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Angular momentum projection from nonaxial intrinsic states

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Abstract. An exact method of angular momentum projection from nonaxial intrinsic states is described. It is shown that the symmetries usually imposed on Hartree–Fock solutions lead to important simplifications in angular momentum projection.

1. Introduction

Angular momentum projection from Hartree–Fock (HF) intrinsic states has become an established technique in the study of nuclear structure. The HF method has long been used to construct intrinsic states giving general information about the nucleus (Ripka 1968 and Kelson 1963), but it is only comparatively recently that manageable projection techniques have become available to allow extraction of more detailed information about particular states of the nucleus. (MacDonald 1970 and Raynal 1970.) Angular momentum projection is indeed a vital link between HF calculation and comparison with experiment.

The Hartree–Fock method and angular momentum projection can be combined in essentially three ways called projection after variation, the mixing method and projection before variation. In projection after variation the HF solution of lowest energy is chosen as an intrinsic state and generates on projection a set of states which are usually taken to represent the ground state band of the nucleus. This approach has been extensively used to calculate energy levels and electromagnetic transition rates (Bassichis *et al* 1965, Gunye and Warke 1967a, 1967b).

Hartree–Fock calculations usually yield several solutions with low energy. On projection these give a number of states with the same angular momentum which can be used as a basis in which to diagonalize the Hamiltonian (Tewari and Grillot 1969, Do Dang 1970, Glen and MacDonald 1971 and Watt 1971a). Alternatively one can generate different intrinsic states by particle–hole excitations from HF solutions (Tewari 1969 and Friedman 1970).

The projection before variation method does not make direct use of HF solutions. Instead it is assumed that a single intrinsic state can on projection yield the J state of lowest energy in the nuclear spectrum, and the parameters of this intrinsic state are found by minimizing the energy of the projected wavefunction. This method has been used in the 2s1d shell (Dreizler *et al* 1968 and Watt 1970) and very interesting results have been obtained in the 1p shell where more complete calculations have been possible (Bouten *et al* 1967). The HF solution with lowest energy always seems to be an excellent first approximation in a projection before variation calculation.

The purpose of this paper is to show that the projection methods introduced by Unna (1963) and Redlich (1958) can be adapted for use with an important class of HF solutions, namely those with ellipsoidal symmetry (Bar-Touv and Kelson 1965 and Ripka 1968). The advantage of Unna's method over others which have been proposed is that it is purely algebraic and therefore especially amenable to further development in particular instances where the intrinsic states possess symmetries.

2. Angular momentum projection in general

Some general features of the problem of projecting states of definite angular momentum from intrinsic wavefunctions will be considered in this section. Consider a set of intrinsic wavefunctions $|\phi_1\rangle, |\phi_2\rangle, \ldots$. Any such wavefunction $|\phi_u\rangle$ can be written as a linear combination of normalized states $|uKJK\rangle$ with definite angular momentum J and component K along the intrinsic z axis

$$|\phi_u\rangle = \sum_{JK} A^{(u)}_{JK} |uKJK\rangle. \tag{1}$$

A projection operator P^J_{MK} may be used to separate the terms on the right side of equation (1), giving

$$P^J_{MK}|\phi_u\rangle = A^{(u)}_{JK}|uKJM\rangle \tag{2}$$

where M is the z component of angular momentum in the space-fixed system of axes.

The identities (Lamme and Boeker 1969 and MacDonald 1970)

$$(P^J_{MK})^\dagger = P^J_{KM}$$

and

$$P^J_{K'M'}P^J_{MK} = \delta_{MM'}P^J_{K'K}$$

allow the following expression to be derived for the overlap $N^J_{K'K}(uv)$ of two wavefunctions of the type appearing in equation (2):

$$\begin{aligned} N^J_{K'K}(uv) &= \langle\phi_u|(P^J_{MK'})^\dagger P^J_{MK}|\phi_v\rangle \\ &= A^{(u)*}_{JK'}A^{(v)}_{JK}\langle uK'JM|vKJM\rangle. \end{aligned} \tag{3}$$

The Hamiltonian H is invariant under rotations and so commutes with the operators P^J_{MK}. Hence

$$\begin{aligned} H^J_{K'K}(uv) &= \langle\phi_u|(P^J_{MK'})^\dagger H P^J_{MK}|\phi_v\rangle \\ &= A^{(u)*}_{JK'}A^{(v)}_{JK}\langle uK'JM|H|vKJM\rangle. \end{aligned} \tag{4}$$

The states

$$|(n)JM\rangle = \sum_{vK} C^{nJ}_{vK} P^J_{MK}|\phi_v\rangle$$

are orthonormalized eigenvectors of the Hamiltonian with energies E^n_J in the space spanned by the states of definite J projected from $|\phi_1\rangle, |\phi_2\rangle \ldots$ if

$$(H^J - E^n_J N^J)\boldsymbol{C}^{nJ} = 0. \tag{5}$$

Here H^J and N^J are matrices whose elements are $H^J_{K'K}(uv)$ and $N^J_{K'K}(uv)$, rows and columns being labelled by the indices uK' and vK respectively. The coefficients C^{nJ}_{vK} form the vector $\boldsymbol{C}^{nJ}$.

