ITERATION NO*13,* FOR*13,* PROTONS AND*13,* NEUTRONS,
    INUCLEUS= *A10/)
203 FORMAT(///58X20H*****//5X*TOTAL BINDING ENERGY=*F12
    1.5,* MEV, TOTAL PROTON POTENTIAL ENERGY=*F12.5,* MEV, TOTAL NEUTRO
    IN POTENTIAL ENERGY=*F12.5//25X*DELTAPN ENERGY=*F12.5,* MEV, TOTAL
    3ONE-BODY ENERGY=*F12.5,* MEV//58X20H*****//)
205 FORMAT(// 1X*COMPUTATION OF EXPECTATION VALUE OF THE 21 SYMPLECTI
    IC BILINEAR OPERATORS, IN DIMENSIONLESS UNITS, OSC. PAR. BSQUARE=*F
    18.3,* FERMISQ*///13X*NAME*3(10XA10)/)
207 FORMAT(13XA10,2X3(F12.5,8X))
209 FORMAT(/// * HARTREE-FOCK ITERATIONS WITH THE PARAMETER LIST,*5X*RO
    INI      ROPI      FPR      FNE      FDN      SPE*//26X*MASS STO
    2RAGE ARRAY NAMES,*3X6A10)
    END
    SUBROUTINE WAVPUN(BR,BI,NA,KIND,NAME)
*
*   TO PUNCH WITH A UNIQUE HEADER AND NO. OF COMP. TRAILER THE COMP.
*   OF THE WF WHICH ARE GT EPS/3
    COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
    1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IL3J,JAR(14,2),IDAC(14,14),JMPO,
    2 NBT,HBOM,OSPA2
    COMMON /PRINLIM/EPSP
    COMMON /CONTRSN/IDUM(280),IBLK,HBOW,TNAME
    COMMON /DUMPN/IPOS(10),COA(10),NCOM,IBUF,ILA,EPS
    DIMENSION BR(1),BI(1),NA(2)
    EPS= EPSP/3$ CALL TIME(NOW)$ CALL DATE(WHEN)
    PUNCH 103,NAME,NA,KIND,TNAME,IBLK,HBOW,WHEN,NOW
    PRINT 105,NAME,NA,KIND,TNAME,IBLK,HBOW,WHEN,NOW
    NCOM=IBUF=0$ ILA=M=1$ DO 1 K = 1 , 2
    CALL WAVPUP(BR(M),NA(K),NB(K))$ ILA= 1+NB(K)**2
1   M= M+NB(K)**2$ IBUF= IBUF+1$ IPOS(IBUF)= NCOM$ COA(IBUF)= 0
    IF(IBUF.LT.08) GO TO 3$ PUNCH 101,(IPOS(J),COA(J),J=1,08)
    IBUF=0
3   NCOM=0$ ILA=M=1$ DO 5 K = 1 , 2$ CALL WAVPUP(BI(M),NA(K),NB(K))
    ILA= 1+NB(K)**2
5   M= M+ NB(K)**2$ IBUF=IBUF+1$ IPOS(IBUF)= NCOM$ COA(IBUF)=0
    PUNCH 101,(IPOS(J),COA(J),J=1,IBUF)$ RETURN
101 FORMAT(08(I4,F6.4))
103 FORMAT(A10,2I4,2X2A10,I5,F10.2,2A10)
105 FORMAT(* WAVEFUNCTION PUNCHED WITH HEADER= *A10,2I4,2X2A10,I5,F10.
    12,2A10)
    END
    SUBROUTINE WAVPUP(BR,NPA,NBP)
    COMMON /DUMPN/IPOS(10),COA(10),NCOM,IBUF,ILA,EPS
    DIMENSION BR(NBP,NBP)
    DO 1 K = 1 , NPA$ DO 3 I = 1 , NBP$ IF(ABS(BR(I,K)).LT.EPS)GOTO 3
    IBUF=IBUF+1$ IPOS(IBUF)=ILA
    COA(IBUF)= SIGN(AMIN1(ABS(BR(I,K)),.9999),BR(I,K))$ NCOM=NCOM+1
    IF(IBUF.LT.08) GO TO 3$ IBUF= 0$ PUNCH 101,(IPOS(J),COA(J),J=1,08)
101 FORMAT(08(I4,F6.4))
3   ILA= ILA+1
1   CONTINUE$ RETURN
    END
    SUBROUTINE GAMEXT(ST,BET,GAMD,QZOR,NPAT,NAME)
*
*   ST(K)= XK2AV. , BET AND GAMD ARE RETURNED ALONG WITH R.M.S. RAD.
    DIMENSION ST(3), TAU(3)
    DATA PI/3.14159265358/

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CNUM= 2.*SQRT(5./(4.*PI))$ CNP= 140./PI
QZOB= (ST(1)*ST(2)*ST(3))* (1./3.)$ A= 0.$ DO 1 K= 1 , 3
TAU(K)= ALOG(ST(K)/QZOB)/CNUM
1  A= A+ TAU(K)**2
  BET= SQRT(2.*A/3.)
  GAMD= 0$ IF(BET.LT.1.E-5) GOTO3 $ CGAM= TAU(3)/BET
  IF(CGAM.GT.1.)CGAM=1.$ IF(CGAM.LT.-1.) CGAM=-1.
  GAMD= CNP*ACOS(CGAM)
*  GAMD= CNP*ACOS(CGAM)$ QZOB= SQRT(QZOB/NPAT)
3  QZOB= SQRT((ST(1)+ST(2)+ST(3))/FLOAT(NPAT))
  PRINT 101, NPAT, NAME , QZOB ,BET,GAMD
101 FORMAT(/* R.M.S. S.P. RADIUS FOR *I3,1XA10,*= *F9.5,
1 * F., BET =*F8.5,*, GAM = *F8.2,* DEG.*/)
  RETURN
  END

  FUNCTION TRVEROJ(VB,RO,NAME)
*
*  TO COMPUTE THE TRACE OF VB*RO WHERE VB AND RO ARE IN N J,M BASIS .
*  IF NAME .NE. 0 PRINT THE COMPONENTS WHICH ARE .GT. EPSP AND THE
*  PARTIAL SUMS OF .5*VB*RO .
  COMMON/HASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1  ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2  NBT,HBOM,OSPA2
  DIMENSION VB(2,1),RO(2,1),ILAB(100),IGN(12),DR(12),DI(12),VR(12),
1  VI(12)$ LOGICAL WESKIP$ COMMON /PRINLIM/ EPS,IPR,QNO(82)
  DATA LSQB,RSQB/1L[,1L]/
  WESKIP= NAME.EQ.0$ XTE= 0.$EPSP=1000.*EPS**2$ IF(WESKIP) GO TO 41
  PRINT 201, NAME, EPSP$ IBUF= 0
41  ILA= 1$ DO 31 JPO= 1 , JMPO$ J= JPO-1$ IF(WESKIP) GO TO 43
*
*  PREPARE DICTIONARY IN ILAB .
  INC= 0$ DO 11 IPL= 1 , 2$ DO 13 KC= 1 , NOLV
  IF(MOD(IPL-1+IPAR(KC),2).NE.0) GO TO 13$ JPHC= ISTA(KC)
  DO 15 KA= 1 , NOLV$ IF(MOD(IPL-1+IPAR(KA),2).NE.0) GO TO 15
  JPHA= ISTA(KA)
  IF(IABS(JPHC-JPHA)+1.GT.JPO.OR.JPHC+JPHA.LT.JPO) GO TO 15
  INC= INC+1$ ILAB(INC)= 100*ICODE(KC)+ ICODE(KA)
15  CONTINUE
13  CONTINUE
11  CONTINUE
  IF(JAR(JPO,1).NE.INC) CALL ERREXIT(JPO,ILAB,2HFL,INC)
43  INC= JAR(JPO,1)
  TRJP= 0.$ DO 3 MPO= 1 , JPO$ EPSM= 1.$ IF(MPO.EQ.1) EPSM= .5
  SUMT= 0.$ DO 5 IAC= 1 , INC
  X= RO(1,ILA)*VB(1,ILA)+RO(2,ILA)*VB(2,ILA)
  IF(ABS(X).LE.EPSP.OR.WESKIP) GO TO 21
  IBUF= IBUF+ 1$ IGN(IBUF)= 10000*ILAB(IAC)+ 100*(JPO-1)+MPO-1
  VR(IBUF)=VB(1,ILA)$ VI(IBUF)=VB(2,ILA)$ DR(IBUF)=RO(1,ILA)
  DI(IBUF)=RO(2,ILA)$ ASSIGN 21 TO IRET$ IF(IBUF.GE.12) GO TO 101
21  SUMT= SUMT+X
5  ILA= ILA+1
3  TRJP= TRJP+ EPSM*SUMT$ IF(WESKIP) GO TO 31$ ASSIGN 1 TO IRET
  IF(IBUF.GT.0) GO TO 101
1  PRINT 103 , J,TRJP
31  XTE= XTE+ TRJP$ TRVEROJ= 2.*XTE$ RETURN
101 PRINT .05, (LSQB,IGN(I),RSQB,I=1,IBUF)$ PRINT 107,(VR(I),I=1,IBUF)
  PRINT 109,(VI(I),I=1,IBUF)$ PRINT 111,(DR(I),I=1,IBUF)
  PRINT 113,(DI(I),I=1,IBUF)
  IBUF= 0$ GO TO IRET,(1,21)
103 FORMAT(* FOR MULTIPOL. LAM=*I3,*, THE TOTAL CONTRIB. TO THE POT. E
  1NERGY IS*F13.5,* MEV*/)
105 FORMAT(* QN=*I2(1XA1,I8,A1))

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107 FORMAT(* VR=*12(F11.5))
109 FORMAT(* VI=*12(F11.5))
111 FORMAT(* DR=*12(F11.5))
113 FORMAT(* DI=*12(F11.5))
201 FORMAT(//10X*MULTIPOLE ANALYSIS OF *A10,* H-F POT. V AND DENS. MA
1TR, D, WITH LISTING OF ALL COMPS WITH EN. CONTR. GT*F7.4//)
END
SUBROUTINE DIAGON(E,BR,BI,VAL,NO)
*
* FIRST CONVERT E BACK TO (JC,MC/E/JA,MA) BASIS, THEN CALL MATRIX
* DIAGONALISATION, ORDER THE STATES IN INCREASING ENERGY AND
* FINALLY REDISTRIBUTE THE PARTICLES IF NEED BE .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
DIMENSION E(1),BR(1),BI(1),VAL(1),NO(2)
CALL ROCONV(BR,E,-1)$ DO 5 K = 1 , IDSC
5 E(K)= BR(K)
MA=1$ MB=1$ DO 1 K = 1 , MUD$ ND= NB(K)$ INC= ND+1
CALL RHERMAD(E(MB),BR(MB),BI(MB),ND,ND,0,IRES,1.E-12)
IF= MB
DO 3 L = 1 , ND$ VAL(MA)= E(IF) $ MA= MA+1
3 IF= IF+ INC
1 MB= MB+ ND**2
IS= ISH= 1$ DO 11 K = 1 , MUD$ ND= NB(K)
CALL ORDR(VA(1S),BR(ISH),BI(ISH),ND,ND)$ IS= IS+ND
11 ISH= ISH+ ND**2$ CALL REORDER(VA,NO)$ RETURN
END
SUBROUTINE ORDER(E,BR,BI,NB,ND)
*
* E IS THE LINEAR EIGENVALUE ARRAY .
COMMON/DUMPN/ TA(100),ITAG(100),TAP(100)
DIMENSION E(ND) ,BR(ND,ND),BI(ND,ND)
DO 3 J = 1 , NB$ TA(J)= E(J)
3 ITAG(J)= JS CALL SORTAG(TA,1,NB,ITAG)$ DO 5 J = 1 , NB
5 E(J)= TA(J)$ DO 7 I = 1 , NB$ DO 9 J = 1 , NB$ TAP(J)= BI(I,J)
9 TA(J)= BR(I,J)$ DO 11 J = 1 , NB$ JP=ITAG(J)$ BI(I,J)= TAP(JP)
11 BR(I,J)= TA(JP)
7 CONTINUE $ RETURN
END
SUBROUTINE WAVPRT(BR,BI,VAL,NNU,NAME,SMPR)
*
* TO DO A CONTROLLED PRINTOUT OF THE WAVEFUNCTION .
COMMON/PRINLIM/ EPS,IFR,QNO(82)$ LOGICAL SMPR
COMMON/DUMPN/ EN(100),ITA(100),QN(20),CR(20),CI(20),DDD(40)
COMMON/BASIS/ ICODE(16),ISTA(16),IPPP(16),INPO(16),INUC(16),
1 LCC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
DIMENSION BR(1),BI(1),VAL(1)
NS= MIN0(NBT,NNU+12)$ IF(SMPR) NS= 0
PRINT 101,NS,NAME,EPS$ DO 1 K = 1 , NBT$ EN(K)= VAL(K)
1 ITA(K)= KS CALL SORTAG(EN,1,NBT,ITA)$ NSP1= NS+1$ IF(SMPR) GO TO 4
DO 3 K = 1 , NS$ KP= ITA(K)$ IF(KP-NB(1)) 5,5,7
5 M=1$ KPP= KPS IPAR=1$ IDB= NB(1)$ IND=1$ GO TO 9
7 M= 1+NB(1)**2$ KPP= KP-NB(1)$ IPAR=-1$ IDB= NB(2)$ IND= 1+NB(1)
9 ILA= M+ IDB*(KPP-1)$ ILB= ILA+ IDB-1$ ILC= 0$ ASSIGN 11 TO IRET
IOCC= NAME$ IF( K.GT,NNU) IOCC=0$ PRINT 103,K,EN(K),IPAR,IOCC
DO 11 KS= ILA,ILE$ CRT= BR(KS)$ CIT= BI(KS)$ QNT= QNO(IND)
IND= IND+1$ IF(ABS(CRT).LT.EPS.AND.ABS(CIT).LT.EPS) GO TO 11
ILC= ILC+1$ QN(ILC)= QNT$ CR(ILC)= CRT$ CI(ILC)= CIT
IF(ILC.GE.12) GO TO 13
11 CONTINUE$ IF(ILC.LT.1) GO TO 3$ ASSIGN 3 TO IRET$ GO TO 13

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3  CONTINUE$ IF(NS.GE.NBT) RETURN
4  PRINT 111,(EN(I),I=NSP1,NBT)$ RETURN
   RETURN
13  PRINT 105,(QN(J),J=1,ILC)$ PRINT 107,(CR(I),I=1,ILC)
   PRINT 109,(CI(J),J=1,ILC)$ ILC=0$ GO TO IRET,(3,11)
101  FOPMAT(//30X10H***** * THE LOWEST *I2,1XA10,
1    * STATES, ALL COMP. .GT. *F5.3,1X10H***** //)
103  FORMAT(/* STATE NO.*I3*, WITH S.P. EN.=*F12.6,* MEV., PAR.=*I3*,
1    OCCUPIED BY A *A10)
105  FORMAT(4H QN=12(1XA10))
107  FORMAT(4H RP= 12(1XF10.7))
109  FORMAT(4H IP= 12(1XF10.7))
111  FORMAT(/* REMAINING S.P. ORBITS AT ENERGIES(MEV)*//(2X10F12.5 ))
   END
   SUBROUTINE RHERMAD(E,BR,BI,NBE,IDIM,IBT,IRES,R2)
*
*  E= HERM. MATRIX TO BE DIAGONALISED.
*  E(I,J), I.GE.J, CONTAINS REAL PART OF E,
*  E(I,J), I.LT. J, CONTAINS IMAGINARY PART OF E .
*  B(IDM,IDM)= ARRAY CONTAINING EIGENVECTORS BY COLUMNS.
*  BR= REAL PART OF B, BI= IM. PART OF B.
*  NBE= DIM OF MATRIX TO BE DIAGONALISED.
*  IDIM= DECLARED DIM OF E AND B, EG, A(IDIM,IDIM), B(IDIM,IDIM).
*  IBT= 0, NO TRIAL EIGENVECTORS, SET B TO 1 INITIALLY.
*  IBT=1, USE CURRENT B.
*  IRES= 0, HERMAD HAS FAILED, IRES=1 IF DIAG. IS COMPLETED.
*
   COMMON/DUMPN/XMS(100),JS(100),DDD(100)
   DIMENSION E(1),BR(1),BI(1)
   N=NBE$ NO=IDIM$ IRES=1$RL=R2*R2
   IF(RL.GT..1.OR.RL.LT.1.E-24) RL= 1.E-12
10  FORMAT(/5X,* HERMAD FAILS, R= *1PE8.2/)
   IF(N.LT.2) GO TO 501$ IF(IBT.GT.0) GO TO 55
   DO 59 I= 1 , N
     IJ= I
     DO 59 J= 1 , N
       BR(IJ)=0.$ BI(IJ)=0.$ IF(I.EQ.J) BR(IJ)=1.
59  IJ= IJ+ ND
55  TEST= 0.$ MI=0
   DO 20 I= 1 , N
     IJ= IS$ JI= MI+1
     DO 22 J= 1 , I
       EPSP= 2.$ IF(I.EQ.J) EPSP= 1.
       H=1.$ IF(I.EQ.J) H= 0.
       TEST= TEST+ (E(IJ)**2+H*E(JI)**2)*EPSP$ IJ= IJ+ ND
22  JI= JI+1
20  MI= MI+ ND
   IF(TEST.EQ.0.) GO TO 502
   XNOM= (N*N-N)/TEST$ NMAX= 5*N*N$ KT=0$ MK=ND
   DO 123 K= 2 , N
     XM=0.$ J=1$ KK=K-1$ KL=K$ LK=MK+1
     DO 32 L= 1 , KK
       Q= E(KL)**2+ E(LK)**2$ KL=KL+ND$ LK=LK+1
       IF(Q.LE.XM) GO TO 32$ XM=Q$ J=L
32  CONTINUE$ XMS(K)= XM$ JS(K)= J
123  MK= MK+ND
27  XM=0.
   DO 222 K= 2 , N
     Q=XMS(K)$ IF(Q.LE.XM) GO TO 222$ XM=Q$ I=K
222  CONTINUE
   R= XNOM*XMS IF(R.LT.RL ) GO TO 502
   KT= KT+1$ IF(KT.GT.NMAX) GO TO 26

