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TRANSFORMATION BRACKETS FOR HARMONIC OSCILLATOR FUNCTIONS

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Abstract: We define the transformation brackets connecting the wave functions for two particles in an harmonic oscillator common potential with the wave functions given in terms of the relative and centre of mass coordinates of the two particles. With the help of these brackets we show that all matrix elements for the interaction potentials in nuclear shell theory can be given directly in terms of Talmi integrals. We obtain recurrence relations and explicit algebraic expressions for the transformation brackets that will permit their numerical evaluation.

1. Introduction

The increased importance acquired by the nuclear shell model [1]) in the past decade, has served as a spur to develop mathematical methods that would simplify the evaluation of the matrix elements involved in this model. It is well known [1]) that all matrix elements for the interaction forces can be reduced to two particle interaction matrix elements [1]), and that these, in turn, can be evaluated in terms of Slater coefficients by the standard methods of atomic spectroscopy. The evaluation of the Slater coefficients in nuclear shell theory is more troublesome than in atomic spectroscopy, as there are more types of forces and these are not yet very well defined. It was shown by Talmi [2]) that when the common potential of the nucleons is of the harmonic oscillator type, the evaluation of the Slater coefficients simplifies considerably. The method of Talmi supplemented by Thieberger's [3]) tables, as well as by other more recent developments [4]), is widely used in nuclear shell theory calculations.

In the Talmi method [2]) one could say that the evaluation of the matrix elements is given in two steps: a) The matrix element is reduced to Slater coefficients by means of the standard methods of Racah [5]) and b) the Slater coefficients are evaluated assuming an harmonic oscillator common potential, taking advantage of the relations between the wave functions for two

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nucleons in this potential, with the wave functions associated with the relative and centre of mass coordinates for the same two nucleons.

In the present paper we show that by introducing a transformation bracket connecting the two nucleon wave function to the relative and centre of mass wave function, the two nucleon matrix elements are given directly in terms of Talmi radial integrals, without the intermediate step of the Slater coefficients. Furthermore, we indicate how the transformation brackets, in combination with fractional parentage coefficients, reduce any matrix element in nuclear shell theory to Talmi integrals. Finally, we give recurrence relations and explicit expressions for the transformation brackets, which will permit their numerical evaluation.

We start by introducing the hamiltonian for two nucleons in a harmonic oscillator potential of frequency ω as

$$H = \tfrac{1}{2}(p_1^2/m)+\tfrac{1}{2}m\omega^2 r_1^2+\tfrac{1}{2}(p_2^2/m)+\tfrac{1}{2}m\omega^2 r_2^2 \tag{1}$$

where $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{p}_1$, $\mathbf{p}_2$ are the coordinates and momenta of the two nucleons and m their mass. We now introduce the relative coordinate $\mathbf{r}$ and the centre of mass coordinate $\mathbf{R}$ by the definitions

$$\mathbf{r} = \frac{1}{\sqrt{2}}(\mathbf{r}_1-\mathbf{r}_2), \quad \mathbf{R} = \frac{1}{\sqrt{2}}(\mathbf{r}_1+\mathbf{r}_2). \tag{2}$$

These definitions will have the advantage over the customary ones [2,3]) that the harmonic oscillator functions will have the same form for all the coordinates involved. The corresponding momenta are

$$\mathbf{p} = \frac{1}{\sqrt{2}}(\mathbf{p}_1-\mathbf{p}_2), \quad \mathbf{P} = \frac{1}{\sqrt{2}}(\mathbf{p}_1+\mathbf{p}_2), \tag{3}$$

so that the hamiltonian can also be written as

$$H = \tfrac{1}{2}(p^2/m)+\tfrac{1}{2}m\omega^2 r^2+\tfrac{1}{2}(P^2/m)+\tfrac{1}{2}m\omega^2 R^2. \tag{4}$$

The angular momenta associated with the different coordinates will be designated by $\mathbf{l}_1$, $\mathbf{l}_2$, $\mathbf{l}$, $\mathbf{L}$ and from (2) and (3) we see that

$$\mathbf{l}_1+\mathbf{l}_2 = \mathbf{l}+\mathbf{L} = \boldsymbol{\lambda}, \tag{5}$$

where $\boldsymbol{\lambda}$ stands for the vector representing the total angular momentum of the two particles.

The wave function for a single harmonic oscillator will be given by

$$\mathscr{R}_{nl}(r)Y_{lm}(\theta, \varphi) \tag{6}$$

where Y_{lm} are spherical harmonics and $\mathscr{R}_{nl}(r)$ the radial functions. In what follows we shall always assume that r is given in units of

$$(\hbar/m\omega)^{\frac{1}{2}}, \tag{7}$$

so that the radial function takes the form

$$\mathscr{R}_{nl}(r) = [2(n!)/\Gamma(n+l+\tfrac{3}{2})]^{\frac{1}{2}} r^l \exp(-\tfrac{1}{2}r^2)L_n^{l+\frac{1}{2}}(r^2), \tag{8}$$

where $L_n^{l+\frac{1}{2}}$ is a Laguerre polynomial as defined in Magnus and Oberhettinger's book [6]), and Γ is a gamma function. The energy associated with this wave function in units of $\hbar\omega$ is