The order of the matrices N^J and H^J is not large in practice. Hence the solution of the eigenvalue problem (5) is trivial compared with the calculation of the matrices themselves. In practice one normally obtains only a very small fraction of all the possible states of a nucleus with given angular momentum, and it seems very unlikely that these few states would ever be linearly dependent. Nevertheless, this has occurred in ^{28}Si (Watt 1971b).

3. Angular momentum projection from Slater determinants

The methods of the previous section may be used with any set of intrinsic wavefunctions $|\phi_1\rangle, |\phi_2\rangle \ldots$. Here the angular momentum projection necessary to initiate such a calculation is considered in detail under the assumption that the intrinsic wavefunctions are Slater determinants. The single particle orbitals from which the determinant $|\phi_u\rangle$ is generated will be denoted by $|up\rangle|\tau_{up}\rangle$ in which the second ket describes the isospin only and the first may be expanded in terms of single particle states $|nljm\rangle$ in some suitable central potential

$$|up\rangle = \sum_{nljm} a^{up}_{nljm}|nljm\rangle.$$

Let us consider the calculation of the quantities $N^J_{K'K}(uv)$ and $H^J_{K'K}(uv)$. The indices uv are an inessential encumbrance at this stage and will be omitted whenever possible. The overlap $N^J_{K'K}$ is defined in equation (3) and is

$$N^J_{K'K} = \frac{2J+1}{8\pi^2}\int \mathrm{d}\Omega\, \mathscr{D}^{J*}_{K'K}(\Omega)\langle\phi_u|R(\Omega)|\phi_v\rangle. \tag{6}$$

Here $R(\Omega)$ is the operator which rotates a wavefunction through Euler angles Ω and $\mathscr{D}^J_{MK}(\Omega)$ is a matrix element of $R(\Omega)$. Hence all the overlaps $N^J_{K'K}$ may be obtained from the numerical determinant

$$D^{(12)}(\Omega) = \langle\phi_u|R(\Omega)|\phi_v\rangle$$

whose pqth element is a single particle matrix element of the rotation operator

$$D^{(12)}_{pq}(\Omega) = \delta_{\tau_{up}\tau_{vq}} \sum_{nljmm'} a^{up*}_{nljm} a^{vq}_{nljm'} \mathscr{D}^j_{mm'}(\Omega).$$

The presence of the isospin delta function implies that $D^{(12)}$ may be written as a product of two determinants, $D^{(1)}$ whose elements come only from proton orbitals and $D^{(2)}$ whose elements come only from neutron orbitals.

The elements of $D^{(1)}$ and $D^{(2)}$ are linear combinations of rotation matrix elements which depend on the Euler angles Ω. For convenience, such a sum will be referred to as a $\mathscr{D}$ number.

The $\mathscr{D}$ numbers have certain properties which are crucial to the projection method. Methods of combining $\mathscr{D}$ numbers which are functions of the same Euler angles will be discussed since other cases do not appear in the applications considered here. First,

it is clear that two $\mathscr{D}$ numbers can be added or subtracted to give a new $\mathscr{D}$ number. Secondly, the relation

$$\mathscr{D}^{j_1}_{m_1m_1'}\mathscr{D}^{j_2}_{m_2m_2'} = \sum_{JMM'} (j_1m_1j_2m_2|j_1j_2JM)(j_1m_1'j_2m_2'|j_1j_2JM')\mathscr{D}^{J}_{MM'} \tag{7}$$

is well known in angular momentum algebra and is proved in Edmonds (1957) whose notation for Clebsch–Gordan coefficients $(j_1m_1j_2m_2|j_1j_2JM)$ and other quantities connected with angular momentum will be used throughout. Equation (7) allows us to define multiplication of $\mathscr{D}$ numbers, for if

$$\mathscr{D}_1 = \sum_{JMM'} A^J_{MM'}\mathscr{D}^J_{MM'}$$

and

$$\mathscr{D}_2 = \sum_{JMM'} B^J_{MM'}\mathscr{D}^J_{MM'} \tag{8}$$

it follows that:

$$\mathscr{D}_1\mathscr{D}_2 = \sum_{JMM'} \left(\sum_{\substack{J_1M_1M_1' \\ J_2M_2M_2'}} A^{J_1}_{M_1M_1'}B^{J_2}_{M_2M_2'}(J_1M_1J_2M_2|J_1J_2JM) \right.$$

$$\left. \times (J_1M_1'J_2M_2'|J_1J_2JM') \right) \mathscr{D}^J_{MM'}. \tag{9}$$

The $\mathscr{D}$ numbers form a ring under the operations of addition and multiplication.

