## MATRIX ELEMENTS IN NUCLEAR SHELL THEORY

T. A. BRODY, G. JACOB† and M. MOSHINSKY††
Instituto de Física, Universidad de México, México, D.F.

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Abstract: In a previous paper, transformation brackets for harmonic oscillator function were defined and used for the evaluation of matrix elements for nuclear forces. Numerical tables for the transformation brackets are now available. The purpose of this paper is to show how these tables, combined with those given in the present note, can be used to evaluate the matrix elements of nuclear shell theory directly in terms of Talmi integrals. For comparison between present methods and those used previously, a relation between Slater coefficients and Talmi integrals is also obtained.

#### 1. Introduction

In a recent paper <sup>1</sup>) (to be referred to as I), one of us (M.M.) defined and gave explicit expressions for the transformation brackets for harmonic oscillator functions. These transformation brackets have been tabulated numerically <sup>2</sup>) by one of us (T.A.B.). The purpose of this paper is to show how these tables, combined with those given in the present note, can be used to evaluate the matrix elements of nuclear shell theory directly in terms of Talmi <sup>3</sup>) integrals.

We start by giving the definition of the transformation brackets. If we have a particle in an harmonic oscillator potential, its wave function is

$$\Re_{nl}(r)Y_{lm}(\theta,\varphi),\tag{1}$$

where  $Y_{lm}(\theta, \varphi)$  is a spherical harmonic and  $\Re_{nl}(r)$  is the radial function. Taking, as in I, r in units of  $(\hbar/m\omega)^{\frac{1}{2}}$ , the radial function has the form

$$\mathfrak{R}_{nl}(r) = r^{l} \exp\left(-\frac{1}{2}r^{2}\right) \sum_{k=0}^{n} (a_{nlk}r^{2k}), \tag{2}$$

where

$$a_{nlk} = \left[\frac{2(n!)}{\Gamma(n+l+\frac{3}{2})}\right]^{\frac{1}{2}} \binom{n+l+\frac{1}{2}}{n-k} \frac{(-1)^k}{k!},\tag{3}$$

and  $\Gamma$  stands for a gamma function. The two-particle wave function with total angular momentum  $\lambda$  is then given by

<sup>†</sup> On leave of absence from Faculdade de Filosofía e Instituto de Física, Universidade do Rio Grande do Sul, Pôrto Alegre, Brasil.

<sup>††</sup> Member of the Instituto Nacional de la Investigación Científica México, D.F.

$$|n_{1}l_{1}, n_{2}l_{2}, \lambda\mu\rangle = \sum_{m_{1}m_{2}} \{\langle l_{1}l_{2}m_{1}m_{2}|\lambda\mu\rangle\Re_{n_{1}l_{1}}(r_{1})Y_{l_{1}m_{1}}(\theta_{1}, \varphi_{1})\Re_{n_{2}l_{2}}(r_{2})Y_{l_{2}m_{2}}(\theta_{2}, \varphi_{2})\},$$

$$(4)$$

where  $\langle l_1 l_2 m_1 m_2 | \lambda \mu \rangle$  is a Clebsch-Gordan coefficient. If we now introduce the relative and centre-of-mass coordinates by the definition

$$\mathbf{r} = \frac{1}{\sqrt{2}} (\mathbf{r}_1 - \mathbf{r}_2), \qquad \mathbf{R} = \frac{1}{\sqrt{2}} (\mathbf{r}_1 + \mathbf{r}_2),$$
 (5)

we can construct a wave function of the same total angular momentum  $\lambda$  by

$$|nl, NL, \lambda\mu\rangle = \sum_{mM} \{\langle lLmM | \lambda\mu\rangle \Re_{nl}(r) Y_{lm}(\theta, \varphi) \Re_{NL}(R) Y_{LM}(\Theta, \Phi) \}.$$
 (6)

The transformation brackets we referred to are those connecting (6) and (4), i.e.