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J=JS(I)$ JT=MAX0(2,J)$ MJ=ND*(J-1)$ IJ=MJ+I$ MI=ND*(I-1)
JI= MI+J$ JJ= MJ+J$ II= MI+I
PU= E(JI)$ YU= E(IJ)$ PSQ=PU**2+ YU**2$ E(IJ)=0.$ E(JI)=0.
P= SIGN(SQRT(PSQ),YU)$ Y= (E(JJ)-E(II))*0.5
X= P/SIGN(ABS(Y)+SQRT(Y*Y+PSQ),Y)
XU= PU/SIGN(ABS(YU)+ ABS(P),YU)
C= 1./SQRT(1.+X*X)$ S= X*C
CU= 1./SQRT(1.+XU**2)$ SU= XU*CU
P= P*X$ E(JJ)= E(JJ)+P$ E(II)= E(II)-P
KJ= MJ+1$ KI= MI+1$ JK=J$ IK=I
DO 25 K= 1 , N
YR= CU*BR(KJ)-SU*BI(KJ)$ YI=SU*BR(KJ)+CU*BI(KJ)
ZR=CU*BR(KI)+SU*BI(KI)$ ZI=-SU*BR(KI)+CU*BI(KI)
BR(KJ)=C*YR+S*ZR$ BR(KI)= -S*YR+C*ZR
BI(KJ)=C*YI+S*ZI$ BI(KI)=-S*YI+C*ZI
IF(K-I) 29,24,28
28 YR=CU*E(KJ)+SU*E(JK)
YI= SU*E(KJ)- CU*E(JK)
ZR= CU*E(KI)- SU*E(IK)
ZI= -SU*E(KI)- CU*E(IK)
E(KJ)= YR*C + S*ZR
E(KI)= -S*YR+ C*ZR
E(JK)= -C*YI- S*ZI
E(IK)= S*YI- C*ZI$ GO TO 24
29 IF(K-J) 31, 24, 30
31 YR= CU*E(JK)- SU*E(KJ)
YI= -SU*E(JK)- CU*E(KJ)
ZR= CU*E(IK)+ SU*E(KI)
ZI= SU*E(IK)- CU*E(KI)
E(JK)= C*YR+ S*ZR
E(IK)= -S*YR+ C*ZR
E(KJ)= -C*YI- S*ZI
E(KI)= S*YI- C*ZI$ GO TO 24
30 YR= CU*E(KJ)+ SU*E(JK)
YI= SU*E(KJ)- CU*E(JK)
ZR= CU*E(IK)+ SU*E(KI)
ZI= -SU*E(IK)+ CU*E(KI)
E(KJ)= C*YR+ S*ZR
E(IK)= -S*YR+ C*ZR
E(JK)= -C*YI- S*ZI
E(KI)= -S*YI+ C*ZI
24 KJ= KJ+1$ KI= KI+1$ JK= JK+ND$ IK= IK+ND
25 CONTINUE $ MK= ND*(JT-1)
DO 301 K= JT, N
JSK= JS(K)$ IF(K-I) 308,309,310
310 IF(J.EQ.JSK.OR.I.EQ.JSK) 309,301
308 IF(J.NE.JSK.AND.J.NE.K) GO TO 301
309 KK= K-1$ XM=0.$ JJ=1$ KL=K$ LK= MK+1
DO 305 L= 1 , KK
Q= E(KL)**2+E(LK)**2$ LK= LK+1$ IF(Q.LE.XM) GO TO 305
XM= Q$ JJ=L
305 KL= KL+ND$ XMS(K)= XMS$ JS(K)= JJ
301 MK= MK+ND$ GO TO 27
26 IRES=0$ PRINT 10,R$ GO TO 502
501 BR(1)=1.$ BI(1)=0.
502 RETURN
END
SUBROUTINE VEERAR(VR,F,ROJ,IPR)
* TO FIND THE AVERAGE ONE-BODY POTENTIAL GIVEN F THE FORCE ARRAY
* AND ROJ THE DENSITY MATRIX IN THE J,M REPRESENTATION .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),

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1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
   DIMENSION VB(2,1),ROJ(2,1),F(1)
   ITSS= 1$ GO TO 15$ ENTRY VEERAF$ ITSS= 0
15  IF(IPR.GT.0) CALL TIMEPRT(X)$ IF(ITSS.EQ.0) GO TO 13
   IF(INT(F(1)).NE.NOLV) CALL ERREXIT(NOLV,F,2HFL,200)
   DO 25 K = 1 , NOLV$ IF(INT(F(K+1)).NE.ICODE(K))
1  CALL ERREXIT(K,ICODE,2HFL,NOLV,F,2HFL,200)
25  CONTINUE
13  IFL= NOLV+1$ IF(IPR.GT.4) PRINT 409,IDSJ,(ROJ(I,1),I=1,IDSJ)
409  FORMAT(/* ROJ ARRAY,*15,* ELEMENTS*/1P(1X10E13.5))
   ILR= 0$ ILV= 1$ DO 1 JPO= 1 , JMPO$ JARJ= JAR(JPO,1)
   IF(ITSS.EQ.0) GO TO 17$ IF(INT(F(IFL+1)).NE.SHIFT(JPO-1,6)+JARJ)
1  CALL ERREXIT(JPO,IFL,JAR,2HFL,14,F(IFL-100),2HFL,200)
17  IFL= IFL+1$ DO 3 MPO= 1 , JPO$ IF(JARJ.EQ.0) GO TO 3
   DO 5 L = 1 , JARJ$ VB(1,ILV)=VB(2,ILV)+0.$ LMF= L+IFL
   DO 7 M = 1 , JARJ$ VB(1,ILV)= VB(1,ILV)+ F(LMF)*ROJ(1,ILR+M)
   VB(2,ILV)= VB(2,ILV)+ F(LMF)*ROJ(2,ILR+M)$ IDEL= 1
   IF(M.LI.L) IDEL= JARJ-M
7   LMF= LMF+ IDEL
5   ILV= ILV+1
3   ILR= ILR+ JARJ
1   IFL= IFL+(JARJ*(JARJ+1))/2
   IF(IPR.GT.5) PRINT 411,IDSJ,(VB(I,1),I=1,IDSJ)
411  FORMAT(/* VBJ ARRAY,*15,* ELEMENTS*/1P(1X10E13.5))
   RETURN
   END
   OVERLAY(DENSITY,4,0)
   PROGRAM DENSITY
   COMMON/QUADS/ QUADS(5,3)
   COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
   COMMON/NUHARN/VALN(82),VALP(82),NP(2),NN(2),NAME,ITER,ITCR,ATNO
1 ,NORBA(41),NORB,BET,GAMD,NPTOT,NNTOT
   COMMON /CODAN/ICODAP(16),ICODAN(16),LVP,LVN,IQM(16),NOLT
   COMMON /PLOT1/ LAY,NMAX/ADEN1/DTHE,ITHE,IRAD,MAXX
   COMMON/PLOT3/X(3),IAXIS(3),UNIT1,XNAME(3),DA,BETA,ABSS(9),
1 DAR(9),NPN(2),COMM(2)
   COMMON YLM(4000),HNL(4000),WAVF(328),RMS(3),AS1(2)
*  **** NOTE**** AS1 OVERWRITTEN TO LENGTH 40000 .
*  DATA COMM/10H TOTAL DEN,10HSITY
*  LAY IS THE NO. OF LEVELS OF DENSITIES TO BE PRINTED IN DENPLOT.
*  UNIT1 IS THE UNIT DENSITY IN DENPLOT, E.G. THE SYMBOL 2 IN DEN-
*  PLOT REPRESENTS A DENSITY OF 1.75 TO 2.25 UNIT1(NUCEON/FERMI CUBED).
*  DATA LAY,NMAX,UNIT1/40,54,.017/,MAXX/300/,JWANT/3/
*
   CALL TIMEPRT(YD)$ CALL BUFFIN(4LROPS ,YLM,IDSJ)
   ENCODE(20,101,COMM)HBOM
101  FORMAT(*TT DNS,HBOM=*F6.1)
   CALL ROCONV(AS1,YLM,-1)$ CALL BUFFIN(4LRONS ,YLM,IDSJ)
   CALL ROCONV(HNL,YLM,-1)$ DO 1 I = 1 , 3
1   RMS(I)= QUADS(I,JWANT)$ DO 2 I = 1 , IDSC
2   AS1(I)= AS1(I)+ HNL(I)$ NPN(1)= NPTOT$ NPN(2)= NNTOT
   CALL CALYLM(YLM,5,181,DTHE,ITHE)$ CALL CALHNL(HNL,MAXX,5,IRAD)
   LVP=LVN=0$ DO 3 II = 1 , NOLV$ IF(MOD(IPAR(II),2).EQ.0) GO TO 5
   LVN= LVN+1$ ICODAN(LVN)= ICODE(II)$ GO TO 3
5   LVP= LVP+1$ ICODAP(LVP)= ICODE(II)
3   CONTINUE$ DO 7 K = 1 , LVP
7   IQM(K)= ICODAP(K)$ DO 9 K = 1 , LVN
9   IQM(K+LVP)= ICODAN(K)$ NOLT= NOLV
   CALL DENPLOT(AS1,RMS,WAVF,YLM,HNL,NB,NBT,HBOM,NAME)

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END
SUBROUTINE CALYLM(YLM,LM,NM,DX,IDIM)
*   CALCULATE THE REAL NORMALIZED ASSOCIATED LEGENDRE POLYNOMIALS
*   FOR L=0 TO L=LM IN INTERVALS OF THETA DX=PI/(2*(NM-1)) AND
*   STORE IN THE LINEAR ARRAY YLM. THE DIMENSION OF YLM MUST NOT BE LESS
*   THAN IDIM*NM, WHERE IDIM IS THE NUMBER OF PAIRS (L,M) = (0,0),
*   (1,0), (1,1), (2,0),....., (LM,LM-1), (LM,LM). OR
*   IDIM=((LM+1)*(LM+2))/2. THE ADDRESS OF THE VALUE FOR
*   (L,M,THETA) IS THE SAME AS THE ADDRESS (LM,IX) IN A IDIM*NM
*   MATRIX, WHERE LM=(L*(L+1))/2+M+1, I.E., ADD=IDIM*(IX-1)+LM.
DIMENSION YLM(1)
LMAX=LM+1$ IDIM=((LMAX+1)*LMAX)/2$ DX=3.141592653/(2.*FLOAT(NM-1))
I=1$ DO 1 L1=1,LMAX$ L=L1-1$ X=-DX$ K=1
DO 2 M=1,NM$ X=X+DX$ CALL NLEGEND(X,YLM(K),L)
2 K=K+IDIM
1 I=I+L1$ RETURN
END
SUBROUTINE NLEGEND(THETA,A,N)
*   BASED ON THE ALEGEND SUBROUTINE IN THE CDC 6600 LIB. AT CRNL.
*   A(M+1)= Y(N,M,THETA) = (-1)**M*SQRT((2*N+1)*FACT(N-M)/
*   (4*PI*FACT(N+M)))*P(N,M,THETA). FOR M.GE.0
DIMENSION RTFAC(20),A(1)
LOGICAL IPASS
DATA IPASS/.FALSE./
IF(IPASS) GOTO2$ RTFAC(1)=1.$ DO 1 I=2,20$ P=SQRT(FLOAT(I-1))
1 RTFAC(I)=P*RTFAC(I-1)$ IPASS=.TRUE.
2 P=SQRT(FLOAT(2*N+1)/(4.*3.141592653)) $ IF(N.GE.1)GOTO20
A(1)=P$ RETURN
20 IF(ABS(THETA).GT.1.E-10)GOTO30$ A(1)=P$ DO 21 K=1,N
21 A(K+1)=.0$ RETURN
30 IF(ABS(THETA-3.1415926536).LT.1.E-11)31,40
31 K=N/2$ IF(K*2.EQ.N)311,312
311 A(1)=P$ GOTO313
312 A(1)=-P
313 DO 314 K=1,N
314 A(K+1)=0$ RETURN
40 Y=SIN(THETA)$ PROD=N+1$ K1=N+2$ K2=2*N$ IF(K2.LT.K1) 52,50
50 DO 51 K=K1,K2
51 PROD=K*PROD
52 PNR=A(N+1)=P*PROD*(Y/2.)*N$ PNS=.0$ COT=COS(THETA)/Y
DO 60 MM=1,N$ M=N-MM$ A(M+1)=(2*(M+1)*COT*PNR-PNS)/((N+M+1)*(N-M))
PNS=PNR$ PNR=A(M+1)
60 A(M+1)=RTFAC(N-M+1)*(-1.)*M*A(M+1)/RTFAC(N+M+1)
A(N+1)=(1-2*MOD(N,2))*A(N+1)/RTFAC(N+1)$ RETURN
END
SUBROUTINE CALHNL(HNL,XMAX,NM,IDIM)
*   CALCULATE THE HARMONIC OSC. WAVE FUNC. FOR ALL STATES WITH TOTAL
*   QUANT. NO. LE NM, FROM X=0 TO X=4.-DX IN INTERVALS OF DX AND STORE
*   IN THE LINEAR ARRAY HNL. X=R/BETA, BETA=1./SQRT(.0241145*HW).
*   HNL(I)=RDFUNC(N,L,X), WHERE I=IDIM*(IX-1)+INL,
*   INL=(NQ/2+1)*(NQ/2)+MOD(NQ,2)*((NQ-1)/2+1)+L/2+1, NQ=2*N+L
*   THE DIMENSION OF HNL MUST NOT BE LESS THAN IDIM*XMAX.
INTEGER XMAX
DIMENSION HNL(1)
IDIM=((NM+3)/2)*((NM+1)/2)+MOD(NM+1,2)*(NM/2+1)$ DX=4./FLOAT(XMAX)
NMAX=NM+1$ IK=0$ X=-DX
DO 1 K=1,XMAX$ X=X+DX$ DO 1 N1=1,NMAX$ IF(MOD(N1-1,2))6,3,4
3 LMIN=1$ GOTO5
4 LMIN=2
5 DO 1 L1=LMIN,N1,2$ L=L1-1$ N=(N1-L1)/2$ IK=IK+1
1 HNL(IK)=RDFUNC(N,L,X)$ RETURN

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6 CALL ERREXIT(N1)
END
FUNCTION RDFUNC(N,L,X)
C NORMALIZED H.O. RADIAL-FUNCTION UPTO NOSC=20 (NOSC=2*N+L)
  DIMENSION FL(11),GL(21)
  LOGICAL IPASS$ DATA IPASS/.F./
  DATA N1MAX,L1MAX/11,21/
  N1= N+1$ L1= L+1$ RDFUNC=0$ IF(N.LT.0.OR.L.LT.0) RETURN
  NL= N+L+1$ IF(N1.GT.N1MAX.OR.NL.GT.L1MAX) GO TO 5
  IF(IPASS) GO TO 2$ IPASS= .T.$ FL(1)=0.$ GL(1)= ALOG(0.5)
  DO 1 M = 2 , L1MAX$ A= M-1$ IF(M.GT.N1MAX) GO TO 1
  FL(M)= FL(M-1)*ALOG(A)
1  GL(M)= GL(M-1)+ALOG(A+0.5)
  A= 2./SQRT(3.141593)
2  XSQ= X*X
C EVALUATE LAGUERRE POLYNOMIAL POLAG(N,L+1/2,XSQ)
  POLAG= EXP(GL(NL)-GL(L1)-FL(N1))$ IF(N.EQ.0) GO TO 4$ B= 1.
  DO 3 M=1,N$ B= -B*XSQ
3  POLAG= POLAG*B*EXP(GL(NL)-GL(L1+M)-FL(N1-M)-FL(M+1))
4  B= EXP(FL(N1)-GL(NL))$ B= SQRT(A*B)
  RDFUNC= B*(X*L)*EXP(-0.5*XSQ)*POLAG$ RETURN
5  PRINT6,N,L$ RETURN
6  FORMAT(/1X,*XXXXX N=*,I2,2X,*L=*,I2,2X,*N OR L TOO LARGE*,
11* CANNOT CALCULATE RADFNC.CHANGE DIMENSION AND DATA XXXXX*)
  END
  SUBROUTINE DENPLOT(RO,RMS,WAVF,YLM,HNL,NB,NBT,HW,NAME)
  * ROUTINE ONLY CALCULATES THE FIRST QUADRANT DENSITY FOR ANY GIVEN
  * CROSS-SECTION. IN OTHER WORDS, PARITY CONSERVATION IS ASSUMED.
  COMMON/PLOT3/X(3),IAXIS(3),UNIT1,XNAME(3),DA,BETA,ABSS(9),
1  DAR(9),NPN(2),COMM(2)
  COMMON/PLOT2/AS2(4000)
  COMMON /PLOT1/LAY,NMAX
  * COMMON/SYMB/LIT(40)$ INTEGER TAG(3)$ REAL NAME
  COMMON/SYMB/LIT(40)
  LOGICAL R1,R2,R3,FLIP,IPASS
  DIMENSION RO(1),RMS(1),YLM(1),HNL(1),NB(1),WAVF(1),ADEN(60),Y(3)
  DIMENSION DA9(9),DB9(9)
  EQUIVALENCE(I,IAXIS(1)), (I2,IAXIS(2)), (I3,IAXIS(3))
  DATA DB/10H+ /, IPASS/.F./
  IF(IPASS)GOTO7$ ENCODE( 90,51,DA9)DA,DA,DA,DA,DA,DA,DA,DA,DA,DA
  ID=DATE(T)$ ENCODE(90,51,DB9)DB,DB,DB,DB,DB,DB,DB,DB,DB$IPASS=.T.
7  JKX=1$ IF(NAME.EQ.5LMG 24.OR.NAME.EQ.5LS 32) JKX=0
  BETA=1./SQRT(.0241145*HW)$ R2=ABS(RMS(1)-RMS(2)).LT..1
  * 0.17 PER FERMI CUBED IS THE NUCLEAR MATTER DENSITY.
  B3=BETA**3$ DDEN1=0.17*B3$ UNIT=UNIT1*B3/2
  R1=ABS(RMS(2)-RMS(3)).LT..1$ R3=ABS(RMS(1)-RMS(3)).LT..1
  * N2=NMAX/2$ DO10 I=1,3$ Y(I)=(RMS(I)*3.0/BETA)**2
  * 10 TAG(I)=I$ CALL SORTAG(RMS,1,3,TAG)$ X(TAG(1))=X(TAG(2))=0
  * XM=AMIN1(3.9,RMS(TAG(3))*3.0/BETA)$ DX=XM/N2$ XMAX=XM+.5*DX$ XM=XM+DX
  * XM=AMIN1(3.9,3.6/BETA)$ DX=XM/NMAX$ XMAX=XM+.5*DX$ XM=XM+DX
  * I1=TAG(3)$ X(I1)=-DX$ W=0$ DO 11 I=1,N2$ X(I1)=X(I1)+DX
  * CALL CWVFNC(X,NBT ,WAVF,YLM,HNL)$ DEN=DENSD(RO,WAVF,1.,1.,NB,2)
  * 11 W=AMAX1(DEN,W)$ DDEN=W/FLOAT(LAY)$ FLIP=.F.$ DZ=6*BETA*DX
  * N7=NMAX/2$ FLIP=.F.$ DO10 I=1,3$ Y(I)=(RMS(I)*3.0/BETA)**2
  * 10 CONTINUE$ XM=AMIN1(3.9,3.6/BETA)$ DX=XM/NMAX$ XMAX=XM+.5*DX
  * XM=XM+DX$ DZ=6*BETA*DX
  * DO 1 I=1,3$ IF(I.EQ.2.AND.R2)GOTO1$ IF(I.EQ.3.AND.(R1.OR.R3))GOTO1
  * I2=MOD(I,3)+1$ I3=MOD(I+1,3)+1$ IF(Y(I3)-Y(I2))3,6,6
  * 3 K=I2$ I2=I3$ I3=K
  * 6 YY=SQRT(Y(I2)/Y(I3))$ X(I2)=-DX $ X(I1)=.0$ KK=0
  * 13 X1=X(I)*X(I)/Y(I)
  PRINT1000,ID$ PRINT1001, DA9