$$E_{nl} = 2n+l+\tfrac{3}{2}. \tag{9}$$

As $\boldsymbol{\lambda}$ commutes with the hamiltonian, we can construct eigenfunctions of H, λ^2, λ_z starting either from (1) or (4), to obtain the eigenkets

$$|n_1l_1, n_2l_2, \lambda\mu\rangle = \sum_{m_1m_2} \langle l_1l_2m_1m_2|\lambda\mu\rangle \mathscr{R}_{n_1l_1}(r_1)Y_{l_1m_1}(\theta_1, \varphi_1)\mathscr{R}_{n_2l_2}(r_2)Y_{l_2m_2}(\theta_2, \varphi_2), \tag{10}$$

$$|nl, NL, \lambda\mu\rangle = \sum_{mM} \langle lLmM|\lambda\mu\rangle \mathscr{R}_{nl}(r)Y_{lm}(\theta, \varphi)\mathscr{R}_{NL}(R)Y_{LM}(\Theta, \Phi), \tag{11}$$

where $\langle l_1l_2m_1m_2|\lambda\mu\rangle$, etc., are Clebsch-Gordan coefficients.

The brackets we are interested in are those connecting (10) and (11), i.e.

$$|n_1l_1, n_2l_2, \lambda\mu\rangle = \sum_{nlNL} |nl, NL, \lambda\mu\rangle\langle nl, NL, \lambda|n_1l_1, n_2l_2, \lambda\rangle. \tag{12}$$

As is well known [5]), the bracket in (12) is independent of the magnetic quantum number μ, and this parameter was therefore not included in the bracket. Because of conservation of energy the bracket will only be different from zero if the following relation is satisfied:

$$2n_1+l_1+2n_2+l_2 = 2n+l+2N+L. \tag{13}$$

As all the parameters in (13) are non-negative integers, it is clear that the summation involved in (12) is a finite one. The condition (13) guarantees also the conservation of parity in the wave function as

$$(-1)^{l_1+l_2} = (-1)^{l+L}. \tag{14}$$

In the next section we shall show how the brackets defined in (12) can be used to determine the matrix elements for different types of nuclear forces.

2. Matrix Elements for Nuclear Forces

2.1. CENTRAL FORCES

Let us consider first a central interaction $V(r)$ between the two nucleons. Using (12) we see that a general matrix element could be written as

$$\begin{aligned}\langle n_1l_1, n_2l_2, \lambda\mu|V(r)|n'_1l'_1, n'_2l'_2, \lambda'\mu'\rangle \\ = \sum_{nlNL}\sum_{n'l'N'L'} \{\langle n_1l_1, n_2l_2, \lambda|nl, NL, \lambda\rangle\langle n'l', N'L', \lambda'|n'_1l'_1, n'_2l'_2, \lambda'\rangle \\ \langle nl, NL, \lambda\mu|V(r)|n'l', N'L', \lambda'\mu'\rangle\}.\end{aligned} \tag{15}$$

But as $V(r)$ depends only on the magnitude of the relative coordinates, we have

$$\langle nl, NL, \lambda\mu|V(r)|n'l', N'L', \lambda'\mu'\rangle = \langle nl||V(r)||n'l'\rangle\, \delta_{ll'}\delta_{NN'}\delta_{LL'}\delta_{\lambda\lambda'}\delta_{\mu\mu'}, \tag{16}$$

where

$$\langle nl||V(r)||n'l'\rangle = \int_0^\infty \mathscr{R}_{nl}(r)V(r)\mathscr{R}_{n'l'}(r)r^2\mathrm{d}r. \tag{17}$$

From the relation(13) we also see that

$$n'-n = n'_1-n_1+n'_2-n_2+\tfrac{1}{2}(l'_1+l'_2-l_1-l_2) \tag{18}$$

where, because of parity considerations, the term in the parenthesis of (18) must be even.

Substituting (16) in (15) we obtain

$$\langle n_1l_1, n_2l_2, \lambda\mu|V(r)|n'_1l'_1, n'_2l'_2, \lambda\mu\rangle = \sum_{nlNL} \{\langle nl, NL, \lambda|n_1l_1, n_2l_2, \lambda\rangle\langle n'l, NL, \lambda|n'_1l'_1, n'_2l'_2, \lambda\rangle \langle nl||V(r)||n'l\rangle\} \tag{19}$$

where n' and n are related by (18), and we have used the fact that the brackets are real, as shown in the following sections, to invert the order in the first bracket.

Using the explicit expressions [6]) for the Laguerre polynomials, the matrix elements (17) can be given in terms of the Talmi integrals

$$I_p = [2/\Gamma(p+\tfrac{3}{2})]\int_0^\infty r^{2p}\exp(-r^2)V(r)r^2\mathrm{d}r. \tag{20}$$

It is clear, therefore, that a matrix element for central forces could be directly determined in terms of Talmi integrals provided that the transformation brackets involved in (19) were available.