The determinant $D^{(12)}$ can be evaluated by performing multiplications and additions of $\mathscr{D}$ numbers and is therefore itself a $\mathscr{D}$ number. Indeed the orthogonality of the rotation matrix elements (Edmonds 1957) and equation (6) imply that

$$D^{(12)} = \sum_{JK'K} N^J_{K'K}\mathscr{D}^J_{K'K}. \tag{10}$$

Hence the overlaps may be obtained by expressing $D^{(12)}$ as a $\mathscr{D}$ number by successive multiplications and additions, and the coefficient of $\mathscr{D}^J_{K'K}$ in the resulting expansion is $N^J_{K'K}$. This method has several advantages over other methods. It is exact as it avoids numerical integration. It works for Slater determinants without special symmetries, and gives the complete set of $N^J_{K'K}$ in one operation. Alternatively, if some values of J are not of interest, as frequently occurs in practice, the multiplications (9) can often at quite an early stage be truncated by omitting terms which will give no contribution.

The determinants $D^{(1)}$ and $D^{(2)}$ may be computed in a variety of ways, but it has been found that the Laplace expansion of a determinant (Ferrar 1957) can be used very effectively.

From equation (4)

$$H^J_{K'K} = \frac{2J+1}{8\pi^2} \int \mathrm{d}\Omega\, \mathscr{D}^{J*}_{K'K}\langle\phi_u|HR(\Omega)|\phi_v\rangle.$$

If the quantity $\langle\phi_u|HR(\Omega)|\phi_v\rangle$ is expressed as a $\mathscr{D}$ number the arguments leading to equation (10) give

$$\langle\phi_u|HR(\Omega)|\phi_v\rangle = \sum_{JK'K} H^J_{K'K}\mathscr{D}^J_{K'K}. \tag{11}$$

The hardest part of any projection calculation is to procure expansion (11).

The Hamiltonian H will be assumed to contain only one-body and two-body operators t_i and V_{ij}, but since for a nucleus of A particles

$$H = \sum_{i=1}^{A} t_i + \sum_{i<j} V_{ij} = \sum_{i<j} \left(\frac{1}{A-1}(t_i + t_j) + V_{ij} \right) = \sum_{i<j} H_{ij}$$

it is unnecessary to consider single particle operators at this stage. Standard manipulation of determinants then gives

$$\langle \phi_u | HR(\Omega) | \phi_v \rangle = \sum_{\substack{p<q \\ r<s}} M^{(12)}_{pqrs} H_{pqrs} (-1)^{p+q+r+s}$$

where

$$H_{pqrs} = \langle up\tau_{up}; uq\tau_{uq} | HR(\Omega) | vr\tau_{vr}; vs\tau_{vs} \rangle$$

and $M^{(12)}_{pqrs}$ is the minor of $D^{(12)}$ obtained by omitting rows pq and columns rs. The multiplication of $M^{(12)}_{pqrs}$ by H_{pqrs} is of course a $\mathscr{D}$ number multiplication. The term H_{pqrs} is antisymmetrized and can be written explicitly as a $\mathscr{D}$ number by coupling states pq and rs to total angular momentum J and isospin T. Setting $\alpha_p = n_p l_p j_p$ the result is

$$\begin{aligned} H_{pqrs} = \sum_{\substack{\alpha_p m_p \alpha_q m_q \\ \alpha_r m_r \alpha_s m_s \\ JMM'TM_T}} & a^{up*}_{\alpha_p m_p} a^{uq*}_{\alpha_q m_q} a^{vr}_{\alpha_r m_r} a^{vs}_{\alpha_s m_s} (G \langle \alpha_p \alpha_q JT | H_{12} | \alpha_r \alpha_s JT \rangle) \\ & \times (\tfrac{1}{2}\tau_{up}\tfrac{1}{2}\tau_{uq} | \tfrac{1}{2}\tfrac{1}{2} TM_T)(\tfrac{1}{2}\tau_{vr}\tfrac{1}{2}\tau_{vs} | TM_T) \\ & \times (j_p m_p j_q m_q | j_p j_q JM)(j_r m_r j_s m_s | j_r j_s JM') \mathscr{D}^J_{MM'} \end{aligned} \tag{12}$$

$$= \sum_{JMM'TM_T} (H_{pqrs})_{JTMM'} \mathscr{D}^J_{MM'}. \tag{13}$$

The symbols $(H_{pqrs})_{JTMM'}$ are defined through equations (12) and (13). The quantities $\langle \alpha_p \alpha_q JT | H_{12} | \alpha_r \alpha_s JT \rangle$ are matrix elements between antisymmetrized and normalized two particle states which require the normalization factor G.