$$|n_1l_1, n_2l_2, \lambda\mu\rangle = \sum_{nlNL} |nl, NL, \lambda\mu\rangle\langle nl, NL, \lambda|n_1l_1, n_2l_2, \lambda\rangle.$$
 (7)

Because both kets must correspond to the same energy, nlNL are restricted to those non-negative integers for which

$$2n+l+2N+L = 2n_1+l_1+2n_2+l_2. (8)$$

With the help of the brackets defined in (7), it was shown that all matrix elements of nuclear shell theory for central, spin-orbit coupling and tensor forces, could be given in terms of the reduced matrix elements

$$\langle nl||V(r)||n'l'\rangle = \int_0^\infty \Re_{nl}(r)V(r)\Re_{n'l'}(r)r^2 dr, \qquad (9)$$

where V(r) is the radial part of the force between the particles and  $\Re_{nl}$  is given by (2).

The transformation brackets

$$\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda \rangle$$
 (10)

have been tabulated <sup>2</sup>) for  $n_1=n_2=0$  and for all values of  $l_1$ ,  $l_2$  up to 6, i.e. the i-shell <sup>†</sup>. The values of the brackets for  $n_1$ ,  $n_2 \neq 0$  can be obtained by recurrence <sup>1</sup>) relations from those in which  $n_1=n_2=0$ , and a general table will be available by the time this article is in print.

The tables published so far 2)  $(n_1=n_2=0)$  are arranged to give for each value of the set  $l_1l_2\lambda$ , all compatible values of nlNL, taking into account (8) and that

$$|l - L| \le \lambda \le l + L. \tag{11}$$

<sup>†</sup> The tables are available upon request from Instituto de Física, Apdo. Postal 31364, México 20, D.F.

An example, for  $l_1=1$ ,  $l_2=2$ ,  $\lambda=1$ , is given by table 1. In this table,  $\rho$  stands for the total energy (8) of the state in units of  $\hbar\omega$ , and the number

$l_1$	$l_2$	λ	n	l	N	L	ρ	$\langle nl, NL, \lambda   0l_1, 0l_2, \lambda \rangle$	p
1	2	1	0	0	1	1	3	0.408 248 29	0
			0	1	0	2		$0.235\ 702\ 26$	1
			0	1	1	0		$-0.527\ 046\ 28$	1
			0	<b>2</b>	0	1		$0.235\ 702\ 26$	2
			1	0	0	1		$-0.527\ 046\ 28$	0, 1, 2
			1	1	0	0		0.408 248 29 6	1, 2, 3

TABLE 1

in the lower right corner, before the vertical line, gives the number of brackets in the set. The number was shown to have the value 2)

$$\frac{1}{8}(\lambda+1)(\rho-\lambda+2)(\rho-\lambda+4), \quad \text{if } \rho-\lambda \text{ even,} \\ \frac{1}{8}\lambda(\rho-\lambda+1)(\rho-\lambda+3), \quad \text{if } \rho-\lambda \text{ odd.}$$
 (12)

The column marked p in table 1, which is separated from the table by a vertical line, indicates the index of the Talmi integrals compatible with each bracket, as discussed in the following sections.

To express the matrix elements of nuclear shell theory in terms of the Talmi integrals

$$I_{p} = 2[\Gamma(p + \frac{3}{2})]^{-1} \int_{0}^{\infty} r^{2p} \exp(-r^{2}) V(r) r^{2} dr, \tag{13}$$

we must first give the reduced matrix elements (9) in terms of  $I_p$ . From the definition (2, 3) of the radial functions it is clear that we can write

$$\langle nl||V(r)||n'l'\rangle = \sum_{p} B(nl, n'l', p)I_{p}, \qquad (14)$$

where B(nl, n'l', p) are certain coefficients whose explicit expression is given in the next section.