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DO 2 J=1,NMAX$ X(I2)=X(I2)+DX$ X(I3)=-DX $ DO 4 K=1,NMAX
4 ADEN(K)=.0$ X2=X(I2)*X(I2)*YY/Y(I2)$ DO 5 K=1,NMAX$ X(I3)=X(I3)+DX
IF(X1+X2+X(I3)*X(I3)/Y(I3).GT.1.) GOTO5
CALL CWFVNC(X,NBT,WAVF,YLM,HNL)$ ADEN(K)=DENS(DRO,WAVF,1.,1.,NB,2)
5 CONTINUE$ IF(J.EQ.NMAX) FLIP=.T.$ DO12 N=1,NMAX
* 12 AS2(KK+N)=ADEN(N)$ CALL LINPLT1(ADEN,DDEN,LAY,NMAX,FLIP)
12 AS2(KK+N)=ADEN(N)$CALL LINPLT2(ADEN,UNIT,LAY,NMAX,DAR)
CALL FORMT(J,NAME)
2 KK=KK+NMAX$ PRINT1001,DA9$ PRINT1002,DB9$ PRINT1003,ABSS,XNAME(I3)
CALL LINPRT1(AS2,DDEN1,NMAX,B3)
IF(I.NE.3.OR.JKX.NE.0)GOTO1$X(I)=JKX=1$X(I2)=-DX$KK=0$ GOTO13
1 CONTINUE$ RETURN
51 FORMAT(9A10)
1000 FORMAT(1H1,18X'DENSITY PLOT FROM EVALIN ( R.Y. CUSSON/ H.C. LEE )
1C,R,N,L. DATE=A10//)
1001 FORMAT(9X**9A10***)
1002 FORMAT(10X,9A10)
1003 FORMAT(9X,9(F5.3,5X)/44X,A1*-AXIS(FERM1)*)
END
SUBROUTINE JWFVNC1(X,NBT,WFJS,YLM,HNL)
* CALCULATE THE SPIN PROJECTED SINGLE PARTICLE WAVE FUNCTIONS AT X
* AND STORE IN THE LINEAR ARRAY WFJS. IN THE FIRST 2*NBT LOCATIONS
* THE SPIN UP COMPONENTS ARE STORED IN THE ORDER GIVEN BY ICODAP AND
* ICODAN. ICODAP CONTAINS THE POSITIVE PARITY STATES IN CODA AND ICODAN
* THE NEGATIVE PARITY STATES. FOR A GIVEN J-STATE THE ORDER OF M IS
* M=J, M=J-1,....., M=-J. THE TOTAL NO. OF STATES IS NBT.
* THE IMAGINARY PART FOLLOWS IMMEDIATELY AFTER THE REAL PART FOR EACH
* (J,M) STATE. THE 2*NBT LOCATIONS STARTING FROM 2*NBT+1 STORE THE
* REAL AND IMAGINARY SPIN DOWN COMPONENTS.
*
COMMON/CLEBDAT/ALOGF(30),SQRF(30)
DIMENSION WFJS(1),YLM(1),HNL(1),X(3)
COMMON /CODAN/ICODAP(16),ICODAN(16),LVP,LVN,IQM(16),NOLT
COMMON/ADEN1/DTHETA,ITHE,IRAD,MAXX
DIMENSION CS(4),SN(4),CSL(10),SNL(10)
COMMON/CODATPR/IBAQ(30)
LOGICAL XX2,LTHE
DATA CS,SN/1.,0.,-1.,0.,0.,1.,0.,-1./
DATA PI,PI2/3.1415 92653 5898,1.5707 96326 7949/
*
* SCG IS THE C-G COEFF. ( J,M I L,.5,M-S,S ) . MU=2*(J-L), NU=2*S.
* X1,X2,X3 ARE THE CARTESIAN COORDINATES X,Y,Z.
ENTRY CWFVNC
21 X1=X(1)$ X2=X(2)$ X3=X(3)
R=X1*X1+X2*X2$ THE=ATAN2(SQRT(R),X3)$ PHI=ATAN2(X2,X1)
R=SQRT(R+X3*X3)$ IF(ABS(X3).LT.1.E-5) THE=PI2
IF(ABS(X1).LT.1.E-5) PHI=SIGN(PI2,X2)$ GOTO1
ENTRY SWFVNC
*
* X1,X2,X3 ARE THE POLAR COORDINATES R,THETA,PHI.
22 R=X(1)$ THE=X(2)$ PHI=X(3)
1 KK=SHIFT(NBT,2)$ DO11 K=1,KK
11 WFJS(K)=0$ DO 16 L=1,10$ PHL=(L-1)*PHI$ CSL(L)=COS(PHL)
16 SNL(L)=SIN(PHL)$ XX2=.FALSE.$ KS=2*NBT$ IF((THE-PI/2.)2,2,3
3 THE =PI-THE$ XX2=.TRUE.
2 LTHE=(PI-.5-THE).GT.0$THETAS XT=THE/0$THETAS K2=XT$ DK2=XT-FLOAT(K2)
XR=R*MAXX/4.$ K1=XR$ DK1=XR-FLOAT(K1)$ YL=IK=1
DO 24 I = 1 , NOLTS IQ= IQM(I)$ IQNT= IBAQ(IQ)$ JPH= IQNT/10000
IT= MOD(IQNT,10000)$ NT= IT/100$ L= MOD(IT,100)$ M22= SHIFT(JPH,1)
M2= M22-1$ NQ= NT-1$ MU= M2-SHIFT(L,1)$ SQL= SQRF(2*L+1)
MDL=MOD(L,4)*1$ SRE=CS(MDL)$ SIM=SN(MDL)$ NQ2=SHIFT(NQ,-1)
IR=IRAD*K1*(NQ2+1)*NQ2*MOD(NQ,2)*(SHIFT(NQ-1,-1)+1)*SHIFT(L,-1)+1

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H=HNL(IR)$ H=H+DK1*(HNL(IR+IRAD)-H)$ IL=SHIFT(L*(L+1),-1)+I*THE*K2+1
*
*      IR IS THE ADD. OF N,L,R IN HNL. ILM IS THE ADD. OF L,LM,THETA IN YLM.
DO24 JM=1,M22$ XM=FLOAT(M2)/2$      DO7 NU=1,3,2$ NNU=NU-2$ YM=ZM=1
LM=SHIFT(M2-NU+2,-1)$ IF(XX2) YL=1-2*MOD(L+LM,2)$ IF(LM)6,5,5
6 LM=-LM$ YM=1-2*MOD(LM,2)$ ZM=-1.
5 IF(LM.GT.L) GOTO7$ ILM=IL+LM$ IS=SHIFT(KS*(3-NU),-1)
KK=.5+MU*NNU*XM$ SQK=SQRF(KK+L)$ SCG=.5*(1+MU-NNU+MU*NNU)*SQK/SQK
Y=YLM(ILM)$ IF(LTHE) Y=Y+DK2*(YLM(ILM+I*THE)-Y)
S=YM*YL*Y*H*SCG$ CR=CSL(LM+1)$ SR=SNL(LM+1)*ZM
WFJS(IS+IK)=(SRE*CR-SIM*SR)*S$ WFJS(IS+IK+1)=(SIM*CR+SRE*SR)*S
7 CONTINUE$ M2=M2-2
24 IK=IK+2$ RETURN
END
FUNCTION DENSD(RO,WAVF,G1,G2,NB,MUD)
*
*      THIS CODE GENERATES MUD CALLS TO DENSP TO GET TOTAL DENSITY
DIMENSION RO(1),WAVF(2,1),NB(1)
M= NBB=1$ X= 0.$ NBT= 0$ DO 11 K= 1 , MUD
11 NBT= NBT+ NB(K)
DO 1 K= 1 , MUD$ ND= NB(K)
X= X+DENSP(RO(M),WAVF(1,NBB),WAVF(1,NBB+NBT),G1,G2,ND)
M= M+ ND**2
1 NBB= NBB+ ND$ DENSD= X$ RETURN
END
FUNCTION DENSP(RO,FI1,FI2,H1,H2,NR)
*
*      ASSUMING THAT RO(I,J) IS REAL COMPUTE SPATIAL DENSITY USING WAVF .
DIMENSION RO(NB,1),FI1(1),FI2(1)
ND= NB$ DENSP= 0.$ II= 1$ DO 1 I= 1 , ND$ JJ= 1$ G1= 2.*H1
G2= 2.*H2$ DO 3 J= 1 , 1$ IF(ABS(RO(I,J)).LT.1.E-6) GO TO 3
IF(I.GT.J) GO TO 4$ G1= .5*G1$ G2= .5*G2
4 DENSP= DENSP+ RO(I,J)*(G1*(FI1(JJ)*FI1(II)+FI1(JJ+1)*FI1(II+1))
1 +G2*(FI2(JJ)*FI2(II)+FI2(JJ+1)*FI2(II+1)))
3 JJ= JJ+ 2
1 II= II+2$ RETURN
END
SUBROUTINE LINPLT2(A,UNIT,LAY,N,X)
COMMON/SYMB/LIT(40)$ DIMENSION X(1),A(1)$ INTEGER X
DATA LIT/1R,1R1,1R,1R2,1R,1R3,1R,1R4,1R,1R5,
1 1R,1R6,1R,1R7,1R,1R8,1R,1R9,1R,1RA,
2 1R,1RB,1R,1RC,1R,1RD,1R,1RE,1R,1RF,
3 1R,1RG,1R,1RH,1R,1RJ,1R,1RK,1R,1RL/
* N1=N-1$ A0=A(1)$ A1=A(2)$ DO3 I=1,13
* 3 X(I)=0B$ DO4 I=2,N1$ A2=A(I+1)$ A(I)=(A0+A1+A2)/3.$ A0=A1
* 4 A1=A2$ M=(5*N)/3$ M1=M-1$ DEL=.5*UNIT$ MS=M1/10+1$ IF(M-100)1,1,99
DO3 I=1,9
3 X(I)=0B$ M=(5*N)/3$ M1=M-1$ DEL=.5*UNIT$ MS=M1/10+1$ IF(M-100)1,1,99
1 K=(A(1)+DEL)/UNIT+1.$ X(1)=SHIFT(LIT(K),54)$ K=(A(N)+DEL)/UNIT+1.
X(MS)=SHIFT(LIT(K),54-6*MOD(M-1,10))$ DO2 I=2,M1$ I1=I-1
I2=I1/10$ I1=MOD(I1,10)$ X1=I2*6.+I1*5./9+1.$ IX=X1
K=(A(IX)+(X1-FLOAT(IX))*(A(IX+1)-A(IX))+DEL)/UNIT+1. $ J=I2+1
2 X(J)=X(J)+SHIFT(LIT(K),54-6*I1)$ RETURN
99 PRINT1002$ RETURN
1002 FORMAT(* MESSAGE FROM LINPLT. N.GT.60. DECREASE NO. OF POINTS CAL
ICULATED, N=NMAX, TO LESS THAN 60.*)
END
SUBROUTINE FORMT(NL,NAME)
COMMON/PLOT3/X(3),IAXIS(3),UNIT1,XNAME(3),DA,BETA,ABSS(9),
1 DAR(9),NPN(2),COMM(2)
DIMENSION DAR1(6)
EQUIVALENCE (DAR(1),DAR1(1))

```

```

DATA DA/10H+-----/, DB/10H1-----/, DC/10H1 NUCLEUS/,
1 DD/1HI/, DL/2H--/, DE/7H(FERMI)/,
2 DF/5HPLANE/, DG/7HI UNIT/, DH/7HDENSITY/,
3 DI/9H/F CUBED /, DJ/10HI COMMENT/, XNAME/1HX,1HY,1HZ/.
XX1=BETA*X(IAxis(1))$ XX2=BETA*X(IAxis(2))
IF((NL-45)*(NL-54))10,10,1
1 IF(NL.EQ.28)GOTO2$ IF(MOD(NL,6).EQ.1)GOTO3
PRINT1001,DD,DAR,DD$ RETURN
2 PRINT1002,XNAME(IAxis(2)),DD,DAR,DD$ RETURN
3 PRINT1003,XX2,DL,DAR,DL$ ABSS(NL/6+1)=XX2$ RETURN
10 IF(MOD(NL,2))12,11,12
11 PRINT1004,DD,DAR1,DD,DD$ RETURN
12 NI=(NL-43)/2$ GOTO(21,22,23,24,25) NI
21 PRINT1001,DD,DAR1,DA,DB,DB,DD$ RETURN
22 PRINT1006,DD,DAR1,DC,NAME,NPN,DD$ RETURN
23 PRINT1007,XX2,DL,DAR1,XNAME(IAxis(1)),XX1,DE,DF,DL
ABSS(NL/6+1)=XX2$ RETURN
24 PRINT1008,DD,DAR1,DG,DH,UNIT1,DI,DD$ RETURN
25 PRINT1009,DD,DAR1,DJ,COMM,DD$ RETURN
1001 FORMAT(9X,A1,9A10,A1)
1002 FORMAT(1X,A1*-AXIS *A1,9A10,A1)
1003 FORMAT(3X,F5.3,A2,9A10,A2)
1004 FORMAT(9X,A1,6A10,A1,29X,A1)
1006 FORMAT(9X,A1,7A10,1X,A5* Z=*I3* N=*I3,1X,A1)
1007 FORMAT(3X,F5.3,A2,6A10*-2X,A1*=*F5.3,A7,1X,A5,7X,A2)
1008 FORMAT(9X,A1,6A10,A7,1X,A7,1X,F5.3,A9,A1)
1009 FORMAT(9X,A1,9A10,A1)
END
SUBROUTINE LINPRT1(RO,DD,N,B3)
* LEFT-RIGHT SYMMETRY OF RO IS NOT CONSERVED. TO CONSERVE SYMMETRY
* USE SUBROUTINE LINPRT.
INTEGER A(40)
DIMENSION RO(N,N)
DATA M/30/
S=100./DD$ SB3= S*B3$ PRINT 1001,SB3$ M1= M-1$ DO 2 J = 1 , N
A(1)= RO(1,J)*S+.5
A(M)=RO(N,J)*S+.5$ DO1 K=2,M1$ XK=FLOAT(K*N)/FLOAT(M)$ I=XK
1 A(K)=(RO(I,J)+(XK-FLOAT(1))*(RO(I+1,J)-RO(I,J)))*S+.5
2 PRINT1000,(A(I),I=1,M)$ RETURN
1000 FORMAT(5X,40I3)
1001 FORMAT(*1 DENSITY PRINT, THE INTEGER PRINTED IS= (RHO IN FERM.*
18H**(-3))*F5.1//)
END
OVERLAY(MULTIP,6,0)
PROGRAM MULTIP
*
* TO COMPUTE THE MULTIPOLE MOMENTS OF THE PROTON WAVEFUNCTIONS .
COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1 ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMPO,
2 NBT,HBOM,OSPA2
COMMON AS1(4000),AS2(4000),AS3(1)
CALL TIMEPRT(YD)
PRINT 103
CALL BUFIN (4LROPS,AS1,IDSJ)
DO 1 KPOLL= 1 , 7 , 2$ KPOL= KPOLL-1$ DO 1 MPOLL= 1 , KPOLL,2
MPOL= MPOLL-1
CALL MULME(AS2,KPOL,MPOL)
CALL ROCONV(AS2,AS3,+1)
HEXAD= TRVEROJ(AS3,AS1,0)*(1-2*MOD(KPOL/2,2))
* DHEXAD=H**L*(4*PI/2*L+1)**.5*(Y(L,M)+(-1)**M*Y(L,-M))/2,IN F**L
DHEX= HEXAD*(OSPA2)**(KPOL/2)
1 PRINT 101,KPOL,MPOL,HEXAD,DHEX

```

```

101  FORMAT(/* FOR KPOL,MPOL=*2I4,* ,MOMENT=*1PE14.5,* ,IN UNITS OF BSQ
1R, MOMENT=*E14.5,* ,IN UNITS OF *7HF**KPOL)
103  FORMAT(///52X*COMPUTATION OF MULTIPOLE MOMENTS*)
      END
      SUBROUTINE MULME(RME,KPOL,MPOL)
*
*   TO COMPUTE THE MATRIX ELEMENTS OF (I*R)**KPOL*C(KPOL,MPOL), IN THE
*   T.R.I. BASIS, WHERE THEY ARE REAL. C(KPOL,MPOL)=(4*PI/(2*K+1))
*   **5*YLM. IF MPOL.NE.0 COMPUTE .5*(C(K,M)+(-1)**(K-M)*C(K,-M)) SINCE
*   THIS IS THE REAL SYMMETRIC HERMITIAN PART .
      COMMON/BASIS/ ICODE(16),ISTA(16),IPAR(16),INPO(16),INUC(16),
1  ILC(16),NOLV,NB(2),MUD,IDF,IDSC,IDSJ,JAR(14,2),IDAC(14,14),JMP0,
2  NBT,HBOM,OSPA2
      DIMENSION RME(1)
      IHA= 1-SHIFT(IABS(KPOL-MPOL).A.1,1)$ RKPO= KPOL
      CNOR= 1./SQRT(1.+2*KPOL)$ DO 2 KK = 1 , IDSC
2  RME(KK)=0 $ ILS= 0$ DO 1 IPL= 2 , 3$ ND= NB(IPL-1)$ ILAP=0
      DO 3 KP = 1 , NOLV$ IF(((IPL+IPAR(KP)).A.1).NE.0) GO TO 3
      JPHP= ISTA(KP)$ MLMP= SHIFT(JPHP,1)$ LP= ILC(KP)
      NUP1= SHIFT(INPO(KP)-LP+1,-1)$ JMLP2= MLMP-SHIFT(LP,1)-1$ILA= 0
      DO 7 K = 1 , KP $ IF(((IPL+IPAR(K)).A.1).NE.0) GO TO 7$JPH=ISTA(K)
      MLM= SHIFT(JPH,1)$ L= ILC(K)$ IF(L+LP-KPOL.LT.0) GO TO 8
      JML2= MLM-SHIFT(L,1)-1$ NUL= SHIFT(INPO(K)-L+1,-1)
      IPE= IABS(L-LP+KPOL)
      RMX= CNOR*RAD(NUP1,LP,NUL,L,KPOL)*RMECK(LP,JMLP2,KPOL,L,JML2)*
1  (1-SHIFT(SHIFT(IPE,-1).A.1,1))$ IF(RMX.EQ.0) GO TO 8
      DO 9 MLP= 1 , MLMP$ ILBP= ILAP+MLP$ RFASM= .5
      DO 11 ML= 1 , MLM$ ILB= ILA+ML$ IF(ILB.GT.ILBP) GO TO 11
      MPMM= ML-MLP+JPHP-JPH$ C1=C2=0
      IF(MPOL.EQ.MPMM) C1= CLEBSCH(JPHP-.5,JPH-.5,JPHP+.5-MLP,ML-.5-JPH,
1  RKPO)
      IF(MPOL.EQ.-MPMM) C2= CLERSCH(JPHP-.5,JPH-.5,JPHP+.5-MLP,ML-.5-JPH
1  ,RKPO)*IHA
      RME(ILS+ILBP+ND*(ILB-1))= RFASM*(C1+C2)*RMX
11  RFASM= -RFASM
9  CONTINUE
8  ILA= ILA+ MLM
7  CONTINUE$ ILAP= ILAP+ MLMP
3  CONTINUE
1  ILS= ILS+ ND*ND$ RETURN
      END
      FUNCTION RMECK(LP,JMLP,K,L,JML)
*
*   TO COMPUTE THE REDUCED MATRIX ELEMENTS OF THE UNNORMALISED
*   SPHERICAL HARMONICS C(K), IN J-J COUPLING BASIS, USING
*   FORMULAE 7.1.9 AND 7.1.10 OF EDMUNDS P 113.
*   JMLP AND JML CAN BE ANY REAL OR INTEGER NUMBERS HAVING THE SIGN OF
*   JP-LP AND J-L .THE MOSHINSKY PHASE FOR YLM IS USED THROUGHOUT AND
*   EDMONDS EXPRESSION FOR THE WIGNER-ECKART THEOREM IS ASSUMED .
*   /ALGFN/ MUST HAVE BEEN PRESET TO LOG(GAMMA(N)) .
      COMMON /CLEBDAT/ALOGF(30),SQRF(30)
      COMMON/RMECKOT/I1,I2,I3,I4,I5,I6,I7,I8,IFASN,RJP,RJ
      VAL=0.$ IF(MOD(L+LP+K,2)) 99,1
1  RSH=1.$ RK=K$ IF(JMLP) 3,99,5
3  RJP= FLOAT(LP)-.5$ IF(JML) 7,99,9
5  RJP= FLOAT(LP)+.5$ IF(JML) 11,99,13
7  RJ= FLOAT(L)-.5$ GO TO 15
9  RJ= FLOAT(L)+.5$ GO TO 17
11 RJ= FLOAT(L)-.5$ GO TO 17
13 RJ= FLOAT(L)+.5
15 RSH=0.
17 SM= RJ+RJP+RK$ IFASN=2- 4*MOD(IABS(IFIX(.5*(RJ-RJP+RK+RSH))),2)