A moment's thought shows that a vast amount of numerical work would be required to carry out the procedure outlined above. It is therefore important to look for ways of simplifying the calculation and in the next section it will be shown that any symmetries in the intrinsic states can be used to advantage.

4. Consequences of symmetries in the intrinsic states

It will now be assumed that the intrinsic states have the ellipsoidal and time reversal symmetries familiar from Hartree–Fock theory (Ripka 1968). Nuclei with an even number of protons and an equal number of neutrons will be considered, and the number of active protons will be denoted by N. The essential simplifications in the intrinsic states implied by these assumptions are that neutrons and protons occupy the same orbitals if the nuclear force is charge independent, and that for each occupied orbital $|p\rangle$, the time reversed orbital $|\tilde{p}\rangle$ is also occupied. For a Hartree–Fock solution in a single major shell calculation (Ripka 1968) this implies that the expansion

$$|p\rangle = \sum_{nljm} a^p_{nljm} |nljm\rangle$$

is over only even (or odd) values of $m-\frac{1}{2}$, and the coefficients a^p_{nljm} are real. Then

$$|\tilde{p}\rangle = \sum_{nljm} a^p_{nljm}(-1)^{j-m}|nlj-m\rangle$$

to a phase factor which may be omitted. It follows that

$$|\tilde{\tilde{p}}\rangle = -|p\rangle. \tag{14}$$

The symmetries also imply certain relations among the overlaps $N^J_{KK'}$ and energies $H^J_{KK'}$. The only allowed values of K, K' are $0, \pm 2, \pm 4, \ldots, \pm(J-1)$ or $\pm J$, and

$$N^J_{K-K'} = (-1)^{J-K'}N^J_{KK'} \qquad N^J_{-KK'} = (-1)^{J-K}N^J_{KK'}$$

with similar relations among the $H^J_{KK'}$. In particular $K = 0$ or $K' = 0$ do not occur for odd J, and hence no $J = 1$ state can be projected from these intrinsic states.

For definiteness the single particle orbitals $|p\rangle$ will be labelled by integral values of $p = 1, 2, \ldots, N$ and the label of the time reversed orbital $|\tilde{p}\rangle$ will be defined to be

$$\tilde{p} = N+1-p. \tag{15}$$

Since neutrons occupy the same orbits as protons, the two determinants $D^{(1)}$ and $D^{(2)}$ introduced in § 3 are equal element by element and the superscripts may be omitted.

The matrix element $\langle\phi_u|HR(\Omega)|\phi_v\rangle$ now becomes

$$\langle\phi_u|HR(\Omega)|\phi_v\rangle = 2D \sum_{\substack{p<q \\ r<s}} (-1)^{p+q+r+s} M_{pqrs} H^{(1)}_{pqrs} + \sum_{pqrs} M_{pr} M_{qs} H^{(0)}_{pqrs} (-1)^{p+q+r+s}. \tag{16}$$

Here M_{pqrs} is the minor of order $N-2$ obtained by omitting rows pq and columns rs of D, and hence DM_{pqrs} is a minor of the determinant $D^{(12)}$; also M_{pr} is a minor of order $N-1$ of D. The first term arises from the interactions between two protons (or two neutrons, giving the factor 2) while the second arises from interactions between one proton and one neutron. The superfix 0 or 1 on H_{pqrs} labels the $|M_T|$ value of the two-particle states $|pq\rangle$ and $|rs\rangle$. The labels p, r refer to proton states in both terms while labels q, s refer to proton states in the first term but to neutron states in the second. The isospin factors in equation (12) therefore reduce to

$$(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}M_T - \tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}TM_T)^2 = \tfrac{1}{2}(1+|M_T|).$$

Hence

$$H^{(0)}_{pqrs} = \tfrac{1}{2}H^{(1)}_{pqrs} + \sum_{JMM'} (H_{pqrs})_{JT=0MM'} \mathscr{D}^J_{MM'}$$

so that the $T = 1$ term need not be computed separately for both $M_T = 0$ and $M_T = 1$. All multiplications in equation (16) are of course $\mathscr{D}$ number multiplications.