2.2. SPIN-ORBIT COUPLING FORCES

For forces of the type

$$V_{lS} = V(r)\mathbf{l}\cdot\mathbf{S} \tag{21a}$$

where

$$\mathbf{l} = \mathbf{r}\times\mathbf{p}, \quad \mathbf{S} = \tfrac{1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2), \tag{21b}$$

the matrix elements in LS coupling can be easily obtained [7]) once

$$\langle n_1l_1, n_2l_2, \lambda||V(r)\mathbf{l}||n'_1l'_1, n'_2l'_2, \lambda'\rangle, \tag{22}$$

is known. Using (12), we see that to determine (22) we need the matrix element

$$\langle nl, NL, \lambda||V(r)\mathbf{l}||n'l', NL, \lambda'\rangle = (-1)^{L+1-l'-\lambda}\langle nl||V(r)\mathbf{l}||n'l'\rangle[(2\lambda+1)(2\lambda'+1)]^{\frac{1}{2}}W(ll'\lambda\lambda'; 1L), \tag{23}$$

where W stands for a Racah coefficient, and the right hand side of (23) is due to the fact that $V(r)\mathbf{l}$ is a Racah tensor [5]) of order one depending only on the relative coordinate. It is also well known [5]) that

$$\langle nl||V(r)\mathbf{l}||n'l'\rangle = \delta_{ll'}\langle nl||V(r)||n'l'\rangle[l(l+1)(2l+1)]^{\frac{1}{2}}, \tag{24}$$

where $\langle nl||V(r)||n'l'\rangle$ is given by (17). Collecting terms we see that the matrix element (22) becomes

$$\langle n_1 l_1, n_2 l_2, \lambda || V(r)\mathbf{l} || n'_1 l'_1, n'_2 l'_2, \lambda' \rangle = \sum_{nlNL} \{\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda\rangle \langle n'l, NL, \lambda' | n'_1 l'_1, n'_2 l'_2, \lambda'\rangle \tag{25}$$

$$\langle nl || V(r) || n'l\rangle [l(l+1)(2l+1)(2\lambda+1)(2\lambda'+1)]^{\frac{1}{2}} (-1)^{L+1-l-\lambda} W(ll\lambda\lambda'; 1L)\},$$

where the relation between n' and n is again given by (18).

2.3. TENSOR FORCES

The tensor forces can be written in the form [7])

$$V_{\mathrm{T}} = V(r)(\tfrac{32}{5}\pi)^{\frac{1}{2}} \mathbf{Y}_2 \cdot \mathbf{X}_2, \tag{26a}$$

where $\mathbf{Y}_2$ represents a Racah tensor whose components are the spherical harmonics $Y_{2m}(\theta, \varphi)$, and the $m = 0$ components of the Racah tensor $\mathbf{X}_2$ is

$$X_{20} = \frac{1}{\sqrt{2}} (3S_z^2 - S^2), \tag{26b}$$

with $\mathbf{S}$ given by (21b).

The matrix elements in LS coupling for tensor forces can be easily obtained[7]) once

$$\langle n_1 l_1, n_2 l_2, \lambda || V(r) \mathbf{Y}_2(\theta, \varphi) || n'_1 l'_1, n'_2 l'_2, \lambda' \rangle \tag{27}$$

is known.

Using (12), we see that to determine (27) we need the matrix element [5])

$$\langle nl, NL, \lambda || V(r)\mathbf{Y}_2(\theta, \varphi) || n'l', NL, \lambda'\rangle$$
$$= (-1)^{L+2-l'-\lambda} \langle nl || V(r)\mathbf{Y}_2(\theta, \varphi) || n'l'\rangle [(2\lambda+1)(2\lambda'+1)]^{\frac{1}{2}} W(ll'\lambda\lambda'; 2L) \tag{28}$$

where in turn [5])

$$\langle nl || V(r) \mathbf{Y}_2(\theta, \varphi) || n'l'\rangle = \langle nl || V(r) || n'l'\rangle [5(2l+1)/4\pi]^{\frac{1}{2}} \langle l200 | l'0\rangle. \tag{29}$$

Collecting terms, we find that the matrix element (27) becomes

$$\langle n_1 l_1, n_2 l_2, \lambda || V(r)\mathbf{Y}_2(\theta, \varphi) || n'_1 l'_1, n'_2 l'_2, \lambda'\rangle = \sum_{nlNL} \sum_{n'l'} \{\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda\rangle \langle n'l', NL, \lambda' | n'_1 l'_1, n'_2 l'_2, \lambda'\rangle \tag{30}$$

$$\langle nl || V(r) || n'l'\rangle (-1)^{L-\lambda-l'} [(2\lambda+1)(2\lambda'+1)(2l+1)(\tfrac{5}{4}\pi)]^{\frac{1}{2}} \langle l200 | l'0\rangle \, W(ll'\lambda\lambda'; 2L)\},$$

where l' is restricted to

$$l' = l \pm 2, l, \tag{31a}$$

and n' is given by the relation

$$n' = n + (n'_1 + n'_2 - n_1 - n_2) + \tfrac{1}{2}(l'_1 + l'_2 - l_1 - l_2) + \tfrac{1}{2}(l - l'). \tag{31b}$$