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I1=RJ+RJ-RK+1$ I2= RJ-RJ+RK+1$ I3=RJ+RK-RJP+1$ I4=IFIX(SM)+2
I5= .5*(SM+3.-RSH)$ I6= .5*(RJP+RJ-RK+1.+RSH)
I7= .5*(RJ+RK-RJP+2.-RSH)$ I8= .5*(RJP-RJ+RK+2.-RSH)
I0= MIN0(I1,I2,I3,I4,I5,I6,I7,I8)$ IF(I0.LT.1) GO TO 99
VAL= IFASN*EXP(.5*(ALOGF(I1)+ALOGF(I2)+ALOGF(I3)-ALOGF(I4))
1 + ALOGF(I5)- ALOGF(I6)- ALOGF(I7)- ALOGF(I8))
99 RMECK= VAL$ RETURN
END
FUNCTION RAD1(NQ,LQ,NR,LR,LAM)
*
* USE THE FORMULA OF MORSE-FESHBACH P. 785 WRITTEN IN TERMS OF
* GAMMA FUNCTIONS.
* ALGA(R)= LOG(ABS(GAMMA(R))), R= 2*K FAGA(R)= SIGN(GAMMA(R)).
* IF R= NEG. INT. ALGA,FAGA CONTAIN THE LOG ABS OF THE RESIDUE AT
* THE POLE, AND THE SIGN OF THE RESIDUE RESPECTIVELY .
* ALOGF(N) MUST HAVE BEEN PRESET TO LOG(GAMMA(N)) .
* NQ= NUP+1$ NR= NU+1
*
COMMON /CLEBDAT/ALOGF(30),SQRF(30)
ENTRY RAD
LMPD= LAM+ LQ+ LR$ RLMP= .5*LMPD$ IFAS= 1-2*MOD(NQ+NR,2)
NP= NQ-1$ N= NR-1$ VAL=0.$ LL= MIN0(NP,LQ,N,LR,LAM+1)
IF(LL.LT.0) GO TO 100$ RNLP= NP+ LQ$ RNL= N+ LR
ISU= MIN0(N,NP)+1$ IF(MOD(LMPD,2)) 1, 3
1 ISL=1$ GO TO 5
3 LML=IFIX(RLMP)-LQ $ LML= IFIX(RLMP)-LR$ ISL=1
IF(LML.GE.0) ISL=1+MAX0(0,NP-LML)
IF(LML.GE.0) ISL= 1+ MAX0(ISL-1,N-LML)
5 IF(ISU-ISL) 99,7,7
7 VAL= IFAS*EXP(.5*(ALOGF(NQ)+ ALOGF(NR)-ALGA(RNL+1.5)-ALGA(RNLP
1 + 1.5))+ ALGA(RLMP-FLOAT(LQ-1))+ALGA(RLMP-FLOAT(LR-1)))
2 FAGA(RLMP-FLOAT(LQ-1))*FAGA(RLMP-FLOAT(LR-1))
SR=0.$ R1=RLMP+1.5$ R2= RLMP-RNLP+1.$ R3= RLMP-RNL+1.
DO 9 IS= ISL,ISU$ RS= IS-1
9 SR= SR+EXP(-ALOGF(RS+1.)-ALOGF(FLOAT(N-IS+2)))-ALOGF(FLOAT(NP-IS
1 +2))+ ALGA(R1+RS)-ALGA(R2+RS)-ALGA(R3+RS))*
2 FAGA(R1+RS)*FAGA(R2+RS)*FAGA(R3+RS)
VAL= VAL*SR
99 RAD1=VAL$ RETURN
100 PRINT 102, NQ,LQ,NR,LR,LAM
102 FORMAT( * BAD CALL TO RAD NQ,LQ,NR,LR,LAM= *5I5,
1 *LOWER LIMITS ARE 1, 0, 1, 0, -1 *)
GO TO 99
END
FUNCTION ALGA(RN)
* TO COMPUTE LOG(ABS(GAMMA(RN))) , USING /ALGFN/ WHICH MUST HAVE
* BEEN FRESET TO LOG(GAMMA(N)) .
* RN MUST BE + K/2 OR -(K+.5)
* THE ENTRY FAGA RETURNS WITH THE PHASE OF GAMMA(-K-.5) FOR K
* NEGATIVE .
* NONSENSE MAY BE RETURNED IF RN.NE. 2*K .
* IF RN=-N,N=0,1,... ALGA= LOG(ABS(RESIDUE AT THE POLE)),
* FAGA= SIGN(RESIDUE)
*
COMMON /CLEBDAT/ALOGF(30),SQRF(30)
DATA AL2/0.6931 47180 55994/,ALRP/0.5723 64942 92470/
*
ITN= INT(RN+ RN)$ IF(ITN) 1,3,5
3 ALGA= -ALOGF(IFIX(-RN)+1)
17 RETURN
5 IF(MOD(ITN,2)) 9,7
7 ALGA= ALOGF(IFIX(RN))$ RETURN

```

```

9  IF(ITN-1) 13,11
11  ALGA= ALRP$ RETURN
13  ALGA= ALRP+ ALOGF(ITN-1)- AL2*(ITN-2)-ALOGF(IFIX(RN-.5))$RETURN
1  IF(MOD(ITN,2)) 15,3
15  ALGA= ALRP-AL2*ITN+ ALOGF(IFIX(.5-RN))-ALOGF(1-ITN)$RETURN
ENTRY FAGA$ ALGA=1$ IF(RN) 19,17,17
19  ALGA= 1-2*MOD(IFIX(.5-RN),2)$ RETURN
END
FUNCTION CLEBSCH(VJ1,VJ2,VM1,VM2,VJ3)
*
* TO COMPUTE C(J1,J2,J3/M1,M2) . A CLEBSCH-GORDAN COEFFICIENT
* USING THE FORMULA OF SCHWINGER(REF. QUANTUM THEORY OF ANG. MOM.,
* BY HIEDENHARN,P246), AND THE REGGE SYMMETRIES(REF. IBID,P.296) .
* COMMON /CLEORD/ ZN(1),VN(3,3),NR(1),NN(3,3)
* COMMON /CLEQUAT/ALOGF(30),SQRF(30)
*
* PREPARE THE REAL REGGE Q.N. IN VN(I,J) .
301 RES= 0.$ ZN(2)= VJ1-VJ3+VJ2$ ZN(6)= VJ1-VM1$ ZN(7)= VJ1+VM1
ZN(9)= VJ2-VM2$ ZN(10)= VJ2+VM2$ RJ= VJ1+VJ2+VJ3
ZN(3)= RJ-ZN(6)-ZN(9)$ ZN(4)= RJ-ZN(7)-ZN(10)
ZN(5)= RJ-ZN(6)-ZN(7)$ ZN(8)= RJ-ZN(9)-ZN(10)$ JJ= MOD(INT(RJ),2)
*
* CHECK THAT THEY ARE NON-NEG. INTEGERS AND FIND NZE.
NZE= 101$ DO 1 I = 1 , 3$ DO 1 J = 1 , 3$ NT= IABS(INT(VN(I,J)))
IF(FLOAT(NT)-NE.VN(I,J)) GO TO 99$ IF(NT.GE.NZE) GO TO 1
NZE= NT$ IZE= 1$ JZE= J
1  NN(I,J)= NT$ IFSE= NR(7)+ NR(9)
*
* C-G EXISTS, BRING NZE TO NN(1,1) POSITION, SAVE THE PHASE .
IF(IZE.EQ.1) GO TO 3$ IF(JJ.NE.0) IFSE= IFSE+1$ DO 5 J = 1 , 3
NT= NN(1,J)$ NN(1,J)= NN(IZE,J)
5  NN(IZE,J)= NT
3  IF(JZE.EQ.1) GO TO 7$ IF(JJ.NE.0) IFSE=IFSE+1$ DO 9 I = 1 , 3
NT= NN(I,1)$ NN(I,1)= NN(I,JZE)
9  NN(I,JZE)= NT
*
* CONSTRUCT DELTA-NORMALISATION .
7  IFAS= 1-2*MOD(IFSE+NR(3)+NR(5),2)
SUM= -ALOGF(INT(RJ)+2)$ DO 11 K = 2 , 10
11  SUM= SUM+ ALOGF(NR(K)+1)$ SUM= .5*SUM
*
* DO THE SUM WITHOUT ALOGF .
SUM= SUM-ALOGF(NR(2)+1)- ALOGF(NR(6)+1)- ALOGF(NR(10)+1)
1  -ALOGF(NR(9)-NR(2)+1)- ALOGF(NR(7)-NR(2)+1) $ PROD= EXP(SUM)
SUM= 1.$ NMX= NR(2)$ IF(NMX.LT.1) GO TO 13
ZA= NR(6)- NMX$ ZB= NR(10)-NMX$ ZC= NMX+1$ ZD= NR(9)+1
ZE= NR(7)+1$ DO 15 K = 1 , NMX$ ZK= K
15  SUM=1.-SUM*ZK*(ZA+ZK)*(ZB+ZK)/((ZC-ZK)*(ZD-ZK)*(ZE-ZK))
13  RES= SUM*PROD*IFAS*SQRT(2.*VJ3+1.)
99  CLEBSCH= RES$ RETURN
END
END EVALIN

```

BLOCK DATA EVAPREP

```

C
C THE SHELL STRUCTURE IS 0S1/2,0P3/2,/P1/2,0D5/2,1S1/2,
C 0D3/2,0F7/2,1P3/2,0F5/2,1P1/2,0G9/2,1D5/2,0G7/2,2S1/2,
C 1D3/2,0H11/2,0H9/2,1F7/2,1F5/2,2P3/2,2P1/2,0I13/2,1G9/2,
C 0I11/2,2D5/2,3S1/2,1G7/2,2D3/2,0J15/2,0J13/2.
C

```

```

COMMON/SHELL/NX(30),Lx(30),XJx(30)
COMMON/UPLOWA/IMIN,IMAX,I1MIN,I1MAX,I2MIN,I2MAX,I3MIN,I3MAX,

```

```

1I4MIN,I4MAX,JMIN,JMAX,ICODE
COMMON/NUMB/NUM,NUMIN,IPARITY
COMMON/IPRI/ IPRINT$ LOGICAL IPRINT
COMMON /TCON/NAME,HBWA(30),IUNIT(30),IADV(30)

```

```

* DATA NAME,HBWA/10H234-016.6L ,13.5,10.5,13.5,10.5,0/
* DATA IUNIT/30*5/
* DATA IADV/30*1/
* DATA NAME,HBWA/10H021SP2,6LV,13.5,17.5,20.0,10.5,25.0,8.0,30.0,
DATA NAME,HBWA/10H020SP2,16L,13.5,17.5,20.0,10.5,25.0,8.0,30.0,
1 15.0,0.00/
DATA IUNIT/5,7*6/
DATA IADV/3,7*1/

```

234-016
234-016

```

* DATA NX,LX,XJX/
1 4*0,1,2*0,1,0,1,0,1,0,2,0,1,0,1,0,2,1,2,0,1,0,2,1,3,2,0,
20,2*1,2,0,2,3,1,3,1,4,2,4,0,5,2,5,3,6,1,3,1,6,4,7,2,4,0,2,7,
30,5,1,5,0,5,2,5,0,5,1,5,3,5,1,5,2,5,0,5,4,5,2,5,3,5,0,5,5,5,
41,5,4,5,3,5,6,5,1,5,2,5,0,5,5,5,4,5,7,5,2,5,3,5,0,5,1,5,6,5,

```

```

C ICODE=0, NO GA PRINTOUT. ICODE=2, FOR GA MATR. PRINTOUT.
DATA IMAX,ICODE/16,2/

```

```

* DATA NUM,NUMIN,IPARITY/0,0,1/

```

```

* DATA IPRINT/.T./
END

```

```

PROGRAM EVAFME(OUTPUT,TAPE1,TAPE2,TAPE5,TAPE9=1,TAPE6)
DIMENSION GA(15000),MAGIC(8),ICODE(16),GPH(2),FCL(5),TLINT(150)
COMMON /TCON/NAME,HBWA(30),IUNIT(30),IADV(30)
COMMON/SHELL/NX(30),LX(30),XJX(30)
COMMON/UPLOWA/IMIN,IMAX,I1MIN,I1MAX,I2MIN,I2MAX,I3MIN,I3MAX,
1I4MIN,I4MAX,JMIN,JMAX,IPUNCH
COMMON/LBL3/IPH(30,30),IJTV(10,2),IIP(100),IIH(100)
COMMON/LBL4/IPMIN,IPMAX,IHMIN,IHMAX,IPHD,IJTD,JJMAX
COMMON/MOSHTN/ NOEN,TABM(1000),NQMS(1000)
COMMON/IPRI/ IPRINT$ LOGICAL IPRINT
COMMON/NUMB/NUM,NUMIN,IPARITY
COMMON/PHGCON/NMAXP,NOENP,IPASS$ LOGICAL IPASS
DATA MAGIC,MAG/2,8,20,28,40,50,82,126,9/
DATA NTYP/2/
CALL ERRSET(IERROR,50)
REWIND 2$ REWIND 5$ REWIND 6
PRINT 101

```

```

101 FORMAT(1HR)
IPMIN=IHMIN=I1MIN=I2MIN=I3MIN=I4MIN=IMIN=1
IPMAX=IHMAX=I1MAX=I2MAX=I3MAX=I4MAX=NV=IMAX
J1P1=1$ DO 21 KP= 1 , NV$ K= KP+IMIN-1

```

```

21 J1P1= MAX0(J1P1,IFIX(2.*XJX(K))+1)
CALL TALMI(TLINT,NTYP)
PRINT1

```

```

1 FORMAT(1H0,5X,45H*****SHELL STRUCTURE*****
1//18X,*N*,7X,*L*,7X,*J*,5X,*NOSC=2N+L */)
DO 3 I=1,30
J=31-I
NOSC=2*NX(J)+LX(J)

```

```

IF (J.NE.22.AND.J.NE.16.AND.J.NE.11.AND.J.NE.10.AND.J.NE.7
1.AND.J.NE.6.AND.J.NE.3.AND.J.NE.1) GO TO 3

```

```

MAG=MAG-1
PRINT2,MAGIC(MAG)

```

```

2 FORMAT(18X,38H***** ,I3)
3 PRINT1002,J,NX(J),LX(J),XJX(J),NOSC

```

```

1002 FORMAT(5X,I2,I12,I8,F9.1,I10)
1003 FORMAT(8X,0I2,5E20.10,I2)
      DO 49 IBL= 1 , 31$ IF (IBL.EQ.1) GO TO 23$ IBL= IBL-1$ WH=H8WA(IB)
      NMAXP=NUENP=0$ IPASS= .F.
      IF (WH.EQ.0) GO TO 99$ CALL PREPSA(IADV(IB),0,IUNIT(IB))
23    REWIND 1$ WRITE(1,1010) NAME
1010  FORMAT(A10)
      IF (IBL.GT.1) CALL LABELF(5,GA)
      JF=JG=F3=F4=F5=IFAS= 0$ F1=F2=NV
      PRINT1003,JF,F1,F2,F3,F4,F5,IFAS
      WRITE(1,1003)JF,F1,F2,F3,F4,F5,IFAS
      DO 7 KP = 1 , NV$ K = KP+IMIN-1$ F1=F2=K$ F3=F4=F5= 0.
      ICODE(KP)= K
      PRINT1003,JF,F1,F2,F3,F4,F5,IFAS
      WRITE(1,1003)JF,F1,F2,F3,F4,F5,IFAS
7    CONTINUE
      IFL= NV+2
      IPI= 1$ DO 4 J1= 1 , J1P1$ J= J1-1$ VJ= J$CALL LABEL3(IPI,J,IDM,1)
      PRINT 1007$ ICNT= 0
1007  FORMAT (/// * THE FIRST 100 F MATRIX ELEMENTS FOR THIS J.*/)
      F1=F2=64*J+IDM$ F3=F4=F5=JF=0
      PRINT1003,JF,F1,F2,F3,F4,F5,IFAS
      WRITE(1,1003)JF,F1,F2,F3,F4,F5,IFAS
      IFL= IFL+1$ IF (IDM.LT.1) GO TO 4
      DO 5 M=1,IDM
        IC=IIP(M)
        ID=IIH(M)
      DO 5 N=M,IDM
        IA=IIP(N)
        IB=IIH(N)
*      JF=ID+64*(IC+64*(IB+64*(IA +64*64*J)))
*      JF=ID+64*(IC+64*(IB+64*(IA+128+64*64*J)))
*      IF (MOD(LX(IA)+LX(IB)+LX(IC)+LX(ID),2))12,11,12
12    F1=F2=0.$ GO TO 13
*    F1= FS, F2= FD, F3= FCS,
11    IF (IBL.EQ.1) GO TO 111
      CALL PHGPHC(IA,IB,IC,ID,J,GPH,GA)$ F1= .5*(GPH(1)-GPH(2))
      F2= .5*(GPH(1)+GPH(2))$ F3=F4=F5=IFAS=0.$ GO TO 13
111  F1=F2=0.
      CALL FMTRX1(IA,IB,IC,ID,J,TLINT,FCL,NTYP,IFAS)
      F3= FCL(3)$ F4= FCL(4)$ F5= FCL(2)
*      F3=FCL(3)*E2B$ F4=FCL(4)$ F5=FCL(2)
*      FCL(1) IS COUL DIRECT, FCL(3) IS COUL DRCT-EXCH,
*      FCL(2) IS R**2 DRCT, FCL(4) IS R**2 DRCT-EXCH.
*      E2B=SQRT(.0241145*WH)*1.44
13    ICNT= ICNT+1$ IF (ICNT.LT.101,A,IPRINT)
1    PRINT1003,JF,F1,F2,F3,F4,F5,IFAS
15  WRITE(1,1003)JF,F1,F2,F3,F4,F5,IFAS
      IFL= IFL+1
5    CONTINUE
4    CONTINUE
      ENDFILE 1
      IFL= IFL-1
      PRINT 1011, IFL
1011  FORMAT (/// * NUMBER OF F MATRIX ELEMENTS COMPUTED*16)
      PRINT2004,NOEN
2004  FORMAT (/// * NUMBER OF TALMAN COEFF. TABULATED=*15///)
      CALL REDFA12(GA,NV,ICODE,NAME,IFL,15000,NUM,WH,IBL)
49  CONTINUE
99  ENDFILE 2
      REWIND 2$ REWIND 5$ REWIND 6
      PRINT 777, IERROR

```

T=0
N=N

E**2/B