The evaluation of equation (16) is by far the most lengthy part of any projection calculation. Consider for example the nucleus ^{24}Mg with eight active particles in the 2s1d shell. There are 36 terms in the first sum on the right side of equation (16). Each product $M_{pqrs}H^{(1)}_{pqrs}$ requires the calculation of the two factors, each of which contains up to 55 nonzero elements with different JMM'. Each of the 55×55 products requires several Clebsch–Gordan coefficients according to equation (7). Finally, the result must be multiplied by D which contains 104 nonzero terms. The second sum in equation (16) is even more formidable. Each matrix element and each minor has up to 91 nonzero

coefficients of rotation matrix elements and there are 256 terms in the sum. Projection before variation calculations of the type carried out to date would be out of the question in ^{24}Mg if these numbers could not be drastically reduced, and it is in this connection that the symmetries play a most crucial role.

Before proceeding further, it is necessary to derive some properties of the $\mathscr{D}$ numbers. Operators T_1, T_2 and T_M may be defined to operate on a $\mathscr{D}$ number, such as $\mathscr{D}_1$ in equation (8), as follows:

$$T_1\mathscr{D}_1 = \sum_{JMM'} (-1)^{J-M} A^J_{MM'} \mathscr{D}^J_{-MM'} \tag{17}$$

$$T_2\mathscr{D}_1 = \sum_{JMM'} (-1)^{J-M'} A^J_{MM'} \mathscr{D}^J_{M-M'} \tag{18}$$

$$T_M\mathscr{D}_1 = \sum_{JMM'} A^J_{MM'} \mathscr{D}^J_{M'M}. \tag{19}$$

Products of these operators may now be defined. In all cases occurring in angular momentum projection, the values of J in the $\mathscr{D}$ numbers are either all integers or all half integers. Hence the operators T_1^2 and T_2^2 applied to $\mathscr{D}_1$ give either $+\mathscr{D}_1$ or $-\mathscr{D}_1$ depending on the values of J, and so are of no practical value. Also $T_M^2 = 1$, T_1 and T_2 commute and $T_1T_M = T_MT_2$. The only useful products are therefore T_1T_2, T_1T_M, T_2T_M and $T_1T_2T_M$. Apart from a possible factor -1, any product may be reduced to an operator in the set

$$S = \{1, T_1\}\otimes\{1, T_2\}\otimes\{1, T_M\}$$

where $\otimes$ indicates a direct product.

The physical significance of these operators may be understood by considering their effect on an element of D such as $\langle up|R(\Omega)|vq\rangle$. The operators T_1 and T_2 replace $\langle up|$ by $\langle u\tilde{p}|$ and $|vq\rangle$ by $|v\tilde{q}\rangle$ respectively, while T_M exchanges the roles of $|up\rangle$ and $|vq\rangle$. That is

$$T_1\langle up|R(\Omega)|vq\rangle = \langle u\tilde{p}|R(\Omega)|vq\rangle\theta(p)$$

$$T_2\langle up|R(\Omega)|vq\rangle = \langle up|R(\Omega)|v\tilde{q}\rangle\theta(q)$$

and

$$T_M\langle up|R(\Omega)|vq\rangle = \langle vq|R(\Omega)|up\rangle.$$

Relation (14) gives the factors θ, defined by

$$\theta(p) = +1 \qquad p \leqslant \tfrac{1}{2}N$$

$$\theta(p) = -1 \qquad p > \tfrac{1}{2}N.$$

The expressions on the right sides of these equations may also be elements of D. The operators T_1 and T_2 certainly relate elements of D, while T_M will relate elements of D if initial and final states are the same, that is, if $u = v$. Clearly products of the operators will also relate elements of D. Thus the operators in the set

$$T = \{1, T_1\}\otimes\{1, T_2\}\otimes\{1, \delta_{uv}T_M\}$$

allow all the elements of D to be generated from a few. This is a rather trivial result but it illustrates the use of these operators.

The real usefulness of the operators in S comes about because they are distributive with respect to $\mathscr{D}$ number addition and multiplication. The property is obvious for addition and will now be proved for multiplication.

Theorem 1. The operators in $S = \{1, T_1\}\otimes\{1, T_2\}\otimes\{1, T_M\}$ are distributive with respect to $\mathscr{D}$ number multiplication, that is, if $\mathscr{T} \in S$,

$$\mathscr{T}(\mathscr{D}_1\mathscr{D}_2 \ldots \mathscr{D}_n) = (\mathscr{T}\mathscr{D}_1)(\mathscr{T}\mathscr{D}_2)\ldots(\mathscr{T}\mathscr{D}_n).$$

The theorem will first be proved for a product of two $\mathscr{D}$ numbers, $\mathscr{D}_1$ and $\mathscr{D}_2$ of equation (8). Consider the operator T_M. From definition (19) and equations (7) and (9),

$$\begin{aligned}(T_M\mathscr{D}_1)(T_M\mathscr{D}_2) &= \left(\sum_{J_1M_1M_1'} A^{J_1}_{M_1M_1'}\mathscr{D}^{J_1}_{M_1'M_1}\right)\left(\sum_{J_2M_2M_2'} B^{J_2}_{M_2M_2'}\mathscr{D}^{J_2}_{M_2'M_2}\right)\\ &= \sum_{\substack{J_1M_1M_1'\\J_2M_2M_2'\\JMM'}} A^{J_1}_{M_1M_1'}B^{J_2}_{M_2M_2'}(J_1M_1J_2M_2|J_1J_2JM)\\ &\qquad\times(J_1M_1'J_2M_2'|JM')\mathscr{D}^{J}_{M'M}\\ &= T_M(\mathscr{D}_1\mathscr{D}_2).\end{aligned}$$

This proves the assertion for T_M.