2.4. j—j COUPLING

In the previous subsections we analyzed with the help of the transformation brackets the matrix elements for nuclear forces in LS coupling. To illustrate the corresponding procedure in j—j coupling, we consider a diagonal matrix element for a central force, and from the relations between the wave functions in j—j coupling and LS coupling [8]), as well as from (19), we immediately obtain

$$\begin{aligned}\langle n_1 l_1 \tfrac{1}{2}, j_1; n_2 l_2 \tfrac{1}{2}, j_2; J|V(r)|n_1 l_1 \tfrac{1}{2}, j_1; n_2 l_2 \tfrac{1}{2}, j_2; J\rangle \\ = \sum_{\lambda S n l N L} \Bigg\{ (2\lambda+1)(2S+1)(2j_1+1)(2j_2+1) \left[\begin{Bmatrix} l_1 & \tfrac{1}{2} & j_1 \\ l_2 & \tfrac{1}{2} & j_2 \\ \lambda & S & J \end{Bmatrix}\right]^2 \\ [\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda\rangle]^2 \langle nl||V(r)||nl\rangle \Bigg\},\end{aligned} \tag{32}$$

where the curly bracket represents a $9j$ coefficient [8]), and the last factor is given by (17). Similar expressions will hold for other types of forces.

2.5. MATRIX ELEMENTS FOR MORE THAN TWO PARTICLES

Let us consider a system of p identical particles in the $n_1 l_1 j_1$ shell, and assume a central force interaction between them of the form

$$\sum_{i<j=1}^{p} V(r_{ij}). \tag{33}$$

Then, as is well known [9]), the diagonal matrix element for the interaction potential is given by

$$\begin{aligned}\langle (n_1 l_1 \tfrac{1}{2} j_1)^p \alpha J M | \sum_{i<j=1}^{p} V(r_{ij}) | (n_1 l_1 \tfrac{1}{2} j_1)^p \alpha J M\rangle \\ = \tfrac{1}{2} p(p-1) \sum_{\alpha'' J'' J'} \{ [\langle (j_1)^2 J', (j_1)^{p-2} \alpha'' J'', J | \} (j_1)^p \alpha J\rangle]^2 \\ \langle n_1 l_1 \tfrac{1}{2}, j_1; n_1 l_1 \tfrac{1}{2}, j_1; J' | V(r) | n_1 l_1 \tfrac{1}{2}, j_1; n_1 l_1 \tfrac{1}{2}, j_1; J'\rangle \},\end{aligned} \tag{34}$$

where α, α'' are additional quantum numbers necessary to specify the states of p and $p-2$ particles respectively, and the first term in the right hand side of (34) is a fractional parentage coefficient in which J' is restricted to even values that satisfy the triangular relation $(J'J''J)$. The matrix element on the right hand side of (34) is a particular case of (32) when $n_2 = n_1$ etc., so that the matrix elements for p particles in a shell are given directly in terms of Talmi integrals and of coefficients which are combinations of fractional parentage coefficients and transformations brackets.

In the previous subsections we have shown that if the transformation brackets

$$\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda\rangle, \tag{35}$$

were available, the coefficients of the Talmi integrals in the explicit expressions for all types of matrix elements, could be tabulated in a direct fashion. In the next sections we obtain recurrence relations and explicit expression for the brackets.

3. Recurrence Relations

It is well known [1,2]) that for the energy levels of interest in nuclear shell theory n_1, n_2 are restricted to the values $n_1, n_2 = 0, 1, 2, 3$. It seems therefore convenient to obtain recurrence relations for the brackets (35) in such a way that a bracket with arbitrary n_1, n_2 could be obtained from the bracket with $n_1 = n_2 = 0$. In this section we shall derive the recurrence relations, while in the next section we obtain the explicit expression for the bracket in which $n_1 = n_2 = 0$.

Let us consider the ket $|n_1+1l_1, n_2l_2, \lambda\mu\rangle$. From the recurrence relations for Laguerre polynomials [10])

$$L_{n+1}^{l+\frac{1}{2}}(r^2) = (n+1)^{-1}[(2n+l+\tfrac{3}{2})-r^2]L_n{}^{l+\frac{1}{2}}(r^2)-(n+1)^{-1}(n+l+\tfrac{1}{2})L_{n-1}^{l+\frac{1}{2}}(r^2), \tag{36}$$

and the form (8) of the radial function we obtain

$$\begin{aligned}|n_1+1l_1, n_2l_2, \lambda\mu\rangle &= [(n_1+1)(n_1+l_1+\tfrac{3}{2})]^{-\frac{1}{2}}[(2n_1+l_1+\tfrac{3}{2})-r_1{}^2]|n_1l_1, n_2l_2, \lambda\mu\rangle \\ &\quad -[n_1(n_1+l_1+\tfrac{1}{2})]^{\frac{1}{2}}[(n_1+1)(n_1+l_1+\tfrac{3}{2})]^{-\frac{1}{2}}|n_1-1l_1, n_2l_2, \lambda\mu\rangle. \end{aligned}\tag{37}$$