```

777 FORMAT(* NUMBER OF INPUT ERRORS= *I3)
END
SUBROUTINE TALMI(TLINT,N)
DIMENSION TLINT(1)
      TLINT(1)=SQRT(2./3.141592653)
      TLINT(31)=3.$          TLINT(61)=1./SQRT(8.)
DO 1 I=2,30$ XI=I-1$ TLINT(I)=XI*TLINT(I-1)/(XI+.5)
      TLINT(30+I)=(XI+1.5)*TLINT(29+I)/(XI+.5)
      TLINT(60+I)=TLINT(59+I)/2.
1 CONTINUE$ NN=N*30$ PRINT1006,(TLINT(I),I=1,NN)$ RETURN
1006 FORMAT(/* TALMI INTEGRALS*//IP(E17.5,9E12.5))
END
SUBROUTINE PPMEXT(J1,J2,J3,J4,KJ,KT,GGG,IPR)
*
* TO OBTAIN FROM MASS STORAGE PREPARED BY PREPSA, THE MATRIX
* ELEMENTS(J1,J2,KJ,KT/ GGG/ J3,J4,KJ,KT) .
* THE SAUNIER MES ARE UNNORMALISED AND USE THE BROD. MOSH. PHASE .
COMMON /SHELL/ NX(30),LX(30),XJX(30)
COMMON/TMP/ IQNA(250),ZA(250),IDIM,IDIM2
COMMON /INDN/ INDEX(71),IFIRS(71),IMS
DATA ICBL/0/
GGT=0.$ IFAS= IABS(LX(J1) + LX(J2) - LX(J3) - LX(J4))/2
IA= MAX0(J1,J2)$ IB= MAX0(J3,J4)$ IF(IA- IB) 20,11,10
11 IA= MIN0(J1,J2)$ IB= MIN0(J3,J4)$ IF(IA-IB) 20,10,10
20 I1= J3$ I2= J4$ I3= J1$ I4= J2$ GO TO 15
10 I1= J1$ I2= J2$ I3= J3$ I4= J4
15 IF(I2.LE.I1) GO TO 30
IA= I1$ I1= I2$ I2= IA$ IFAS= IFAS+ IFIX(XJX(I1)+ XJX(I2))+ KJ+ KT
30 IF(I4.LE.I3) GO TO 40
IA= I3$ I3= I4$ I4= IA$ IFAS=IFAS+FIX(XJX(I3)+XJX(I4))+KJ+KT
40 I= I4+ (I3*(I3-1))/2+ ((I2-1)*((I1-1)*I1+ I2))/2
1 + ((I1-1)*I1*(2-I1+ I1*2))/8
IQN= SHIFT(I,5)+ SHIFT(KJ,1)+ KTS IF(IQN.LT.1) GO TO 99
*
* NOW FIND POSITION OF IQN IN BLOCKS .
LM= IMS-1$ DO 50 L = 1 , LM$ IF(IQN.LT.IFIRS(L+1)) GO TO 51
50 CONTINUE $ GO TO 99
51 IF(L.EQ.ICBL) GO TO 52
ICBL= L$ CALL READMS(9,IQNA,IDIM2,L)
52 IR= INB'NS(IQNA,1,IDIM,IQN)$ IF(IR.LT.1) GO TO 99
GGT= (1- 2*MOD(IFAS,2))*ZA(IR)
99 GGG= GGT$ RETURN
END
SUBROUTINE LABEL3(IPARITY,IJ,IDIM,ISYM)

```

```

C
C IF IPARITY = 1, TWO PARTICLE STATES HAVE POSITIVE PARITY,
C IF IPARITY =-1, TWO PARTICLE STATES HAVE NEGATIVE PARITY,
C IF IPARITY = 0, NO RESTRICTION ON PARITY.
C

```

```

COMMON/SHELL/NX(30),LX(30),XJX(30)
COMMON/LBL3/IPH(30,30),IJTV(10,2),IIP(100),IIH(100)
COMMON/LBL4/IPMIN,IPMAX,IHMIN,IHMAX,IPHD,IJTD,JMAX
VJ=IJ
DO 1 I=1,30
DO 1 J=1,30
1 IPH(I,J)=.0
DO 2 I=1,10
DO 2 J=1,2
2 IJTV(I,J)=.0
N=0$ DO 7 I=1,2$ DO 7 IH=IHMIN,IHMAX
IF(MOD(LX(IH),2).NE.I-1)GOTO7$ IPMIN=IPMINS IF(ISYM.EQ.1)GOTO6
IF(IHMIN.EQ.IPMIN.AND.IHMAX.EQ.IPMAX) IPMIN=IH

```

```

6 DO 3 IP=IPMINP,IPMAX
  IF(IJ.LT.0) GOT04
  IF(XJX(IP)+XJX(IH).LT.VJ.OR.ABS(XJX(IP)-XJX(IH)).GT.VJ) GOT03
4 IF(IPARITY.EQ.0) GOT05
  IF((-1)**(LX(IP)+LX(IH)).NE.IPARITY) GOT03
5 N=N+1
  IPH(IP,IH)=N
  IIH(N)=IH
  IIP(N)=IP
3 CONTINUE
7 CONTINUE$ IDIM=N
  IF(IPASS.NE.125394) PRINT1002,((IPH(J,I),J=1,30),I=1,30)
  IPASS=125394
1002 FORMAT(30I3)
  RETURN
  END
  FUNCTION RACAH(A,B,C,D,E,F)
  FUNCTION RACAT(A,B,C,D,E,F)
*
*
* TO COMPUTE RACAH COEFFICIENTS USING THE REGGE SYMMETRIES
* AND TO BUFFER THE PREVIOUSLY COMPUTED VALUES .
  LOGICAL INITIAL
  COMMON/BUFFN/IGN(1000),SIXJT(1000),NOTA,IOVF,IR,ICU
  COMMON /FACLN/FACLO(100)
  COMMON /ORDTRK/ IZ(1),IX1,IX2,IX3,IY1,IY2,IY3,IY4,
1 RV(1),X1,X2,X3,Y1,Y2,Y3,Y4,SIXJ
  DATA INITIAL/.TRUE./,ICU,NOTA/2*0/,IOVF/500/
  SIXJ=0.$ IFAS=0
  X1=A+B+C+D$ X2=A+D+E+F$ X3= B+C+E+F
  Y1= A+B+E$ Y2= C+D+E$ Y3= A+C+F$ Y4= R+D+F
*
* FIRST CHECK FOR ERRORS IN CALLING SEQUENCE
  DO 1 K = 2 , 8
  Z0=RV(K)$ IT= ABS(Z0)$ IF(FLOAT(IT).NE.Z0) GO TO 999
1 IZ(K)= IT
*
* THEN SORT THE REGGE QUANTUM NUMBERS.
  IFAS=IX1$ IT= IX1$ IE=2$ IF(IX1-IX2) 25,23,23
25 IT= IX2$ IE=3
23 IF(IT-IX3) 29,29,27
27 IZ(IE)= IX3$ IX3= IT
29 IF(IX1-IX2) 31,31,33
33 IT= IX1$ IX1=IX2$ IX2= IT
31 IX0= IX1$ IT= IY1$ IE= 5$ IF(IY1-IY2) 35,37,37
35 IT= IY2$ IE= 6
37 IF(IT-IY3) 39,41,41
39 IT= IY3$ IE= 7
41 IF(IT-IY4) 45,45,43
43 IZ(IE)= IY4$ IY4= IT
45 IT= IY1$ IE=5$ IF(IY1-IY2) 47,49,49
47 IT= IY2$ IE=6
49 IF(IT-IY3) 53,53,51
51 IZ(IE)= IY3$ IY3= IT
53 IF(IY1-IY2) 57,57,55
55 IT= IY1$ IY1=IY2$ IY2= IT
57 IY0= IY4
*
* NEXT TEST FOR TRIANGLE CONDITION .
  IF(IX0.LT.IY0) GO TO 999 $ IF(IX0.LT.1) GO TO 997
*
* DO A TABLE SEARCH .
  IQ= IX0-IY0$ DO 59 K= 3 , 8

```

```

59  IQ= SHIFT(IQ,6)+ IZ(K)
    IR= INBINS(IQN,1,NOTA,IQ)$ IF(IR.LT.1) GO TO 61
    SIXJ= SIXJT(IR) $ GO TO 999
*
*    SO, COMPUTE DEL3
61  IF(.NOT.INITIAL) GO TO 3$ INITIAL= .FALSE.$ FACLO(1)= 0.
    DO 5 K= 2 , 100
5   FACLO(K)= FACLO(K-1)+ ALOG(FLOAT(K-1))
3   DEL3=0.$ CN= FACLO(2+IY0)$ DO 7 K= 1 , 4
    DEL3= DEL3- FACLO(2+IZ(K+4))$ CN= CN-FACLO(1+IY0-IZ(K+4))
    DO 7 L= 1 , 3 $ DEL3= DEL3+ FACLO(1+IZ(L+1)- IZ(K+4))
7   CONTINUE
*
*    THEN INITIALISE THE SUM.
    DO 9 I= 2 , 4
9   CN= CN-FACLO(1+IZ(I)-IY0)
    DEL3CN= (1-2*MOD(IY0,2))*EXP(CN+ .5*DEL3)
    SM=1.$ IRAN= IX0-IY0+1$ IF(IRAN.LT.2) GO TO 13
    Z0=IX0+3$ NX0=IX0+1$ X1=IX1-NX0$ X2= IX2-NX0$ X3= IX3-NX0
    NX0= IX0+2$ Y1= NX0-IY1$ Y2= NX0-IY2$ Y3=NX0-IY3$ Y4=NX0-IY4
*
*    THE SUM IS DONE RECURSIVELY WITHOUT FACLO
    DO 15 K= 2 , IRAN$ XK= K
15  SM= 1.-SM*(Z0-XK)*(X1+XK)*(X2+XK)*(X3+XK)/
    1 ((Y1-XK)*(Y2-XK)*(Y3-XK)*(Y4-XK))
*
*    SIXJ IS THE USUAL 6-J SYMBOL OF WIGNER .
13  SIXJ= DEL3CN*SM
*
*    SAVE THIS VALUE IN ICN .
    NOTA= MIN0(NOTA+1,1000)$ ICU= ICU+1$ ICN= NOTA
    IF(NOTA.EQ.1000) ICN= IOVF$ IQN(ICN)= IQ$ SIXJT(ICN)= SIXJ
    CALL SORTAG1(IQN,1,NOTA,SIXJT,ICN)
    GO TO 999
997 SIXJ=1.
999 RACAH= SIXJ*(1-2*MOD(IFAS,2))
*999 RACAT= SIXJ*(1-2*MOD(IFAS,2))
    RETURN
    END
    SUBROUTINE FMTRX1(IA,IB,IC,ID,J,TLINT,FCL,NTYP,IFAS)
*
*    ROUTINE CALCULATES THE ANTI-SYMMETRIZED F-MATRIX ELEMENTS
*    UTILIZING THE SUBROUTINE FMTRX.
*    FCL(I) I=1, ... ,NTYP, STORES THE DIRECT M.E.,
*    FCL(K), K=NTYP+1, ... ,2*NTYP, STORES THE DIRECT MINUS EXCHANGE M.E.
*
    COMMON/SHELL/NX(30),LX(30),XJX(30)
    DIMENSION FCL(1),TLINT(1),FCL1(10)
    VA=XJX(IA)$ VB=XJX(IB)$ VC=XJX(IC)$ VD=XJX(ID)$ VJ=J
    IFAS= 1-2*MOD(NX(IA)+NX(IB)+NX(IC)+NX(ID)+IABS(LX(IA)+LX(ID)
1   -LX(IB)-LX(IC))/2,2)
    JM=AMIN1(VA+VC,VB+VD)+1.$ JN=AMAX1(ABS(VA-VC),ABS(VB-VD))+1.
    JN=JN+MOD(LX(IA)+LX(IC)+JN+1,2)$ I=VA+VDS PH=(-1)**(I+J)
    CALL FMTRX(IA,IB,IC,ID,J,TLINT,FCL,NTYP)$ DO 1 K=1,NTYP
1   FCL(K+NTYP)=FCL(K)
    DO 2 JX=JN,JM,2$ JP=JX-1$ VJP=JP
    X= (VJP+VJP+1.)*(-1)**JP*RACAH(VA,VB,VC,VD,VJ,VJP)
    CALL FMTRX(IA,IC,IB,ID,JP,TLINT,FCL1,NTYP)
    DO 2 K=1,NTYP$ NK=K+NTYP
2   FCL(NK)=FCL(NK)-X*FCL1(K)*PH$ RETURN
    END
    SUBROUTINE FMTRX(I1,I2,I3,I4,J,TLINT,FCL,NTYP)

```

FUNCTION GENERATES THE DIMENSIONLESS TWO BODY MATRIX
ELEMENTS USING TALMANS FORMULEA FOR CENTRAL FORCES.
THE TALMI INTEGRALS ARE NORMALIZED BY THE INTEGRAL
(0,INF.)R**(2M+2)*EXP(-R**2).
THUS RTAL(S1+1,S2+1,L,N+1) IS EQUAL TO TALMANS R-COEFFICIENT
R(S1,S2,L,N) TIMES THE NORMALIZATION FACTOR.
THE EXTERNALS TALMAN AND RACAH ARE NEEDED.
C(N+1,L+1) ARE THE NORMALISATION CONSTANT OF THE OSC. W.F.(N,L)

```

COMMON/SHELL/NX(30),LX(30),XJX(30)
DIMENSION FCL(1),TLINT(1),T(5),S(5)
DIMENSION FAC(30),DFAC(30),C(5,8)
LOGICAL IPASS
DATA IPASS,RTPI/.FALSE.,1.77245385/
      RTAL(N1,N2,L,M)=      -YY*FLOAT((-1)**(N1+N2+M)*(L+L+1))
1      *EXP(DFAC(2*(L+N1+N2-1))+FAC(L+N1+N2-1)-FAC(N1)-FAC(N2))
2      -DFAC(2*(L+N2))-FAC(M)-FAC(L+N1+N2-M)
3      -DFAC(2*(L+N1)))/2.**(N1+N2)
      IF(IPASS)      GOTO2$ FAC(1)=FAC(2)=DFAC(1)=DFAC(2)=0
DO 1 N=3,30$ X1=N-1$ X1=ALOG(X1)$ FAC(N)=X1+FAC(N-1)
1      DFAC(N)=X1+DFAC(N-2)$ RX=SQRT(2./RTPI**3)$ XL=-3
DO 7 L=1,8$ XL=XL+2.$ X=L+L-1$ C(1,L)=RY=RX=SQRT(ABS(XL)/2.)*RX
DO 7 N=2,5$ XN=N-1$ X=X+2.
7      C(N,L)=RY=-SQRT(XN*X/2.)*RY$ YY=4.*RTPI**6$ IPASS=.TRUE.
N= NTP
2      DO 14 I=1,N
14      FCL(I)=0$ IA=I1$ IB=I2$ IC=I3$ ID=I4
      LA=LX(IA)$LB=LX(IB)$LC=LX(IC)$LD=LX(ID)
      IF(MOD(LA+LB+J,2).NE.0.OR.MOD(LC+LD+J,2).NE.0) RETURN
      IF((LA+LB-J)*(IABS(LA-LB)-J).GT.0) RETURN
      IF((LC+LD-J)*(IABS(LC-LD)-J).GT.0) RETURN
      NA=NX(IA)$NB=NX(IB)$NC=NX(IC)$ND=NX(ID)
      I=XJX(I1)-XJX(I3)$ PH=(-1)**(1+(LC+LB-LA-LD)/2)
      N1MAX=(2*(NA+NB)+LA+LB-J)/2+1$N2MAX=(2*(NC+ND)+LC+LD-J)/2+1
      IF(N2MAX-N1MAX)5,5,6
6      K=N1MAX$N1MAX=N2MAX$N2MAX=K$K=LA$LA=LC$LC=K$K=LB$LB=LD$LD=K
      IA=I3$IB=I4$IC=I1$ID=I2$ NA=NX(IA)$ NB=NX(IB)$ NC=NX(IC)$ND=NX(ID)
5      VLA=LA$ VLB=LB$ VLC=LC$ VLD=LD
      VA=XJX(IA)$VB=XJX(IB)$VC=XJX(IC)$VD=XJX(ID)$VJ=J$ DO 9 I=1,N
9      S(I)=0
      DO 11 N1= 1,N1MAX$ C1=TALMAN(NA,LA,NB,LB,N1-1,J)
      DO 11 N2=1,N2MAX$ C2=TALMAN(NC,LC,ND,LD,N2-1,J)*C1$MAX=N1+N2+J-1
      DO 8 I=1,N
8      T(I)=0$ DO 12 M=1,MAX$ MI=-30$ DO 12 I=1,N$ MI=MI+30
12      T(I)=T(I)+RTAL(N1,N2,J,M)*TLINT(MI+M)$ DO 11 I=1,N
11      S(I)=S(I)+C2*T(I)
      X=C(NA+1,LA+1)*C(NB+1,LB+1)*C(NC+1,LC+1)*C(ND+1,LD+1)
1      *SQRT((VA+VA+1.)*(VB+VB+1.)*(VC+VC+1.)*(VD+VD+1.))/(VJ+VJ+1.)
2      *RACAH(VLA,VLB,VA,VB,VJ,.5)*RACAH(VLC,VLD,VC,VD,VJ,.5)*PH
      DO 10 I=1,N
10      FCL(I)=X*S(I)$ RETURN
END
FUNCTION TALMAN(N1,L1,N2,L2,NC,LC)
COMMON/MOSHTN/NDUM,TAB(1000),NAB(1000)
DATA NMAX/0/,NOEN/0/
      TALMAN=0$ IF(MOD(L1+L2+LC,2).NE.0) RETURN
      IF((2*NC*LC).GT.(2*(N1+N2)+L1+L2)) RETURN
      NA=N1$ NB=N2$ LA=L1$ LB=L2$ IF(NA-NB)4,5,5
4      NB=N1$ NA=N2$ LB=L1$ LA=L2
5      IQ=SHIFT(NA,30)+SHIFT(LA,24)+SHIFT(NB,18)+SHIFT(LB,12)

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1      +SHIFT(NC,6)+LC$ IR=INRINS(NAH,1,NOEN,IQ)$ IF(IR)2,2,7
2      Z=TALMAN1(NA,LA,NR,LC)$ TALMAN=Z$ IF(NMAX-1000)1,9,9
1      NMAX=NMAX+1$ NOEN=MAX0(NMAX,NOEN)$ NOUM=NOEN
3      TAB(NMAX)=Z$ NAB(NMAX)=IQ$ CALL SURTAG1(NAB,1,NOEN,TAB,NMAX)
      RETURN
7      TALMAN=TAB(IR)$ RETURN
9      PRINT100$ NMAX=500$ GOTO3
1000  FORMAT(*      TALMAN TABLE IS FULL... LENGTHIS 1000 *)
      END
      FUNCTION TALMAN1(NA,LA,NB,LC)
*
*      THIS IS THE C-COEFFICIENT OF TALMAN(SEE NUCL.PHYS. A141
*      (1970)273, EQ(15)). THE FUNCTION SUBROUTINE CG000(L1,L2,LC)
*      FOR THE 3-J SYMBOLS IS THE ONLY EXTERNAL NEEDED.
*      FAC(N+1) IS THE LOG OF FACTORIAL N.
*      NA IS ASSUMED TO BE GT NH. IF OTHERWISE CALCULATION
*      WILL BE SLOWER BUT RESULT WILL BE CORRECT.
*
      DIMENSION FAC(30),DFAC(30)
      LOGICAL IPASS
      DATA IPASS/,FALSE./
      IF(IPASS)      GOTO2$ FAC(1)=FAC(2)=DFAC(1)=DFAC(2)=0
      DO 1 N=3,30$ X1=N-1$ X1=ALOG(X1)$ FAC(N)=X1+FAC(N-1)
1      DFAC(N)=X1+DFAC(N-2)$ IPASS=.TRUE.
2      NX=LA+LB+LC-2$ NY=(LA+LB-LC)/2-1$ NZ=(LA+LB-LC)/2-NC-1
      S=0$ LAM=LA+LA$ NAA=NA+1$ NBB=NB+1
      DO 6 M=1,NAA$NMIN=MAX0(1,NC-M+1-NY)$LAM=LAM+2$IF(NMIN.GT.NBB)GOTO6
      NS=NY+M$ NT=NZ+M$      NR=NX+M+M+NMIN+NMIN-2
      LBN=LB+LB+NMIN+NMIN-2$ S1=FAC(M)+FAC(NAA-M+1)+DFAC(LAM)
      DO 7 N=NMIN,NBB$LBN=LBN+2$ NR=NR+2
7      S=S+(1-2*1ABS(MOD(M+N,2)))$EXP(DFAC(NH)+FAC(NS+N)
1      - FAC(N)-FAC(NBB-N+1)-DFAC(LRN)-FAC(NT+N)-S1)
6  CONTINUE$ TALMAN1=(-1)**(NA+NB)*(2*LA+1)*(2*LB+1)*2**(NY+1)
1      *CG000(LA,LC)$S$ RETURN
*      1      *CG000(LA,LB,LC)$S
      PRINT8, NA,LA,NB,LC,TALMAN1$ RETURN
8      FORMAT(10X,6I3,E20.10)
      END
      SUBROUTINE SORTAG1(A,II,JJ,TAG,IOUT)
*      THE ELEMENTS A(II) TO A(JJ) ARE ASSUMED IN INCREASING
*      ORDER EXCEPT FOR A(IOUT), WHICH IS TO BE POSITIONED .
*      TAG IS PERMUTED ALONG WITH A .
      DIMENSION A(1), TAG(1)
      INTEGER A
      IO= IOUT, I=II, J= JJ
      IF(J-I-1) 99,1,1
1      IF(IO-I) 99,13,5
5      IF(J-IO) 99,11,9
9      IF(A(IO)-A(IO+1)) 11,99,3
11     IF(A(IO-1)-A(IO)) 99,99,7
7      T= TAG(IO-1)$ TAG(IO-1)= TAG(IO)$ TAG(IO)= T
      IT= A(IO-1)$ A(IO-1)= A(IO)$ A(IO)= IT$ IO= IO-1
      IF(IO-I) 99,99,11
3      T= TAG(IO+1)$ TAG(IO+1)= TAG(IO)$ TAG(IO)= T
      IT= A(IO+1)$ A(IO+1)= A(IO)$ A(IO)= IT$ IO= IO+1
      IF(J-IO) 99,99,13
13     IF(A(IO)-A(IO+1)) 99,99,3
99     RETURN
      END
      FUNCTION CG000(IA,IB,IC)
C      SUBROUTINE TO CALCULATE THE 3-J SYMBOL (A,B,C/0,0,0)
C      THE TRIANGULAR INEQUALITIES ARE ALREADY SATISFIED.

```