Now consider operator T_1. By definition (17)

$$\begin{aligned}(T_1\mathscr{D}_1)(T_1\mathscr{D}_2) &= \sum_{\substack{J_1M_1M_1'\\J_2M_2M_2'}} A^{J_1}_{M_1M_1'}(-1)^{J_1-M_1}\mathscr{D}^{J_1}_{-M_1M_1'}B^{J_2}_{M_2M_2'}(-1)^{J_2-M_2}\mathscr{D}^{J_2}_{-M_2M_2'}\\ &= \sum_{\substack{J_1M_1M_1'\\J_2M_2M_2'\\JMM'}} A^{J_1}_{M_1M_1'}B^{J_2}_{M_2M_2'}(-1)^{J_1+J_2-M_1-M_2}\\ &\qquad\times(J_1-M_1J_2-M_2|J_1J_2J-M)\\ &\qquad\times(J_1M_1'J_2M_2'|J_1J_2JM')\mathscr{D}^{J}_{-MM'}.\end{aligned}$$

In this expression, $M = M_1 + M_2$ because of the Clebsch–Gordan coefficient, and $J_1 + J_2 + J$ must be an integer. Since

$$\begin{aligned}(-1)^{J_1+J_2-M}(J_1-M_1J_2-M_2|J_1J_2J-M) &= (-1)^{2(J_1+J_2+J)+J-M}\\ &\qquad\times(J_1M_1J_2M_2|JM)\\ &= (-1)^{J-M}(J_1M_1J_2M_2|JM)\end{aligned}$$

the right side of the above expression equals $T_1(\mathscr{D}_1\mathscr{D}_2)$, which proves the result for T_1. The result for T_2 can be derived in a similar way.

Let $\mathscr{T}_1, \mathscr{T}_2 \in S' = \{1, T_1, T_2, T_M\}$. Then

$$\mathscr{T}_1\mathscr{T}_2(\mathscr{D}_1\mathscr{D}_2) = \mathscr{T}_1[(\mathscr{T}_2\mathscr{D}_1)(\mathscr{T}_2\mathscr{D}_2)] = (\mathscr{T}_1\mathscr{T}_2\mathscr{D}_1)(\mathscr{T}_1\mathscr{T}_2\mathscr{D}_2).$$

But any operator $\mathscr{T} \in S$ can be expressed as a product of operators in S' and hence the theorem is true for products of two $\mathscr{D}$ numbers. Since $\mathscr{D}$ number multiplication is associative

$$\begin{aligned}\mathscr{T}(\mathscr{D}_1\mathscr{D}_2\ldots\mathscr{D}_n) &= \mathscr{T}[(\mathscr{D}_1\ldots\mathscr{D}_{n-1})\mathscr{D}_n]\\ &= [\mathscr{T}(\mathscr{D}_1\ldots\mathscr{D}_{n-1})](\mathscr{T}\mathscr{D}_n)\end{aligned}$$

and the theorem follows by induction.

Since the operators in T act on elements of the determinant D to give other elements, it follows from the above theorem that these operators when applied to a minor of D will generate other minors of D. When applied to the matrix elements H_{pqrs}, these operators also generate other matrix elements as can be seen from equation (12). Hence these operators can be used to reduce the number of minors and of matrix elements which need to be calculated explicitly. Another relationship useful in calculating the quantities H_{pqrs} is

$$(H_{pqsr})_{JTMM'} = (-1)^T (H_{pqrs})_{JTMM'} \tag{20}$$

which is not hard to prove.