If we multiply both sides of (37) by the bra $\langle nl, NL, \lambda\mu|$ we see that the left hand side of (37) will be zero unless

$$2n+l+2N+L = 2n_1+l_1+2n_2+l_2+2. \tag{38}$$

For bras that satisfy (38) the brackets on the right hand side of (37) will be zero, so we are left with

$$\begin{aligned}&\langle nl, NL, \lambda|n_1+1l_1, n_2l_2, \lambda\rangle \\ &= [(n_1+1)(n_1+l_1+\tfrac{3}{2})]^{-\frac{1}{2}}\langle nl, NL, \lambda\mu|-r_1{}^2|n_1l_1, n_2l_2, \lambda\mu\rangle \\ &= [(n_1+1)(n_1+l_1+\tfrac{3}{2})]^{-\frac{1}{2}} \sum_{n'l'N'L'} \{\langle nl, NL, \lambda\mu|-r_1{}^2|n'l', N'L', \lambda\mu\rangle \\ &\quad \cdot \langle n'l', N'L', \lambda|n_1l_1, n_2l_2, \lambda\rangle\}. \end{aligned}\tag{39}$$

To evaluate the matrix element in (39), we recall that from (2)

$$r_1{}^2 = \tfrac{1}{2}(r^2+R^2+2\mathbf{R}\cdot\mathbf{r}). \tag{40}$$

Using the standard methods of Racah [5]) we give the matrix elements in table 1 for all the values of n', l', N', L', consistent with the energy conservation rule

$$2n+l+2N+L = 2n'+l'+2N'+L'+2, \tag{41}$$

and the selection rules in the radial integrals, where these integrals were evaluated using (36) and the recurrence relation for Laguerre polynomials [10])

$$r^2 L_n^{l+\frac{3}{2}}(r^2) = (n+l+\tfrac{3}{2})L_n^{l+\frac{1}{2}}(r^2) - (n+1)L_{n+1}^{l+\frac{1}{2}}(r^2). \tag{42}$$

If we had started with the ket $|n_1 l_1, n_2+1 l_2, \lambda\mu\rangle$ we would have got the same expression (39), only with the first factor changed to index 2 instead of index 1, and the matrix element of $-r_2^2$ instead that of $-r_1^2$. As

$$r_2^2 = \tfrac{1}{2}(r^2+R^2-2\mathbf{R}\cdot\mathbf{r}) \tag{43}$$

the table for the matrix element of $-r_2^2$ would be the same table 1, but with the last four lines (that correspond to the matrix element of $\mathbf{R}\cdot\mathbf{r}$) with their signs changed.

TABLE 1

Matrix elements of $(-r_1^2)$

n'	l'	N'	L'	$\langle nl, NL, \lambda \| -r_1^2 \| n'l', N'L', \lambda\rangle$
$n-1$	l	N	L	$\frac{1}{2}[n(n+l+\frac{1}{2})]^{\frac{1}{2}}$
n	l	$N-1$	L	$\frac{1}{2}[N(N+L+\frac{1}{2})]^{\frac{1}{2}}$
$n-1$	$l+1$	$N-1$	$L+1$	$[nN(l+1)(L+1)]^{\frac{1}{2}}(-1)^{\lambda+L+l}W(ll+1LL+1;1\lambda)$
$n-1$	$l+1$	N	$L-1$	$[n(N+L+\frac{1}{2})(l+1)L]^{\frac{1}{2}}(-1)^{\lambda+L+l}W(ll+1LL-1;1\lambda)$
n	$l-1$	$N-1$	$L+1$	$[(n+l+\frac{1}{2})Nl(L+1)]^{\frac{1}{2}}(-1)^{\lambda+L+l}W(ll-1LL+1;1\lambda)$
n	$l-1$	N	$L-1$	$[(n+l+\frac{1}{2})(N+L+\frac{1}{2})lL]^{\frac{1}{2}}(-1)^{\lambda+L+l}W(ll-1LL-1;1\lambda)$

From table 1 and the considerations of the previous section, we see that we could determine straightforwardly the brackets for arbitrary n_1, n_2 once the brackets with $n_1 = n_2 = 0$ are given.

4. The Bracket $\langle nl, NL, \lambda | 0l_1, 0l_2, \lambda\rangle$

For the brackets with $n_1 = n_2 = 0$ we shall give explicit expressions rather than recurrence relations. To derive these expressions we shall need a formula for the translation of multipole fields [11]). This formula concerns the development of the multipole field $r^l Y_{lm}(\theta, \varphi)$ when the vector $\mathbf{r}$, of spherical coordinates (r, θ, φ) is represented by

$$\mathbf{r} = \mathbf{r}' - \mathbf{r}'' \tag{44}$$

where the spherical coordinates of $\mathbf{r}'$ and $\mathbf{r}''$ are given by (r', θ', φ') and $(r'', \theta'', \varphi'')$ respectively. As the multipole field is a solution of the Laplace equation, we see from (44) that

$$\nabla'^2 r^l Y_{lm}(\theta, \varphi) = 0, \quad \nabla''^2 r^l Y_{lm}(\theta, \varphi) = 0, \tag{45}$$