```

C      ALSO (-1)**(A+B+C)=+1 HAS BEEN SATISFIED.
      DIMENSION FL(130)
      DATA IPASS/0/
      IF(1PASS.EQ.1) GOTO25 FL(1)=0$DO1 K=2,130$ A=K-1
1  FL(K)=FL(K-1)+ALOG(A)$ IPASS=1
2  CG000=.0
      IF(IC.GT.(IA+IB).OR.IC.LT.IABS(IA-IB)) RETURN
      IF((-1)**(IA+IB+IC).NE.1) RETURN
      IAB=IA+IB
40  IG2=IAB+IC
      IG2P=IG2+2
      IG=IG2/2
      ICP=IC+1
      IACMBP=IA-IB+ICP
      IBCMAP=IB-IA+ICP
      IABMCP=IAB-IC+1
70  IGP 1=IG+1
      IGMAP1=IGP1-IA
      IGMRP1=IGP1-IB
      IGMCP1=IGP1-IC
      IGD2=IG/2
      NSIG=IG-IGD2-IGD2
      SIG=1-NSIG-NSIG
      X=FL(IGP1)-FL(IGMAP1)-FL(IGMBP1)-FL(IGMCP1)
      DLG=.5*(FL(IACMBP)+FL(BCMAP)+FL(IABMCP)-FL(IG2P))
      YLG=X+DLG
      Y=EXP(YLG)
      TJ=SIG*Y
      CG000=TJ
      RETURN
      END
      SUBROUTINE PREPSA(1BLK,IREW,KU)
*
*      TO PREPARE THE SAUNIER TAPE FOR USE BY PPMEX .
*
*      IF(IREW.EQ.0) DO NOT REWIND 5 ....
      COMMON/TEMP/ IQNA(250),ZA(250),IDIM,IDIM2
      COMMON /INDN/ INDEX(71),IFIRS(71),IMS
      DIMENSION Z(5),IRCT(8)
      LOGICAL INITIAL
      DATA IRC,IRCT/0,17661,17662,17663,17744,17745,17750,17761,17762/
      DATA INITIAL /.T./
      DATA IDIM,IDIM2/250,500/
      IF(IREW.NE.0) REWIND KU
      IMS= 1LA= 1LB= 1 $ IB= 1BLK-1$ IF(.NOT.INITIAL) GO TO 11
      INITIAL= .F.$ CALL OPENMS(9,INDEX,71,0)
11  IF(IB.LT.1) GO TO 5$ DO 1 K = 1 , IB$ DO 1 L = 1 , 8364
1   READ(KU,102) IDUMP
102  FORMAT(I6)
*
*      TAPE IS NOW POSITIONED AT CORREXT BLOCK .
5   DO 7 L = 1 , IDIM2
7   IQNA(L)= 0
      DO 3 L = 1 , 8364$ IF(KU.EQ.6) IRC= IRC+1
30  READ(KU,1013) I1,I2,I3,I4,J,(Z(K),K=1,5)
      DO 201 JC= 1 , 8$ IF(IRC.NE.IRCT(JC)) GO TO 201
      PRINT 1015,I1,I2,I3,I4,J,(Z(K),K=1,5),IRC
201  CONTINUE
1015 FORMAT(1X5I2,5E14.6,I5/)
1013 FORMAT(5I2,5E14.6)
      I= I4+ (I3*(I3-1))/2+ ((I2-1)*((I1-1)*I1+ I2))/2
      1 + ((I1-1)*I1*(2-I1+ I1**2))/8
      IQN= SHIFT(I,5)+ SHIFT(J,1)

```

```

DO 3 IT= 1 , 2$ IF(Z(IT).EQ.0.) GO TO 3
IQNA(ILB)= IQN+ IT-1$ ZA(ILB)= Z(IT)$ ILB= 1LB+1
IF(1LB.GT.IDIM.OR.( L .GE.8364.AND.IT.EQ.2)) GO TO 150
3 CONTINUE$ IMS= IMS-1$ RETURN
150 IFIRS(IMB)= IQNA(1)$ CALL WRITMS(9,IQNA,IDIM2,IMS)
IMS= IMS+1$ ILB=1$ DO 9 LT= 1 , IDIM2
9 IQNA(LT)=0$ GO TO 3
END
SURROUTINE LABELF(M,GA)

C
C ROUTINE PUTS TWO PARTICLE M.E.S (IA,IB,2J,2TIGIIC,1D,2J,2T)
C INTO A ONE-DIMENSIONAL ARRAY.
C IF M=0, M.E.S ARE READ IN ON DATA CARDS,
C IF M=2, M.E.S ARE CALCULATED BY CALLING PPME.
C THE GENERAL RULE OF THE ORDER OF THE INPUT M.E.S IS
C IB.GE.IA.AND.ID.GE.IC. IN PARTICULAR IF THE INPUT ARE
C PPME TO BE CONVERTED TO PHME. THEN IN ADDITION WE HAVE
C IC.GE.IA, AND ID.GE.IB IFF IC.EQ.IA.
C

COMMON/SHELL/NX(30),LX(30),XJX(30)
LOGICAL IABCD,IPAULI,I12,I34
COMMON/LBL5/IA,IB,IC,ID,JJ2,JT2,N,IP2
COMMON/UPLWA/IMIN,IMAX,I1MIN,I1MAX,I2MIN,I2MAX,I3MIN,I3MAX,
I4MIN,I4MAX,JMIN,JMAX,ICODE
COMMON/NUMB/NUM,NUMIN,IPARITY
DIMENSION I12(200),GA(1)
COMMON/GMTRXB/GB(32)
LOGICAL IPRINT,IWRITE
PRINT 105,M$ ICNT= 0
ENTRY LABELC
ENTRY LABELD
ENTRY LABELF

105 FORMAT(//* THE FIRST 200 G MAT ELEM OBTAINED BY LABELING ROUTINE,M
1=*I3//)
IPRINT=ICODE.EQ.2.OR.ICODE.GE.4$ IWRITE=ICODE.EQ.3.OR.ICODE.GE.4
IQAB=SHIFT(IA,6)+IB$ IQCD=SHIFT(IC,6)+ID
IQABCD=SHIFT(IQAB,12)+IQCD$ DO 25 K=1,32
25 GB(K)=0$ N=NUMIN$ K2=I2MAX-I2MIN+1$ K0=-K2
DO 24 I1=I1MIN,I1MAX$ K0=K0+K2$ I11=I1-I2MIN-1
IF(I11.LE.0) I11=0$ K1=(I11*(I11+1))/2$ I2MN=MAX0(I1,I2MIN)
DO 24 I2=I2MN,I2MAX$ IQ12=SHIFT(I1,6)+I2$ L12=LX(I1)+LX(I2)
IMN=K0-K1+I2-I2MN+1
V1=XJX(I1)$ V2=XJX(I2)$ J12=V1+V2$ J21=ABS(V1-V2)$ I12=I1.EQ.I2
IF(M.NE.1) GOTO103$ IF(IQAB-IQ12)24,50,24
50 N=I12(IMN)$ GOTO104
103 I12(IMN)=N
104 DO 22 I3=I1,I3MAX$ IF(I3-I1) 34,12,11
12 I4=MAX0(I2,I4MIN)$ GOTO10
11 I4MN=MAX0(I3,I4MIN)
10 DO 22 I4=I4MN, I4MAX$ IQ34=SHIFT(I3,6)+I4$ L34=LX(I3)+LX(I4)
IF(MOD(L12-L34,2)) 22,26,22
26 V3=XJX(I3)$ V4=XJX(I4)$ J34=V3+V4$ J43=ABS(V3-V4)$ I34=I3.EQ.I4
J2MAX=MIN0(J12,J34)+1$ J2MIN=MAX0(J21,J43)+1
IF(J2MAX-J2MIN)22,13,13
13 IQ1234=SHIFT(IQ12,12)+IQ34$ IABCD=IQ1234.EQ.IQABCD
DO 23 IT1=1,2$ KT=IT1-1$ KJT=KT+16$ IT2=2*KT
DO 23 JJ1=J2MIN,J2MAX$ KJT=KJT+1$ J=JJ1-1$ IJ2=2*J
IPAULI=MOD(J+KT,2).EQ.0
IF(I12.AND.IPAULI)GOTO23$ IF(I34.AND.IPAULI)GOTO23
N=N+1$ IF(M.EQ.2)GOTO4$ IF(M.EQ.0)GOTO2$ IF(M.EQ.3) GOTO23
IF(M.EQ.5) GO TO 501
IF(IABCD.AND.M.EQ.1) 102,23,102,23

```

```

4 CALL PPME(I1,I2,I3,I4,J,KT,GGG,0)
*   THE TIME-REVERSAL PHASE IS IN PPME.
504 ICNT= ICNT+1$ IF(ICNT.LT.201.A.IPRINT)
1 PRINT5000,N,I1,I2,I3,I4,J,KT,GGG
  IF(IWRITE) WRITE(8,5000)N,I1,I2,I3,I4,J,KT,GGG
  GOT01
2 READ(8,5000)NN,IA,IB,IC,ID,J,KT,GGG
  JJ2=J*2$ JT2=KT*2
  IQABCD=ID+SHIFT(IC,6)+SHIFT(IB,12)+SHIFT(IA,18)
  JNJ2=IQABCD+SHIFT(JJ2,24)+SHIFT(JT2,30)
  INJ2=IQ1234+SHIFT(IJ2,24)+SHIFT(I12,30)
C 2 READ 5000, NN,IA,IB,IC,ID,JJ2,JT2,GGG,JP1
5000 FORMAT(15,5X,6I5,5X,E20.8,15)
  IF(NN.NE.N.OR.INJ2.NE.JNJ2) GOT034
1 GA(N-NUMIN)=GGG
  GOT023
102 IF(JJ2-IJ2) 41,42,41
42 IF(JT2-IT2) 41,33,41
41 GB(KJT)=GA(N-NUMIN)
23 CONTINUE
  IF(IABCD.AND.M.EQ.1) RETURN
22 CONTINUE
24 CONTINUE$ IF(M-1)27,28,27
28 N=0$ RETURN
27 NUM=N$ IF(IWRITE) ENDFILE8$ RETURN
34 PRINT2000,N,I1,I2,I3,I4,IJ2,IT2,NN,IA,IB,IC,ID,JJ2,JT2
  RETURN
2000 FORMAT(2X,49H***** ERROR IN CARD INPUT *****/
15X,14I5)
33 GB(KJT)=GA(N-NUMIN)$ RETURN
501 CALL PPME(I1,I2,I3,I4,J,KT,GGG,n)$ GO TO 504
END
SUBROUTINE REDFA12(AL1,NOLV,CODA,FLNAME,IDF,IDM,IDG,HBOM,IBL)
*
* READ FROM SCRATCH TAPE1, INTO TAPE2 THE 7 ARRAYS .
* LOOK FOR FLNAME, THEN READ TO ENDFILE MARK.
* NOLV= F(1)= NUMBER OF LEVELS .
* CODA(NOLV)= CODENUMBER ARRAY= F(2,...,NOLV+2) .
* IDF= NUMBER OF F ELEMENTS READ .
* IDM= DIM OF F ARRAY .
* WRITE ON 2 OUT OF TA FLNAME,NOLV,CODA(16),IDF,IDG,HBOM.
*
  DIMENSION AL1(1),CODA(1),NAA(7),FT(5)
  DIMENSION TA(25)
  INTEGER CODA
  DATA NAA/3LFPR,3LFNE,3LFDN,3LRIS,3LRID,3LPTS,3LPTD/
  REWIND 1
  TA(1)= FLNAME$ TA(2)= NOLV$ DO 7 K = 1 , NOLV
7 TA(K+2)= CODA(K)
  TA(21)= IDF$ TA(22)= IDG$ TA(23)= HBOM
  WRITE(2) TA $ PRINT 107, TA
107 FORMAT(//# TA CONTROL 3LOCK//IP5(5E20.6//))
  IF(IBL.GT.1) WRITE(2)(AL1(I),I=1,IDG)
  DO 1 L = 1 , 7$IF((IBL.EQ.1.A.L.LT.3).OR.(IBL.GT.1.A.L.GT.2))GOTO1
  READ(1,1010) TITLES IDF=0
1010 FORMAT (A10)
  IF(TITLE.NE.FLNAME) GO TO 101
  READ(1,1003) JF,FT,IPH$ IF(FT(1).LT.1) GO TO 101
1003 FORMAT(8X,012,5E20.10,12)
  NOLV= FT(1)$ IFL=2$ AL1(1)= FT(L)$ IF(L.GT.5) AL1(1)=FT(L-2)
  DO 31 K = 1 , NOLV$ READ(1,1003) IFD,FT,IPH
  CODA(K)= FT(1)$ AL1(IFL)= FT(L) $ IF(L.GT.5)AL1(IFL)=FT(L-2)

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```

31 IFL= IFL+1
33 IF(IFL.GT.IDM) GO TO 101$ READ(1,1003) IFD,FT,IPH
   AL1(IFL)= FT(L)$IF(L.GT.5) AL1(IFL)= IPH*FT(L-2)
5   IFL= IFL+1$ IF(EOF(1)) 35,33
35 IDF= IFL-2
   REWIND 1
   WRITE(2)(AL1(I),I=1,IDF)
1   CONTINUE
105 RETURN
101 PRINT 103
103 FORMAT (/* F ARRAY NOT ON TAPE1 */)
   GO TO 105
END
SUBROUTINE PHGPHD(IU,IV,IW,IX,J,GPH,GA)
*
*   CALCULATES THE F-MATRIX ELEMENT F(A,B,C,D,J) FROM THE FORMULA
*   
$$F(A,B,C,D,J,T) = -\text{SUM}(JP) (.5*(2*JP+1)*\text{RACAH}(A,D,B,C,JP,J)*$$

*   
$$(-G(0)+3*G(1))*D(T,0) + (G(0)+G(1)))$$

*   WHERE G(T) IS THE G-MATRIX G(D,A,B,C,JP,T),
*   AND D(T,TP) IS THE KRONEKER DELTA-FUNCTION.
*   GPH(T+1)=F(A,B,C,D,J,T)
*
COMMON/SHELL/NX(30),LX(30),XJX(30)
COMMON/PHGCON/NMAX ,NOEN ,IPASS
DIMENSION GA(1),GPH(1),GX(2),TAB(200,2),NAB(200)
COMMON/GMTRXB/GB(32)$ INTEGER TAG(200)$ LOGICAL IPASS
COMMON/LBL5/IP,IQ,IR,IS,JJ2,JDUM,N,IDUM
DATA NMAX,NOEN/0,0/,IPASS/.F./
ENTRY PHGPHC
IF(IPASS)GOTO3$ DO 4 I=1,200
4   TAG(I)=I $ IPASS=.T.
3   IF(IU-IV)30,31,31
30  IA=IV$ IB=IU$ IC=IX$ ID=IW$ FAT=1$ IF(IA-IC)33,32,32
31  IA=IU$ IB=IV$ IC=IW$ ID=IX$ FAT=0$ IF(IA-IC)33,32,32
33  II=IA$ IA=IC$ IC=II$ II=IB$ IB=ID$ ID=II
32  II=SHIFT(J,24)+SHIFT(IA,18)+SHIFT(IB,12)+SHIFT(IC,6)+ID
   VC=XJX(IC)$ VD=XJX(ID)$ VJ=J$ VA=XJX(IA)$ VB=XJX(IB)
   IFAT=FAT*(VA+VB+VC+VD)$FAT=1-2*MOD(IFAT,2)$ JJ2=-1$GPH(1)=GPH(2)=0
   IF(NOEN.LT.1)GOTO8$ JJ=INBINS(NAB,1,NOEN,II)$ IF(JJ)8,8,17
17  GPH(1)=TAB(TAG(JJ),1)*FAT$ GPH(2)=TAB(TAG(JJ),2)*FAT$ RETURN
8   JAD=VA+VD$ JBC=VB+VC$ JDA=ABS(VA-VD)$ JCB=ABS(VB-VC)$ J2MAX=MIN0(
1JAD,JBC)+1$ J2MIN=MAX0(JDA,JCB)+1$ IF(J2MAX-J2MIN)11,10,10
10  IP=MIN0(IA,ID)$ IQ=MAX0(IA,ID)$ IR=MIN0(IB,IC)$ IS=MAX0(IR,IC)
   IF(IP.GT.IR.OR.(IP.EQ.IR.AND.IQ.GT.IS))6,7
6   JJ=IP$ IP=IR$ IR=JJ$ JJ=IQ$ IQ=IS$ IS=JJ
7   CALL LAHEL(1,GA)$ IF(N) 1,1,12
12  DO 2 J2=J2MIN,J2MAX$ JP=J2-1$ VJP=JP$ DO 5 JT1=1,2$ JT=JT1-1
   IFAS=0$ IF(ID.GT.IA) IFAS=IFAS+JP+JT+JAD
   IF(IB.GT.IC) IFAS=IFAS+JP+JT+JBC$ PH=1-2*MOD(IFAS,2)
5   GX(JT1)=GB(JT*16+J2-J2MIN+1)*PH
   S0=(-GX(1)+3.*GX(2))/2.$ S1=(GX(1)+GX(2))/2.
   XX=RACAH(VA,VD,VB,VC,VJP,VJ)*(VJP+VJP+1.)
   GPH(1)=GPH(1)-XX*S0*FAT
2   GPH(2)=GPH(2)-XX*S1*FAT$ IF(NMAX=200)20,21,21
20  NMAX=NMAX+1$ NOEN=MAX0(NMAX,NOEN)
22  NAB(NMAX)=II$ DO 19 I=1,2
19  TAB(TAG(NMAX),I)=GPH(I)*FAT$ CALL SORTAG1(NAB,1,NOEN,TAG,NMAX)
   RETURN
21  PRINT2002$ NMAX=1$ GOTO22
2002 FORMAT(* MESSAGE FROM PHGPHD. TABLE TAB(200) IS FULL.*)
1   PRINT2001,IA,IB,IC,ID,J
2001 FORMAT(* MESSAGE FROM PHGPHD. G-MATRIX ELEMENTS NEEDED FOR