It is now possible to simplify equation (16). The expression

$$A = \sum_{\substack{p<q \\ r<s}} (-1)^{p+q+r+s} M_{pqrs} H^{(1)}_{pqrs} \tag{21}$$

will be considered first. It is convenient to use the notation of set theory (Kahan 1965) to keep track of the ranges of the variables $pqrs$ over which the summation must be performed. In equation (21), $pqrs$ belongs to the set S_1 given by

$$S_1 = \{pqrs : 1 \leqslant p < N, p < q \leqslant N; 1 \leqslant r < N, r < s \leqslant N\}.$$

Consider the effect of operator T_1 on a typical term in equation (21). It will change labels pq into $\tilde{p}\tilde{q}$. But only $p < q$ belong to S_1 and hence $\tilde{q} < \tilde{p}$ by definition (15), and so

$$(pqrs) \in S_1 \Rightarrow (\tilde{q}\tilde{p}rs) \in S_1$$

since

$$1 \leqslant p < N, p < q \leqslant N \Rightarrow 1 \leqslant \tilde{q} < N, \tilde{q} < \tilde{p} \leqslant N.$$

From equations (17) and (20)

$$T_1 H^{(1)}_{pqrs} = \theta(p)\theta(q) H^{(1)}_{\tilde{p}\tilde{q}rs} = -\theta(p)\theta(q) H^{(1)}_{\tilde{q}\tilde{p}rs}.$$

It is easy to show from the theory of determinants that

$$T_1 M_{pqrs} = -\theta(p)\theta(q) M_{\tilde{q}\tilde{p}rs}$$

and hence

$$T_1[(-1)^{p+q+r+s} M_{pqrs} H^{(1)}_{pqrs}] = (-1)^{\tilde{q}+\tilde{p}+r+s} M_{\tilde{q}\tilde{p}rs} H^{(1)}_{\tilde{q}\tilde{p}rs}.$$

This result shows that the operator T_1 may be applied to a complete term in expression (21) to give another complete term in the expansion. If $p = \tilde{q}$ (and hence $\tilde{p} = q$), the operator T_1 leaves the term unaltered. Expression (21) may therefore be written

$$A = (1 + T_1) \sum_{pqrs \in S_2} (-1)^{p+q+r+s} M_{pqrs} H^{(1)}_{pqrs} (1 + \delta_{p\tilde{q}})^{-1}$$

where $S_2 \subset S_1$ and has still to be determined. The members $pqrs$ of S_2 must satisfy the conditions of S_1 and obey the auxiliary conditions that either $\tilde{p} = q$ or

$$(pqrs) \in S_2 \Rightarrow (\tilde{q}\tilde{p}rs) \in' S_2.$$

There are in all $2^{N(N-2)/4}$ ways of choosing the set S_2. One possibility is as follows. Pairs of indices (pq) may be ordered by the conditions $(pq) < (p'q')$ if $p < p'$ or $p = p'$ and

$q < q'$, and $(pq) = (p'q')$ if $p = p'$, $q = q'$. Then S_2 contains all sets $(pqrs) \in S_1$ which satisfy $(pq) \leqslant (\tilde{q}\tilde{p})$. This implies that

$$S_2 = \{pqrs : 1 \leqslant p \leqslant \tfrac{1}{2}N, p < q \leqslant \tilde{p}; 1 \leqslant r < N, r < s \leqslant N\}.$$

If operator T_2 is used, the summation reduces to

$$A = (1+T_2)(1+T_1) \sum_{pqrs \in S_3} (-1)^{p+q+r+s} M_{pqrs} H^{(1)}_{pqrs} (1+\delta_{p\tilde{q}})^{-1} (1+\delta_{r\tilde{s}})^{-1}$$

where

$$S_3 = \{pqrs : 1 \leqslant p \leqslant \tfrac{1}{2}N, p < q \leqslant \tilde{p}; 1 \leqslant r \leqslant \tfrac{1}{2}N, r < s \leqslant \tilde{r}\}.$$

If initial and final wavefunctions are the same, operator T_M may be used and

$$A = (1+T_1)(1+T_2)(1+T_M) \sum_{pqrs \in S_4} (-1)^{p+q+r+s} M_{pqrs} H^{(1)}_{pqrs} \Delta_1^{-1}(pqrs)$$

where

$$\Delta_1(pqrs) = (1+\delta_{p\tilde{q}})(1+\delta_{r\tilde{s}})(1+\delta_{pr}\delta_{qs})$$

and

$$S_4 = \{pqrs : (pqrs) \in S_3 \text{ and } (pq) \leqslant (rs)\}.$$

The convention defined above is used to order the pairs (pq) and (rs).

The total number of members of the various sets is important when deciding on the feasibility of an actual calculation. These numbers are presented in table 1 for N active protons along with representative numbers for the nuclei ^{24}Mg and ^{28}Si with respectively eight and twelve active particles in the 2s1d shell.