so $r^l Y_{lm}(\theta, \varphi)$ should be expanded in terms of multipole fields in $\mathbf{r}'$, $\mathbf{r}''$. Furthermore, the multipole fields are basis for the representation of the rotation group [5]). Combining these two facts we see immediately that

$$r^l Y_{lm}(\theta, \varphi) \\ = \sum_{l', l''=0}^{l} \delta_{l'+l'', l} G(l'l''l) \sum_{m'm''} \langle l'l''m'm''|lm\rangle r'^{l'} Y_{l'm'}(\theta', \varphi') r''^{l''} Y_{l''m''}(\theta'', \varphi'') \tag{46}$$

where $G(l'l''l)$ is a coefficient to be determined. Assuming now that $\theta' = \theta'' = 0$, we see from (44) that $\theta = 0$ and $r = r' - r''$, so that (46) becomes

$$[(2l+1)4\pi]^{\frac{1}{2}}(r'-r'')^l \\ = \sum_{l', l''=0}^{l} \delta_{l'+l'', l} G(l'l''l) \langle l'l''00|l0\rangle [(2l'+1)(2l''+1)]^{\frac{1}{2}} r'^{l'} r''^{l''}. \tag{47}$$

As (47) is valid for any r', r'' we obtain, using the explicit expression [5]) for Clebsch Gordan coefficients, that [11])

$$G(l'l''l) = (-1)^{l''}(4\pi)^{\frac{1}{2}}[(2l+1)!]^{\frac{1}{2}}[(2l'+1)!(2l''+1)!]^{-\frac{1}{2}}. \tag{48}$$

Let us now consider the ket $|0l_1, 0l_2, \lambda\mu\rangle$. From the definition of the Laguerre polynomials we have [6,10])

$$L_0^{l+\frac{1}{2}}(r^2) = 1 \tag{49}$$

so from (8) and (10) we obtain

$$|0l_1, 0l_2, \lambda\mu\rangle = 2[\Gamma(l_1+\tfrac{3}{2})\Gamma(l_2+\tfrac{3}{2})]^{-\frac{1}{2}} \exp[-\tfrac{1}{2}(r_1^2+r_2^2)]|l_1 l_2 \lambda\mu\rangle \tag{50}$$

where $|l_1 l_2 \lambda\mu\rangle$ stands for

$$|l_1 l_2 \lambda\mu\rangle = \sum_{m_1 m_2} \langle l_1 l_2 m_1 m_2|\lambda\mu\rangle r_1^{l_1} Y_{l_1 m_1}(\theta_1, \varphi_1) r_2^{l_2} Y_{l_2 m_2}(\theta_2, \varphi_2). \tag{51}$$

From (2) we have

$$\mathbf{r}_1 = \frac{1}{\sqrt{2}}\mathbf{R} + \frac{1}{\sqrt{2}}\mathbf{r}, \quad \mathbf{r}_2 = \frac{1}{\sqrt{2}}\mathbf{R} - \frac{1}{\sqrt{2}}\mathbf{r}. \tag{52}$$

Applying (46) to the multipole fields in (51), and using the relation [12])

$$Y_{l'm'}(\theta, \varphi) Y_{l''m''}(\theta, \varphi) = \sum_{l,m} H(l'l''l) \langle l'l''m'm''|lm\rangle Y_{lm}(\theta, \varphi), \tag{53}$$

where

$$H(l'l''l) = [(2l'+1)(2l''+1)/4\pi(2l+1)]^{\frac{1}{2}} \langle l'l''00|l0\rangle, \tag{54}$$

as well as the relation that reduces the summation of products of Clebsch-Gordan coefficients to $9j$ coefficients [13]), we obtain

$$
\begin{aligned}
|l_1 l_2 \lambda\mu\rangle = 2^{-\frac{1}{2}(l_1+l_2)} \sum_{L,l} \sum_{l'L'l''L''} \Big\{ (-1)^{l'} \delta_{L'+l',l_1} \delta_{L''+l'',l_2} \\
G(L'l'l_1)G(L''l''l_2)H(l'l''l)H(L'L''L) \\
[(2L+1)(2l+1)(2l_1+1)(2l_2+1)]^{\frac{1}{2}} \begin{Bmatrix} l' & l'' & l \\ L' & L'' & L \\ l_1 & l_2 & \lambda \end{Bmatrix} \\
r^{l'+l''-l} R^{L'+L''-L} [\sum_{M,m} \langle lLmM|\lambda\mu\rangle r^l Y_{lm}(\theta,\varphi) R^L Y_{LM}(\Theta,\Phi)] \Big\}.
\end{aligned}
\tag{55}
$$

From (54) we see that $l'+l''-l$, $L'+L''-L$ are non-negative even numbers, so that using the expansion formula of a power of the variable in terms of Laguerre polynomials † we have

$$
(r^2)^{\frac{1}{2}(l'+l''-l)} = \sum_{n=0}^{\frac{1}{2}(l'+l''-l)} \frac{(-1)^n [\frac{1}{2}(l'+l''-l)]!}{[\frac{1}{2}(l'+l''-l)-n]!} \frac{\Gamma[\frac{1}{2}(l'+l''+l+3)]}{\Gamma(n+l+\frac{3}{2})} L_n^{l+\frac{1}{2}}(r^2) \tag{56}
$$

and a similar expression for $R^{L'+L''-L}$. As the arguments of the factorials must always be non-negative, we see from (56) and the corresponding expression for R that

$$
\begin{aligned}
l'+l''-l-2n \geqq 0, \\
L'+L''-L-2N \geqq 0.
\end{aligned}
\tag{57}
$$