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```
1THE CONSTRUCTION OF THE F-MATRIX ELEMENT** F(*5I3*) DO NOT  
2EXIST IN THE ARRAY GA OF SUBROUTINE LABELD*)  
11 RETURN  
END
```

APPENDIX II

SAMPLE RESULTS FOR ${}^4\text{He}$

This case was run with the S.P. No. 2 potential, $N = 0-2$, $\hbar\omega = 13.5$ MeV. Only 2 iterations were performed to illustrate the output format.

ELLIPSOIDAL MODIFIED HARMONIC OSCILLATOR COMPUTATION

DEF. PAR. OF POTENTIAL ARE, $BETA = .001000$, $GAMMA = 0.000$

MAJOR SHELL N SPIN-ORBIT STRENGTH CHI LSQR STRENGTH D

0	.0700	0.0000
1	.0700	0.0000
2	.0700	0.0000
3	.0700	.3500
4	.0500	.4500
5	.0500	.4500
6	.0500	.4500

STATE ORDERING ACCORDING TO INCREASING ENERGY EIG. VAL., FOR SUMMING PURPOSES

INCR. ORD.NO. J	1	2	3	4	5	6	7	8	9	10	11	12
NATU. ORD.NO. I	1	2	4	3	5	6	8	10	7	9	13	12
EAV. OF JTH ST.	1.125000	1.839774	1.840226	1.945001	2.554636	2.554910	2.555451	2.625002	2.729664	2.730338	3.122557	3.122734
INCR. ORD.NO. J	13	14	15	16	17	18	19	20	21	22	23	24
NATU. ORD.NO. I	15	19	11	20	16	14	18	17	22	23	25	28
EAV. OF JTH ST.	3.123082	3.123619	3.315088	3.315911	3.367535	3.367887	3.368575	3.420510	3.799455	3.799591	3.799864	3.800272
INCR. ORD.NO. J	25	26	27	28	29	30	31	32	33	34	35	36
NATU. ORD.NO. I	34	27	30	32	24	26	29	33	35	21	31	42
EAV. OF JTH ST.	3.800816	4.006932	4.007358	4.008205	4.024429	4.024659	4.025117	4.025795	4.124944	4.132057	4.133014	4.411872
INCR. ORD.NO. J	37	38	39	40	41	42	43	44	45	46	47	48
NATU. ORD.NO. I	45	40	44	49	54	37	47	50	52	41	39	43
EAV. OF JTH ST.	4.411980	4.412195	4.412518	4.412947	4.413484	4.664320	4.664592	4.665135	4.665948	4.686135	4.687002	4.687335
INCR. ORD.NO. J	49	50	51	52	53	54	55	56	57	58	59	60
NATU. ORD.NO. I	48	53	60	62	68	70	69	75	82	46	38	51
EAV. OF JTH ST.	4.687833	4.688493	5.001798	5.001886	5.002061	5.002324	5.002675	5.003113	5.003638	4.826891	4.828090	4.839319
INCR. ORD.NO. J	61	62	63	64	65	66	67	68	69	70	71	72
NATU. ORD.NO. I	55	56	36	72	71	61	76	83	63	66	65	64
EAV. OF JTH ST.	4.839853	4.840847	4.902523	5.299224	5.299418	5.299806	5.300387	5.301159	5.326751	5.326879	5.327137	5.327522
INCR. ORD.NO. J	73	74	75	76	77	78	79	80	81	82	83	84
NATU. ORD.NO. I	74	81	58	59	79	77	67	73	80	57	84	78
EAV. OF JTH ST.	5.328034	5.328673	5.506713	5.507303	5.508472	5.524201	5.524526	5.525168	5.526112	5.624889	5.631934	5.633208

ENERGY EIG.VAL., JZ AVER. AND MAJOR SHELL Q.N. IN THE NATURAL ORDER(ORDER OF COMPUTATION)

NATU. ORD.NO. I	1	2	3	4	5	6	7	8	9	10	11	12
ENE. OF ITH ST.	1.500000	2.429706	2.640001	2.430294	3.359528	3.359883	3.709547	3.360587	3.710456	3.500002	4.380461	3.995672
JZA. OF ITH ST.	.500000	.500000	.500000	-1.500000	.500000	-1.500000	.500000	2.500000	-1.500000	.500000	.500000	-1.500000
NMSH OF ITH ST.	0	1	1	1	2	2	2	2	2	2	3	3
NATU. ORD.NO. I	13	14	15	16	17	18	19	20	21	22	23	24
ENE. OF ITH ST.	3.995453	4.485854	3.996109	4.485400	4.591010	4.486744	3.996764	4.381538	5.514394	4.849332	4.849499	5.299274

JZA. OF ITH ST.	.50000	-1.50000	2.50000	.50000	.50000	2.50000	-3.50000	-1.50000	.50000	.49999	-1.9996	.50000
NMSH OF ITH ST.	3	3	3	3	3	3	3	3	4	4	4	4
NATU. ORD. NO. I	25	26	27	28	29	30	31	32	33	34	35	36
ENE. OF ITH ST.	4.849833	5.299567	5.264263	4.850333	5.300148	5.264816	5.515678	5.265915	5.301012	4.851000	5.499944	6.555023
JZA. OF ITH ST.	2.49997	-1.50000	.50000	-3.50000	2.50000	-1.50000	-1.50000	2.50000	-3.50000	4.50000	.50000	.50000
NMSH OF ITH ST.	4	4	4	4	4	4	4	4	4	4	4	5
NATU. ORD. NO. I	37	38	39	40	41	42	43	44	45	46	47	48
ENE. OF ITH ST.	6.079131	6.450783	6.124378	5.574635	6.124170	5.514248	6.124794	5.575021	5.574377	6.404197	6.279479	6.125416
JZA. OF ITH ST.	.50000	-1.50000	-1.50000	2.50000	.50000	.50000	2.50000	-3.50000	-1.50000	.50000	-1.50000	-3.50000
NMSH OF ITH ST.	5	5	5	5	5	5	5	5	5	5	5	5
NATU. ORD. NO. I	49	50	51	52	53	54	55	56	57	58	59	60
ENE. OF ITH ST.	5.575536	6.080173	6.429112	6.081212	6.128241	5.574179	6.429801	6.431105	7.499891	7.263973	7.264743	6.254180
JZA. OF ITH ST.	4.50000	2.50000	.50000	-3.50000	4.50000	-5.50000	-1.50000	2.50000	.50000	.50000	-1.50000	.50000
NMSH OF ITH ST.	5	5	5	5	5	5	5	5	6	6	6	6
NATU. ORD. NO. I	61	62	63	64	65	66	67	68	69	70	71	72
ENE. OF ITH ST.	6.849756	6.254283	6.504084	6.905027	6.904556	6.904241	7.299389	6.254488	6.255205	6.254795	6.849269	6.849025
JZA. OF ITH ST.	2.50000	-1.50000	.49999	-3.49999	2.49997	-1.49997	-1.50000	2.50000	4.50000	-3.50000	-1.50000	.50000
NMSH OF ITH ST.	6	6	6	6	6	6	6	6	6	6	6	6
NATU. ORD. NO. I	73	74	75	76	77	78	79	80	81	82	83	84
ENE. OF ITH ST.	7.300215	6.905654	6.255716	6.850487	7.298972	7.515935	7.266273	7.301433	6.906436	6.256330	6.851459	7.514207
JZA. OF ITH ST.	2.50000	4.50000	-5.49999	-3.49999	.50000	-1.50000	2.50000	-3.50000	-5.50000	6.50000	4.50000	.50000
NMSH OF ITH ST.	6	6	6	6	6	6	6	6	6	6	6	6

COMP. OF 1TH L. ORB IN SPIN-CART. DEFORM. BASIS: (MU,NX,NY,NZ) .

UN= (0)
 CT= 1.000000
 EXPANSION COEF. IN [NT,J,K,J-K] SPHERICAL BASIS
 UN= (100) [20201] [20302]
 CT= 1.0000000 -0.001727 -0.002116
 UN= (1) [20102] [20203]
 CT= 1.0000000 -0.001727 -0.002116

TIMEPRT CALLED BY NUHART AT LINE 23, CP TIME= 16.568 SEC, SYSTEM TIME 18.34.56.

HARTREE-FOCK ITERATIONS WITH THE PARAMETER LIST, RONI ROPI FPR FNE FDN SPE
MASS STORAGE ARRAY NAMES, RONI ROPI FPF FNF FDF

ITERATION NO 1 FOR 2 PROTONS AND 2 NEUTRONS, NUCLEUS= HE 4

***** THE LOWEST 0 NEUTRON(S) STATES, ALL COMP. .GT. .003 *****

REMAINING S.P. ORBITS AT ENERGIES(MEV)

-11.30798	-11.30798	15.31936	15.31936	15.32285	15.32285	17.87555	17.87555	24.29343	24.29343
27.13201	27.13201	27.13283	27.13283	27.13447	27.13447	29.14350	29.14350	29.14501	29.14501

***** THE LOWEST 0 PROTON(S) STATES, ALL COMP. .GT. .003 *****

REMAINING S.P. ORBITS AT ENERGIES(MEV)

-10.62198	-10.62198	16.30268	16.30268	16.30618	16.30618	18.85888	18.85888	25.21901	25.21901
28.03887	28.03887	28.03968	28.03968	28.04131	28.04131	30.05036	30.05036	30.05185	30.05185

TOTAL BINDING ENERGY= -21.17943 MEV, TOTAL PROTON POTENTIAL ENERGY= -10.26194 MEV, TOTAL NEUTRON POTENTIAL ENERGY= -10.91749

DELTA PN ENERGY= .65555 MEV, TOTAL ONE-BODY ENERGY= 0.00000 MEV

ITERATION NO 2 FOR 2 PROTONS AND 2 NEUTRONS, NUCLEUS= HE 4

MULTIPOLE ANALYSIS OF NEUTRON(S) H-F POT. V AND DENS. MATR. D, WITH LISTING OF ALL COMPS WITH EN. CONTR. GT .0090

GN= [1010000] [1050000] [5010000] [5050000]
VR= -15.98249 -8.92312 -8.92312 34.49191
VI= 0.00000 0.00000 0.00000 0.00000
DR= 1.39870 .14729 .14729 .01551
DI= 0.00000 0.00000 0.00000 0.00000
FOR MULTIPOL. LAMB= 0, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -12.22419 MEV

FOR MULTIPOL. LAM= 1, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -0.00000 MEV
 FOR MULTIPOL. LAM= 2, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -0.00000 MEV
 FOR MULTIPOL. LAM= 3, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -0.00000 MEV
 FOR MULTIPOL. LAM= 4, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -0.00000 MEV
 FOR MULTIPOL. LAM= 5, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -0.00000 MEV

***** THE LOWEST 14 NEUTRON(S) STATES, ALL COMP. .GT. .003 *****

STATE NO. 1, WITH S.P. EN.= -12.383931 MEV., PAR.= 1, OCCUPIED BY A NEUTRON(S)
 QM (0, 1, -1) (2, 1, -1)
 RM .9855973 .1691094
 IP= 0.000000 0.000000

STATE NO. 2, WITH S.P. EN.= -12.383931 MEV., PAR.= 1, OCCUPIED BY A NEUTRON(S)
 QM (0, 1, 1) (2, 1, 1)
 RM .9855973 .1691094
 IP= 0.000000 0.000000

STATE NO. 3, WITH S.P. EN.= 17.094385 MEV., PAR.= -1, OCCUPIED BY A
 QM (1, 3, -1)
 RM .9999999
 IP= 0.000000

STATE NO. 4, WITH S.P. EN.= 17.094085 MEV., PAR.= -1, OCCUPIED BY A
 QM (1, 3, 1)
 RM .9999999
 IP= 0.000000

STATE NO. 5, WITH S.P. EN.= 17.095684 MEV., PAR.= -1, OCCUPIED BY A
 QM (1, 3, 3)
 RM 1.000000
 IP= 0.000000

STATE NO. 6, WITH S.P. EN.= 17.095684 MEV., PAR.= -1, OCCUPIED BY A
 QM (1, 3, -3)
 RM 1.000000
 IP= 0.000000

STATE NO. 7, WITH S.P. EN.= 20.115797 MEV., PAR.= -1, OCCUPIED BY A
 QM (1, 1, 1)
 RM .9999999
 IP= 0.000000

STATE NO. 8, WITH S.P. EN.= 20.115797 MEV., PAR.= -1, OCCUPIED BY A
 QM (1, 1, -1)
 RM .9999999
 IP= 0.000000

STATE NO. 9, WITH S.P. EN.= 25.472066 MEV., PAR.= 1, OCCUPIED BY A
 QM (0, 1, 1) (2, 1, 1)
 RM -.1691094 .9855973
 IP= 0.000000 0.000000

STATE NO. 10, WITH S.P. EN.= 29.472066 MEV., PAR.= 1, OCCUPIED BY A

QNS (0, 1, -1) (2, 1, -1)
RPS -.1691094 .9855973
IPS 0.0000000 0.0000000

STATE NO. 11, WITH S.P. EN.= 29.200555 MEV., PAR.= 1, OCCUPIED BY A

QNS (2, 3, 1)
RPS 1.0000000
IPS 0.0000000

STATE NO. 12, WITH S.P. EN.= 29.200555 MEV., PAR.= 1, OCCUPIED BY A

QNS (2, 5, -1)
RPS 1.0000000
IPS 0.0000000

STATE NO. 13, WITH S.P. EN.= 29.200912 MEV., PAR.= 1, OCCUPIED BY A

QNS (2, 5, 3)
RPS 1.0000000
IPS 0.0000000

STATE NO. 14, WITH S.P. EN.= 29.200912 MEV., PAR.= 1, OCCUPIED BY A

QNS (2, 5, -3)
RPS 1.0000000
IPS 0.0000000

REMAINING S.P. ORBITS AT ENERGIES (MEV)

29.20162 29.20162 31.40131 31.40131 31.40192 31.40192
WAVEFUNCTION PUNCHED WITH HEADER= HE 4 2 0 NEUTRON(S) 021SP2.6LV 1 13.50 11/09/70 18.35.01.

MULTIPOLE ANALYSIS OF PROTON(S) H-F POT. V AND DENS. MATR. D, WITH LISTING OF ALL COMPS WITH EN. CONTR. GT .0090

QNS (1010000) (1050000) (5010000) (5050000)
VR= -15.03117 -8.76113 -8.76113 35.87213
VF= 0.00000 0.00000 0.00000 0.00000
OR= 1.40001 .14103 .14103 .01421
DI= 0.00000 0.00000 0.00000 0.00000
FOR MULTIPOL. LAM= 0, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -11.50264 MEV
FOR MULTIPOL. LAM= 1, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
FOR MULTIPOL. LAM= 2, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
FOR MULTIPOL. LAM= 3, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
FOR MULTIPOL. LAM= 4, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
FOR MULTIPOL. LAM= 5, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV

***** THE LOWEST 14 PROTON(S) STATES, ALL COMP. .GT. .003 *****

STATE NO. 1, WITH S.P. EN.= -11.66504 MEV., PAR.= 1, OCCUPIED BY A PROTON(S)

QNS (0, 1, -1) (2, 1, -1)
RPS .9862931 .1650030
IPS 0.0000000 0.0000000

STATE NO. 2, WITH S.P. EN.= -11.665048 MEV., PAR.= 1, OCCUPIED BY A PROTON(S)
QN= [0, 1, 1] [2, 1, 1]
RP= .9862931 .1650030
IP= 0.0000000 0.0000000

STATE NO. 3, WITH S.P. EN.= 18.098119 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 3, -1]
RP= .9999999
IP= 0.0000000

STATE NO. 4, WITH S.P. EN.= 18.098119 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 3, 1]
RP= .9999999
IP= 0.0000000

STATE NO. 5, WITH S.P. EN.= 18.099721 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 3, -3]
RP= 1.0000000
IP= 0.0000000

STATE NO. 6, WITH S.P. EN.= 18.099721 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 3, 3]
RP= 1.0000000
IP= 0.0000000

STATE NO. 7, WITH S.P. EN.= 21.113161 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 1, 1]
RP= .9999999
IP= 0.0000000

STATE NO. 8, WITH S.P. EN.= 21.113161 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 1, -1]
RP= .9999999
IP= 0.0000000

STATE NO. 9, WITH S.P. EN.= 26.401832 MEV., PAR.= 1, OCCUPIED BY A
QN= [0, 1, 1] [2, 1, 1]
RP= -.1650030 .9862931
IP= 0.0000000 0.0000000

STATE NO. 10, WITH S.P. EN.= 26.401832 MEV., PAR.= 1, OCCUPIED BY A
QN= [0, 1, -1] [2, 1, -1]
RP= -.1650030 .9862931
IP= 0.0000000 0.0000000

STATE NO. 11, WITH S.P. EN.= 30.128003 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, 1]
RP= 1.0000000
IP= 0.0000000

STATE NO. 12, WITH S.P. EN.= 30.128003 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, -1]
RP= 1.0000000
IP= 0.0000000

STATE NO. 13, WITH S.P. EN.= 30.128354 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, 3]
RP= 1.0000000
IP= 0.0000000

STATE NO. 14, WITH S.P. EN.= 30.128354 MEV., PAR.= 1, OCCUPIED BY A

UN= 12, 5, -3)
 NP= 1.0000000
 IP= 0.0000000

REMAINING S.P. ORBITS AT ENERGIES (MEV)

30.12906 30.12906 32.32431 32.32431 32.32491 32.32491
 WAVEFUNCTION PUNCHED WITH HEADER= HE 4 2 0 PROTON(S) 021SP2,6LV 1 13.50 11/09/70 18.35.02.

TOTAL BINDING ENERGY= -23.72683 MEV, TOTAL PROTON POTENTIAL ENERGY= -11.50264 MEV, TOTAL NEUTRON POTENTIAL ENERGY= -12.22419

DELTAPN ENERGY= .72155 MEV, TOTAL ONE-BODY ENERGY= 0.00000 MEV

COMPUTATION OF EXPECTATION VALUE OF THE 21 SYMPLECTIC BILINEAR OPERATORS, IN DIMENSIONLESS UNITS, OSC. PAR. BSQUARE= 3.081 FERMISO

NAME	PROTON(S)	NEUTRON(S)	NUCLEON(S)
NL1	0.00000	0.00000	0.00000
NL2	0.00000	0.00000	0.00000
NL3	-0.00000	-0.00000	-0.00000
NL4	0.00000	0.00000	0.00000
NL5	0.00000	0.00000	0.00000
NL6	0.00000	0.00000	0.00000
NL7	0.00000	0.00000	0.00000
NL8	0.00000	0.00000	0.00000
NL9	0.00000	0.00000	0.00000
AP4	.00000	.00000	.00000
AP5	-0.00010	-0.00010	-0.00020
AP6	0.00000	0.00000	0.00000
AP7	0.00000	0.00000	0.00000
AP8	0.00000	0.00000	0.00000
AP9	3.10890	3.11439	6.22330
AM4	0.00000	0.00000	0.00000
AM5	-0.00036	-0.00035	-0.00071
AM6	0.00000	0.00000	0.00000
AM7	0.00000	0.00000	0.00000
AM8	0.00000	0.00000	0.00000
AM9	.79727	.81653	1.61380

R.M.S. S.P. RADIUS FOR 2 PROTON(S) = 1.88723 F., BET = .00009, GAM = .00 DEG.

R.M.S. S.P. RADIUS FOR 2 NEUTRON(S) = 1.88160 F., BET = .00009, GAM = .00 DEG.

R.M.S. S.P. RADIUS FOR 4 NUCLEON(S) = 1.88442 F., BET = .00009, GAM = .00 DEG.

***** TOTAL R.M.S. RADIUS W.R.T. C.M.= 1.63195 F., PROTON R.M.S. RADIUS W.R.T. TOTAL C.M.= 1.63358 F. *****

COULOMB ENERGY= .74307 MEV.

HARTREE-FOCK ITERATIONS WITH THE PARAMETER LIST,	RONI	ROPI	FPR	FNE	FDM	SPE
MASS STORAGE ARRAY NAMES,	RON	ROP	FPR	FNE	FDM	KEN

ITERATION NO 1 FOR 2 PROTONS AND 2 NEUTRONS, NUCLEUS= HE 4

MULTIPOLE ANALYSIS OF NEUTRON(S) H-F POT. V AND DENS. MATR. D, WITH LISTING OF ALL COMPS WITH EN. CONTR. GT .0090

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QN= ( 1010000) ( 1050000) ( 5010000) ( 5050000)
VR= -40.87687 -17.87368 -17.87368 -15.67061