Table 1. Numbers of elements in the sets defined in the text

Set	Number	^{24}Mg	^{28}Si
S_1	$\frac{1}{4}N^2(N-1)^2$	36	225
S_2	$\frac{1}{8}N^3(N-1)$	24	135
S_3	$\frac{1}{16}N^4$	16	81
S_4	$\frac{1}{32}N^2(N^2+4)$	10	45
S_5	N^4	256	1296
S_6	$\frac{1}{8}N^2(N^2+4)$	40	180
S_7	$\frac{1}{16}N^2(N^2+8)$	24	99

The second term in equation (16) may be reduced in a similar way. We write

$$B = \sum_{pqrs} (-1)^{p+q+r+s} M_{pr} M_{qs} H^{(0)}_{pqrs}. \tag{22}$$

Since neutrons and protons occupy the same orbitals

$$H^{(0)}_{pqrs} = H^{(0)}_{qpsr}$$

and hence

$$M_{pr} M_{qs} H^{(0)}_{pqrs} = M_{qs} M_{pr} H^{(0)}_{qpsr}.$$

The expressions on both right and left of this equation appear in summation (22) which may therefore be written

$$B = \sum_{pqrs \in S_5} (-1)^{p+q+r+s} M_{pr} M_{qs} H_{pqrs} \frac{2}{1+\delta_{pq}\delta_{rs}}$$

where

$$S_5 = \{pqrs : 1 \leqslant p \leqslant q \leqslant N; 1 \leqslant r \leqslant N, 1 \leqslant s \leqslant N, r < s \text{ if } p = q\}.$$

As above

$$T_1 H^{(0)}_{pqrs} = \theta(p)\theta(q) H^{(0)}_{\tilde{p}\tilde{q}rs} = -\theta(p)\theta(q) H^{(0)}_{\tilde{q}\tilde{p}rs}$$

and

$$pqrs \in S_5 \Rightarrow \tilde{q}\tilde{p}rs \in S_5.$$

Also

$$T_1 M_{pr} = -\theta(p) M_{\tilde{p}r}. \tag{23}$$

Similar results hold for T_2 and hence

$$B = 2(1+T_2)(1+T_1) \sum_{pqrs \in S_6} (-1)^{p+q+r+s} M_{pr} M_{qs} H^{(0)}_{pqrs} \times \{1 + (\delta_{pq} + \delta_{p\tilde{q}})(\delta_{rs} + \delta_{r\tilde{s}})\}^{-1}$$

where

$$S_6 = S'_6 \cup S''_6$$

$$S'_6 = \{pqrs : 1 \leqslant p \leqslant \tfrac{1}{2}N, p \leqslant q \leqslant \tilde{p}; 1 \leqslant r \leqslant \tfrac{1}{2}N, r \leqslant s \leqslant \tilde{r}\}$$

$$S''_6 = \{pqrs : 1 \leqslant p \leqslant \tfrac{1}{2}N, p < q < \tilde{p}; 1 \leqslant r \leqslant \tfrac{1}{2}N, s < r \text{ or } s > \tilde{r}\}.$$

If T_M is also applicable, equation (22) becomes finally

$$B = 2(1+T_M)(1+T_1)(1+T_2) \sum_{pr} M_{pr} \sum_{qs} (-1)^{p+q+r+s} M_{qs} H^{(0)}_{pqrs} \Delta_2^{-1}(pqrs)$$

where

$$\Delta_2(pqrs) = 1 + (\delta_{pq} + \delta_{p\tilde{q}})(\delta_{rs} + \delta_{r\tilde{s}}) + (\delta_{pr}\delta_{qs} + \delta_{p\tilde{r}}\delta_{q\tilde{s}}) + (\delta_{ps}\delta_{qr} + \delta_{p\tilde{s}}\delta_{q\tilde{r}}).$$

The indices $pqrs \in S_7 = S'_7 \cup S''_7$ where

$$S'_7 = \{pqrs : pqrs \in S'_6, (pq) \leqslant (rs)\}$$

$$S''_7 = \{pqrs : pqrs \in S''_6, (pq) \leqslant (sr) \text{ if } s < r, (pq) \leqslant (\tilde{s}\tilde{r}) \text{ if } \tilde{s} < r\}.$$

The number of members of sets S_5, S_6 and S_7 are given in table 1.

It can be seen that in the limit of large N, the amount of work involved in calculating A and B is reduced by factors of eight and sixteen respectively. These reductions are especially important in the projection before variation type of calculation where the energy of the projected state is minimized numerically in a space of several variables, and hundreds of projections are therefore necessary. Results have been reported for the nucleus ^{24}Mg (Watt 1971a) and calculations for ^{28}Si are feasible using these methods.

5. Conclusion

It has been shown that angular momentum projection can be greatly simplified if the intrinsic states have the ellipsoidal and time reversal symmetries commonly assumed in Hartree–Fock calculations. The method which has been developed is exact and suffers neither from the formidable computational problems of direct numerical integration nor from the inherent uncertainties of approximation methods. Since the approach is analytical, it should be possible to develop similar methods to cope with other symmetries in the intrinsic states should the need arise.

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