Adding these two expressions, we obtain from the Kronecker deltas in (55), that

$$
l_1+l_2-l-2n-L-2N \geqq 0. \tag{58}
$$

But, from the conservation of energy relation (13), we see that (58) is actually zero, so that in (57) both expressions must be zero. Therefore, when introducing (56) and the corresponding formula for R in (55), we can include the Kronecker deltas

$$
\delta_{l'+l'',2n+l}, \quad \delta_{L'+L'',2N+L}. \tag{59}
$$

Going now back to (50), where we replace $|l_1 l_2 \lambda\mu\rangle$ by its explicit expression in terms of (55), (56) etc., and comparing with the ket (11) as well as with the form (8) of the radial function, it is seen straightforwardly that

$$
\begin{aligned}
\langle nl, NL, \lambda | 0l_1, 0l_2, \lambda\rangle = \left[\frac{(2l+1)(2L+1)(2l_1+1)(2l_2+1)}{\Gamma(l_1+\frac{3}{2})\Gamma(l_2+\frac{3}{2}) n! \Gamma(n+l+\frac{3}{2}) N! \Gamma(N+L+\frac{3}{2})} \right]^{\frac{1}{2}} \\
2^{-\frac{1}{2}(l_1+l_2)} \sum_{l'L'l''L''} \Big\{ (-1)^{l'} \delta_{L'+l',l_1} \delta_{L''+l'',l_2} \delta_{l'+l'',2n+l} \delta_{L'+L'',2N+L} \\
G(L'l'l_1)G(L''l''l_2)H(l'l''l)H(L'L''L) \\
\begin{Bmatrix} l' & l'' & l \\ L' & L'' & L \\ l_1 & l_2 & \lambda \end{Bmatrix} (-1)^n [\tfrac{1}{2}(l'+l''-l)]! \Gamma[\tfrac{1}{2}(l'+l''+l+3)] \\
(-1)^N [\tfrac{1}{2}(L'+L''-L)]! \Gamma[\tfrac{1}{2}(L'+L''+L+3)] \Big\}.
\end{aligned}
\tag{60}
$$

† To obtain this formula we use the relation $L_n^{-n}(x) = (-1)^n (n!)^{-1} x^n$ and the expansion of $L_n^{\alpha}(x)$ in terms of $L_m^{\beta}(x)$.

The expression (60) gives then the explicit evaluation of the transformation bracket when $n_1 = n_2 = 0$. The Kronecker deltas in (60) reduce the quadruple summation to a single sum (the $\delta_{L'+L'', 2N+L}$ is a consequence of the other three δ's and of (13)), but we have in the summation $9j$ coefficients not readily available. We shall use the definition of the $9j$ coefficients in terms of Racah coefficients to simplify the expression (60) for the transformation brackets. It is well known that [13])

$$\begin{Bmatrix} l' & l'' & l \\ L' & L'' & L \\ l_1 & l_2 & \lambda \end{Bmatrix} = (-1)^k \begin{Bmatrix} l & l'' & l' \\ L & L'' & L' \\ \lambda & l_2 & l_1 \end{Bmatrix}$$
$$= \sum_x (2x+1)(-1)^{l+L-\lambda} W(lLl_1l_2; \lambda x) W(l''L''xL; l_2L') W(l'L'lx; l_1l'') \quad (61)$$

where k stands for the sum of all nine coefficients. From (60) we see that $l'+L' = l_1$, $l''+L'' = l_2$, so that the last two Racah coefficients appearing in (61) are expressed as simple products of factorials [14]). Substituting (61) in (60), making use of the explicit form of all factors in (60), and defining

$$q = l_1+l''-l' = l_2+L'-L'' \quad (62)$$

we obtain

$$\langle nl, NL, \lambda | 0l_1, 0l_2, \lambda \rangle$$
$$= \left[\frac{l_1!\, l_2!}{(2l_1)!(2l_2)!} \frac{(2l+1)(2L+1)}{2^{l+L}} \frac{(n+l)!}{n!(2n+2l+1)!} \frac{(N+L)!}{N!(2N+2L+1)!}\right]^{\frac{1}{2}} \quad (63)$$
$$(-1)^{n+l+L-\lambda} \sum_x \{(2x+1) A(l_1l, l_2L, x) W(lLl_1l_2; \lambda x)\},$$

where W is a Racah coefficient, and A is defined by

$$A(l_1l, l_2L, x)$$
$$= \left[\frac{(l_1+l+x+1)!(l_1+l-x)!(l_1+x-l)!}{(l+x-l_1)!}\right]^{\frac{1}{2}} \left[\frac{(l_2+L+x+1)!(l_2+L-x)!(l_2+x-L)!}{(L+x-l_2)!}\right]^{\frac{1}{2}} \quad (64)$$
$$\sum_q \left\{(-1)^{\frac{1}{2}(l+q-l_1)} \frac{(l+q-l_1)!}{[\frac{1}{2}(l+q-l_1)]!\,[\frac{1}{2}(l+l_1-q)]!} \frac{1}{(q-x)!(q+x+1)!} \frac{(L+q-l_2)!}{[\frac{1}{2}(L+q-l_2)]!\,[\frac{1}{2}(L+l_2-q)]!}\right\}.$$