VI= 0.00000 0.00000 0.00000 0.00000
DR= 1.37377 .23571 .23571 .04044
DI= 0.00000 0.00000 0.00000 0.00000
FOR MULTIPOL. LAM= 0, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -32.60764 MEV
FOR MULTIPOL. LAM= 1, THE TOTAL CONTRIB. TO THE POT. ENERGY IS .00000 MEV
FOR MULTIPOL. LAM= 2, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
FOR MULTIPOL. LAM= 3, THE TOTAL CONTRIB. TO THE POT. ENERGY IS .00000 MEV
FOR MULTIPOL. LAM= 4, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
FOR MULTIPOL. LAM= 5, THE TOTAL CONTRIB. TO THE POT. ENERGY IS .00000 MEV

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***** THE LOWEST 14 NEUTRON(S) STATES, ALL COMP. .GT. .003 *****

STATE NO. 1, WITH S.P. EN.= -19.377974 MEV., PAR.= 1, OCCUPIED BY A NEUTRON(S)
 QN= (0, 1, -1) (2, 1, -1)
 RP= .9907529 .1356784
 IP= 0.0000000 0.0000000

STATE NO. 2, WITH S.P. EN.= -19.377974 MEV., PAR.= 1, OCCUPIED BY A NEUTRON(S)
 QN= (0, 1, 1) (2, 1, 1)
 RP= .9907529 .1356784
 IP= 0.0000000 0.0000000

STATE NO. 3, WITH S.P. EN.= 3.057962 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, 1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 4, WITH S.P. EN.= 3.057962 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, -1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 5, WITH S.P. EN.= 3.058400 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, -3)

RP= 1.0000000
IP= 0.0000000

STATE NO. 6, WITH S.P. EN.= 3.058400 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 3, 3]
RP= 1.0000000
IP= 0.0000000

STATE NO. 7, WITH S.P. EN.= 6.351016 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 1, -1]
RP= 1.0000000
IP= 0.0000000

STATE NO. 8, WITH S.P. EN.= 6.351016 MEV., PAR.= -1, OCCUPIED BY A
QN= [1, 1, 1]
RP= 1.0000000
IP= 0.0000000

STATE NO. 9, WITH S.P. EN.= 13.142871 MEV., PAR.= 1, OCCUPIED BY A
QN= [0, 1, 1] [2, 1, 1]
RP= -.1356794 .9907529
IP= 0.0000000 0.0000000

STATE NO. 10, WITH S.P. EN.= 13.142871 MEV., PAR.= 1, OCCUPIED BY A
QN= [0, 1, -1] [2, 1, -1]
RP= -.1356784 .9907529
IP= 0.0000000 0.0000000

STATE NO. 11, WITH S.P. EN.= 17.439012 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, 1]
RP= 1.0000000
IP= 0.0000000

STATE NO. 12, WITH S.P. EN.= 17.439012 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, -1]
RP= 1.0000000
IP= 0.0000000

STATE NO. 13, WITH S.P. EN.= 17.439154 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, 3]
RP= 1.0000000
IP= 0.0000000

STATE NO. 14, WITH S.P. EN.= 17.439154 MEV., PAR.= 1, OCCUPIED BY A
QN= [2, 5, -3]
RP= 1.0000000
IP= 0.0000000

REMAINING S.P. ORBITS AT ENERGIES (MEV)

17.43944 17.43944 19.73509 19.73509 19.73533 19.73533

MULTIPOLE ANALYSIS OF PROTON(S) H-F POT. V AND DENS. MATR. D, WITH LISTING OF ALL COMPS WITH EN. CONTR. GT .0090

QN= [1010000] [1050000] [5010000] [5050000]
VR= -39.90723 -17.78474 -17.78474 -14.32646
VI= 0.00000 0.00000 0.00000 0.00000
OR= 1.37571 .23015 .23015 .03850
DI= 0.00000 0.00000 0.00000 0.00000

FOR MULTIPOL. LAM= 0, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -31.81938 MEV
 FOR MULTIPOL. LAM= 1, THE TOTAL CONTRIB. TO THE POT. ENERGY IS .00000 MEV
 FOR MULTIPOL. LAM= 2, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
 FOR MULTIPOL. LAM= 3, THE TOTAL CONTRIB. TO THE POT. ENERGY IS .00000 MEV
 FOR MULTIPOL. LAM= 4, THE TOTAL CONTRIB. TO THE POT. ENERGY IS -.00000 MEV
 FOR MULTIPOL. LAM= 5, THE TOTAL CONTRIB. TO THE POT. ENERGY IS .00000 MEV

***** THE LOWEST 14 PROTON(S) STATES, ALL COMP. .GT. .003 *****

STATE NO. 1, WITH S.P. EN.= -18.670839 MEV., PAR.= 1, OCCUPIED BY A PROTON(S)
 QN= (0, 1, -1) (2, 1, -1)
 RP= .9911472 .1327677
 IP= 0.0000000 0.0000000

STATE NO. 2, WITH S.P. EN.= -18.670839 MEV., PAR.= 1, OCCUPIED BY A PROTON(S)
 QN= (0, 1, 1) (2, 1, 1)
 RP= .9911472 .1327677
 IP= 0.0000000 0.0000000

STATE NO. 3, WITH S.P. EN.= 4.091875 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, 1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 4, WITH S.P. EN.= 4.091875 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, -1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 5, WITH S.P. EN.= 4.092309 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, -3)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 6, WITH S.P. EN.= 4.092309 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 3, 3)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 7, WITH S.P. EN.= 7.379135 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 1, -1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 8, WITH S.P. EN.= 7.379135 MEV., PAR.= -1, OCCUPIED BY A
 QN= (1, 1, 1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 9, WITH S.P. EN.= 14.071823 MEV., PAR.= 1, OCCUPIED BY A
 QN= (0, 1, -1) (2, 1, -1)
 RP= -.1327677 .9911472
 IP= 0.0000000 0.0000000

STATE NO. 10. WITH S.P. EN.= 14.071823 MEV., PAR.= 1, OCCUPIED BY A
 QN= (0, 1, 1) (2, 1, 1)
 RP= -.1327677 .9911472
 IP= 0.0000000 0.0000000

STATE NO. 11. WITH S.P. EN.= 18.374921 MEV., PAR.= 1, OCCUPIED BY A
 QN= (2, 5, 1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 12. WITH S.P. EN.= 18.374921 MEV., PAR.= 1, OCCUPIED BY A
 QN= (2, 5, -1)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 13. WITH S.P. EN.= 18.375062 MEV., PAR.= 1, OCCUPIED BY A
 QN= (2, 5, 3)
 RP= 1.0000000
 IP= 0.0000000

STATE NO. 14. WITH S.P. EN.= 18.375062 MEV., PAR.= 1, OCCUPIED BY A
 QN= (2, 5, -3)
 RP= 1.0000000
 IP= 0.0000000

REMAINING S.P. ORBITS AT ENERGIES (MEV)

18.37534 18.37534 20.66728 20.66728 20.66751 20.66751

TOTAL BINDING ENERGY= -11.52663 MEV, TOTAL PROTON POTENTIAL ENERGY= -31.81938 MEV, TOTAL NEUTRON POTENTIAL ENERGY= -32.60764

DELTA PN ENERGY= .78826 MEV, TOTAL ONE-BODY ENERGY= 52.90038 MEV

COMPUTATION OF EXPECTATION VALUE OF THE 21 SYMPLECTIC BILINEAR OPERATORS, IN DIMENSIONLESS UNITS, OSC. PAR. BSQUARE= 3.081 FERMISO

NAME	PROTON(S)	NEUTRON(S)	NUCLEON(S)
NL1	0.00000	0.00000	0.00000
NL2	0.00000	0.00000	0.00000
NL3	.00000	.00000	.00000
NL4	0.00000	0.00000	0.00000
NL5	0.00000	0.00000	0.00000
NL6	0.00000	0.00000	0.00000
NL7	0.00000	0.00000	0.00000
NL8	0.00000	0.00000	0.00000
NL9	0.00000	0.00000	0.00000
AP4	.00000	.00000	.00000
AP5	-.00002	-.00002	-.00004
AP6	0.00000	0.00000	0.00000
AP7	0.00000	0.00000	0.00000
AP8	0.00000	0.00000	0.00000

AP9	3.07051	3.07363	6.14414
AM4	0.00000	0.00000	0.00000
AM5	-0.00008	-0.00008	-0.00017
AM6	0.00000	0.00000	0.00000
AM7	0.00000	0.00000	0.00000
AM8	0.00000	0.00000	0.00000
AM9	.64467	.65854	1.30321

R.M.S. S.P. RADIUS FOR 2 PROTON(S) = 1.93329 F., BET = .00002, GAM = .00 DEG.

R.M.S. S.P. RADIUS FOR 2 NEUTRON(S) = 1.92900 F., BET = .00002, GAM = .00 DEG.

R.M.S. S.P. RADIUS FOR 4 NUCLEON(S) = 1.93114 F., BET = .00002, GAM = .00 DEG.

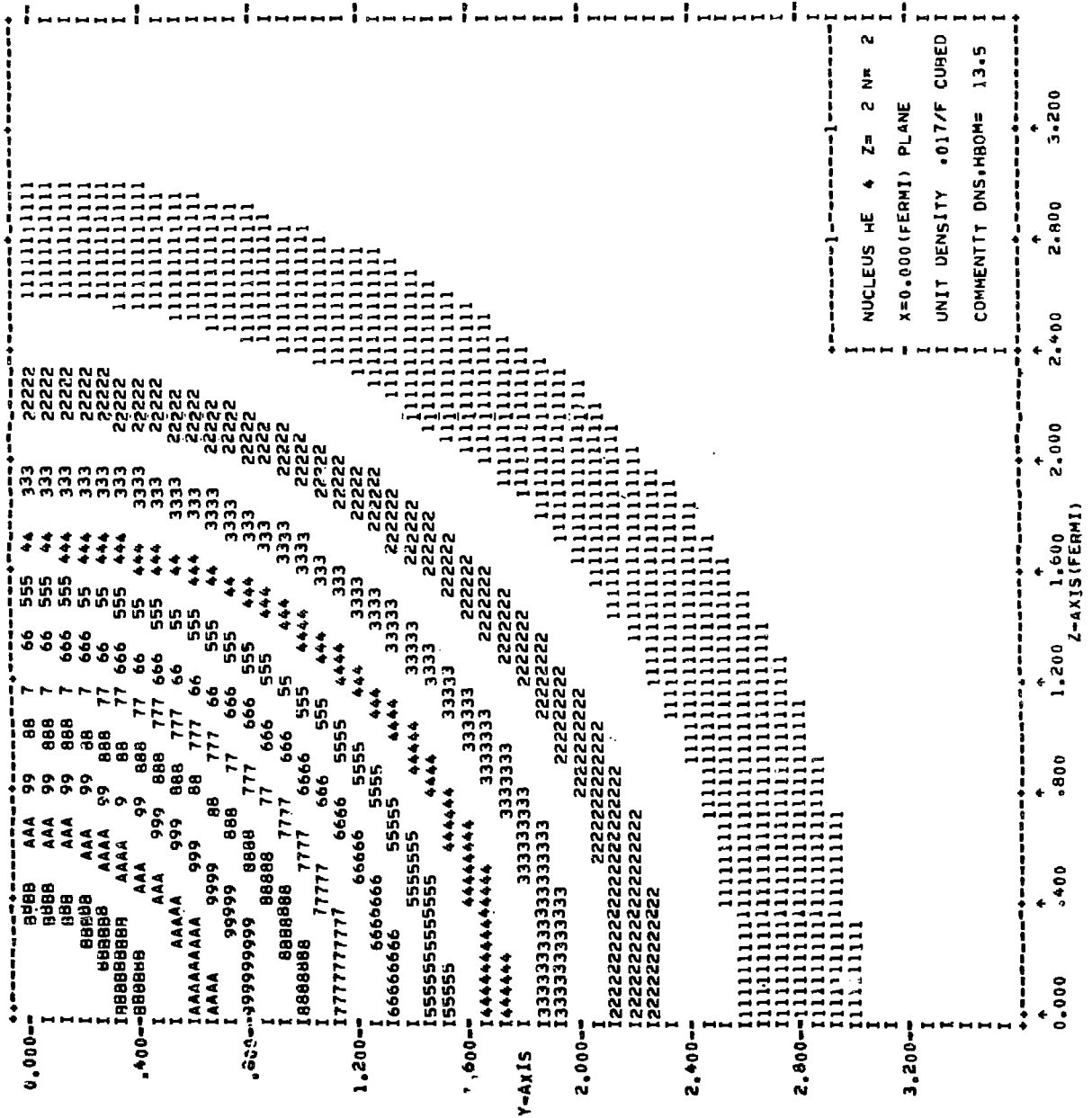
TIMEPRT CALLED BY MULTIP AT LINE 9. CP TIME= 19.055 SEC, SYSTEM TIME 18.35.10.

COMPUTATION OF MULTIPOLE MOMENTS

FOR KPOL,MPOL=	0	0	MOMENT=	2.00000E+00	IN UNITS OF BSQR, MOMENT=	2.00000E+00	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	2	0	MOMENT=	1.31379E-04	IN UNITS OF BSQR, MOMENT=	4.04842E-04	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	2	2	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	4	0	MOMENT=	2.51408E-08	IN UNITS OF BSQR, MOMENT=	2.38725E-07	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	4	2	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	4	4	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	6	0	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	6	2	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	6	4	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL
FOR KPOL,MPOL=	6	6	MOMENT=	0.	IN UNITS OF BSQR, MOMENT=	0.	IN UNITS OF F**KPOL

TIMEPRT CALLED BY OENSITY AT LINE 21. CP TIME= 19.832 SEC, SYSTEM TIME 18.35.12.

DENSITY PLOT FROM EVAL IN (R.Y. CUSSON/ H.C. LEE) C.R.N.L. DATE 11/09/70



APPENDIX III

DEBUGGING & ERREXIT MODES

A COMPASS multiple entry point routine (FTNUTIL) is included in the code for debugging purposes. The statement call TIMEPRT(TIME) will print the CP-time, the system time of day and return the CP-time in TIME. The CALL TRCEBCK statement works out the calling sequence in nested subroutine calls. The CALL TRCEDMP($p_1, p_2, p_3, \dots, p_k$), $k \leq 20$ will print the parameter list p_i either as single variables or as arrays with 3 formats, 1PE25.14, I16, and 020. In the array mode of print out 3 parameters must be given, p_i, p_{i+1}, p_{i+2} with p_i being the location where printing begins, $p_{i+1} = 2HFL$ and p_{i+2} is an integer specifying the number of consecutive locations to be printed. The last entry point is reached with CALL ERREXIT($p_1, \dots, p_k$). This will first trace back then trace-dump as above then dump the xfer package and 4000₈ locations around the call. Finally EXIT is called. All exits from EVALIN result from malfunctions of the program. The trace part of ERREXIT will supply the name of the subroutine and the line number. A list of these exits is given below and the problem which caused it is explained.

<i>SUBROUTINE</i>	<i>LINE</i>	<i>PROBLEMS</i>
EVALIN	58	TA control block on input tape was mis-read by REDFAT1. F array does not exist.
EVALIN	70	ICON array of EVALI should not point to a non positive RNU data set.
ADLONG	7	F array appears to be more than 16000 long, need more core.
ROCONIP	19	R0 is not hermitian, suspect bad symmetry properties of the F array or erroneous matrix diagonalisation during previous iteration.
READIN	33	Last entry of current card set should be the cartesian dimension of IDSC; bad cards, or cards punched for a different basis than the present assumed one.
READIN	35	The present basis is being overwritten, see 33 above.
READIN	37	Too many or bad wavefunction cards.
CARTOJ	100	Too many states for the size of the STUCO array.
POLTRA	17	need a bigger array to handle this state.
TRIMUP	8	bad calling sequence. ND should have been larger than N.
NOLMIN	15	array CP too small.
LINCOM	12	array C appears to be too small.
SCALN2	17	array CP appears to be too small.
DISTRAE	29	array CP appears to be too small.
CNNJKTE	16	array CP appears to be too small.
EXF11BP	41	The required state was not found, bad calling sequence to INBINS.
EXF11BP	48	Missing state or bad matrix elements.

<i>SUBROUTINE</i>	<i>LINE</i>	<i>PROBLEMS</i>
HARFIT	34	RO**2.NE.RO, bad density matrix suspect diagonalisation or F array.
TRVEROJ	27	TRVEROJ and IDACSET disagree on the computed dimension of a J subspace. Suspect bad calling sequences.
VEEBAR	11,12,18	Bad F array, suspect mass storage read operation or the construction of F.
CALHNL	17	number of nodes +1 must be .GE.1.

APPENDIX IV

CONTROL OPTIONS IN BLOCK DATA

All the data cards of EVALI can be set to specify the flow of the program. IPUNCH may be set to .F. to inhibit punching of the wavefunction cards by WAVPUN. The card header is also printed when cards are punched, to facilitate identification of the cards.

The variable EPS may be increased to .1 if only the major components of the wavefunction are to be printed. The amount and detail of the printout can be increased by raising IPR up to 10. The cranking loop in NWHART will be implemented by writing the names of the one body operators etc... (see NUHART) in EXFID. ITER and ITCR give the number of iterations in the main call and in the cranking calls. TNAME, HBWA and IBLK specify the force parameters. TNAME is compared with the name read from tape. HBWA(I) should have the value of $\hbar\omega$ for the Ith block on the tape while IBLK specifies which block is to be used.

The arrays ICON(2,40) and RNU(5,40) specify the sequence of nuclei which will be treated in one run of the program. RNU(5,K) contains 5 pieces of initial data belonging to the Kth nucleus. The first 2 items are the number of protons and neutrons stored as real numbers. The next one contains the name of the nucleus, up to 10 characters left adjusted, in internal BCD mode. The last 2 items

are the real values of gamma, the non-axiality angle in degree, and β_w , the potential deformation parameter. They are used by the overlay ELMOSE to determine the initial trial wavefunction from Nilsson's deformed ellipsoidal oscillator model.

The sequence in which these initial nuclei will be considered is contained in ICON(2,J). For example ICON(1,1) = K1, ICON(1,2) = K2, ICON(1,3) = 0 will process nuclei K1, K2 in the list of RNU, then stop. If ICON(2,KI) = 1, the initial wavefunction is computed using ELMOSE, but if ICON(2,KI) = 0 this wavefunction is read from cards by READIN. Other control values could clearly be added to obtain different sequences.

APPENDIX V

MAGNETIC TAPE CARD IMAGES OF THE CODES

A copy of a 600 foot reel of $\frac{1}{2}$ " magnetic tape (AECL #234-005) may be obtained by sending a similar blanked reel of tape to the Technical Information Branch, Atomic Energy of Canada Limited, Chalk River Nuclear Laboratories, Chalk River, Ontario, Canada.

The returned tape will consist of 3414 physical records of 80 external 7-track BCD characters each, recorded at a density of 556 bpi. Each record is separated by a $\frac{3}{4}$ " interrecord gap and contains one card image. The listing of appendix I was made from this tape.

TABLE 1
THE SINGLE PARTICLE BASIS USED IN EVALIN

I	n	ℓ	j	N = 2n+ℓ	Z _{cumulative}
					82
16	1	2	3/2	4	
15	0	5	11/2	5	
14	2	0	1/2	4	
13	0	4	7/2	4	
12	1	2	5/2	4	
					50
11	0	4	9/2	4	
					40
10	1	1	1/2	3	
9	0	3	5/2	3	
8	1	1	3/2	3	
					28
7	0	3	7/2	3	
					20
6	0	2	3/2	2	
5	1	0	1/2	2	
4	0	2	5/2	2	
					8
3	0	1	1/2	1	
2	0	1	3/2	1	
					2
1	0	0	1/2	0	