From (62) we see that

$$l+q-l_1 = l''-l'+l \quad (65)$$

and as from (54) the right hand side is even, we conclude that the summation over q is restricted to those non-negative integer values of q for which $l+q-l_1$ is even and the arguments of the factorials are non-negative integers. The restrictions on x are given by the Racah coefficient, i.e.

$$|l-l_1| \leqq x \leqq l+l_1, \quad |L-l_2| \leqq x \leqq L+l_2. \quad (66)$$

In (63) we have then an explicit expression for the bracket with $n_1 = n_2 = 0$. Combining these results with the recurrence relations of the previous section, we could evaluate explicitly any transformation bracket for the harmonic oscillator wave functions.

5. Discussion

In section 2 we indicated the application of the transformation brackets to the evaluation of matrix elements for different types of forces, where these matrix elements in turn are of interest in the problems of energy levels, configuration mixing, etc., of nuclear shell theory. To determine the matrix elements, the brackets must be available in numerical form, and we shall estimate the number of brackets we need to tabulate.

We first note that from the definition (10) and (11) of the eigenkets and the relation (2), the brackets have the following symmetry properties:

$$\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda\rangle = (-1)^{L-\lambda}\langle nl, NL, \lambda | n_2 l_2, n_1 l_1, \lambda\rangle$$
$$= (-1)^{l_1-\lambda}\langle NL, nl, \lambda | n_1 l_1, n_2 l_2, \lambda\rangle = (-1)^{l_1+l}\langle NL, nl, \lambda | n_2 l_2, n_1 l_1, \lambda\rangle. \quad (67)$$

We can therefore restrict our evaluation to brackets in which

$$l_2 \geqq l_1, \quad L \geqq l. \quad (68)$$

Furthermore, in nuclear shell theory we are only interested in states in which [15])

$$2n_1+l_1 \leqq 6, \quad 2n_2+l_2 \leqq 6, \quad (69)$$

so that we have the restrictions

$$0 \leqq n_1, n_2 \leqq 3, \quad 0 \leqq l_1, l_2 \leqq 6. \quad (70)$$

Let us now consider brackets in which n_1, n_2 are given and define ρ and σ as

$$\rho = 2n_1+l_1+2n_2+l_2, \quad (71)$$

$$\sigma = l+L. \quad (72)$$

For a given σ and with the restriction (68), the number of possible pairs of values for l, L are given by $F(\sigma)$ where

$$F(\sigma) = \begin{cases} \frac{1}{2}(\sigma+2) & \text{if } \sigma \text{ is even,} \\ \frac{1}{2}(\sigma+1) & \text{if } \sigma \text{ is odd.} \end{cases} \quad (73)$$

Furthermore, from (11) and (68) we have

$$L-l \leqq \lambda \leqq L+l, \quad (74)$$

so that for a given l the number of possible values of λ is $2l+1$. Combining this with (73) we see that for a given σ the number of possible values of l, L, λ is $F^2(\sigma)$. Finally, from (13) we have $n+N = \frac{1}{2}(\rho-\sigma)$, so the number of possible pairs of values of n, N with ρ, σ given is

$$\tfrac{1}{2}(\rho-\sigma)+1. \quad (75)$$

From (13) and (14) we see that $\sigma \leqq \rho$ and $\rho-\sigma$ is even, and the above analysis shows that the number of kets $|nl, NL, \lambda\rangle$ where $L \geqq l$ and ρ is fixed, is

$$U(\rho) = \sum_{\substack{\sigma=0 \\ \rho-\sigma \text{ even}}}^{\rho} \{F^2(\sigma)[\tfrac{1}{2}(\rho-\sigma)+1]\}. \tag{76}$$

If n_1, n_2 are given we see from (71) that the number of possible pairs of values for l_1, l_2 is

$$F(\rho)-(n_1+n_2), \tag{77}$$

so that the total number of brackets becomes

$$\mathcal{N}(n_1, n_2) = \sum_{\rho=2(n_1+n_2)}^{12} \{[F(\rho)-(n_1+n_2)]U(\rho)\}. \tag{78}$$

From (78) we have, for $n_1 = n_2 = 0$, the number of brackets $\mathcal{N}(0, 0) = 6300$. Considering all the possibilities $n_1, n_2 = 0, 1, 2, 3$ allowed by (70), the total number of brackets is 49 680. This number is still reasonable for tabulation, particularly as it is probable that there are, besides (67), other symmetry properties which establish relations between the brackets. A general tabulation is planned using the 650 IBM machine of the University of Mexico.

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