## 2. The coefficients B(nl, n'l', p)

From (9) and (2, 3) we see that

$$\langle nl||V(r)||n'l'\rangle = \sum_{k=-\infty}^{\infty} \sum_{k'=-\infty}^{\infty} a_{nlk} a_{n'l'k'} f(0, k, n) f(0, k', n')$$

$$\int_{0}^{\infty} r^{l+l'+2k+2k'} \exp(-r^{2}) V(r^{2}) r^{2} dr,$$
(15)

where to extend the summations from  $-\infty$  to  $+\infty$ , we introduce the step function f(a, x, b) defined for  $a \le b$  as follows:

$$f(a, x, b) = \begin{cases} 0, & \text{if } x < a, \\ 1, & \text{if } a \le x \le b, \\ 0, & \text{if } x > b. \end{cases}$$
 (16)

We now express k' in terms of a new variable p by  $\dagger$ 

$$k' = p - \frac{1}{2}(l + l') - k. \tag{17}$$

From (15) we obtain

$$\langle nl||V(r)||n'l'\rangle = \sum_{p=-\infty}^{\infty} \left\{ \sum_{k=-\infty}^{\infty} a_{nlk} a_{n'l'p-\frac{1}{2}(l+l')-k} \right.$$

$$f(0, k, n) f(0, p-\frac{1}{2}l-\frac{1}{2}l'-k, n') \frac{1}{2} \Gamma(p+\frac{3}{2}) I_p \right\},$$
(18)

where  $I_p$  is given by (13). Using the properties (16) of the step function f(a, x, b), we can write (18) as

$$\langle nl||V(r)||n'l'\rangle = \sum_{p=\frac{1}{2}(l+l')+n+n'}^{\frac{1}{2}(l+l')+n+n'} B(nl, n'l', p)I_p,$$
 (19)

where

$$B(nl, n'l', p) = \frac{1}{2}\Gamma(p + \frac{3}{2}) \sum_{k=0}^{\beta} a_{nlk} a_{n'l'p - \frac{1}{2}(l+l') - k}.$$
 (20)

The limits of the summation in (20) are given by

$$\alpha \equiv \max \left[0, \left(p - \frac{1}{2}l - \frac{1}{2}l' - n'\right)\right] = \begin{cases} 0 & \text{if } p - \frac{1}{2}(l + l') - n' \leq 0, \\ p - \frac{1}{2}(l + l') - n' & \text{if } p - \frac{1}{2}(l + l') - n' > 0. \end{cases}$$
(21)

$$\beta \equiv \min \left[ n, \left( p - \frac{1}{2}l - \frac{1}{2}l' \right) \right] = \begin{cases} p - \frac{1}{2}(l+l') & \text{if } p - \frac{1}{2}(l+l') \le n \\ n & \text{if } p - \frac{1}{2}(l+l') > n. \end{cases}$$
 (22)

From the explicit expression (3) of the  $a_{nlk}$  we obtain finally

$$B(nl, n'l', p) = \frac{(-1)^{p-\frac{1}{2}l-\frac{1}{2}l'}(2p+1)!}{2^{n+n'}p!} \left[ \frac{n!n'!(2n+2l+1)!(2n'+2l'+1)!}{(n+l)!(n'+l')!} \right]^{\frac{1}{2}}$$

$$\sum_{k=\alpha}^{\beta} \frac{(l+k)!(p-\frac{1}{2}l+\frac{1}{2}l'-k)!}{k!(2l+1+2k)!(n-k)!(2p-l+l'+1-2k)!(n'-p+\frac{1}{2}l+\frac{1}{2}l'+k)!(p-\frac{1}{2}l-\frac{1}{2}l'-k)!}$$
(23)

It will be shown in the next section that for diagonal matrix elements for all types of forces, we need to know only B(nl, nl, p) and B(nl, n-1l+2, p). These coefficients are tabulated at the end of the paper for all values of interest of n, l, p.

<sup>†</sup> As shown in I, l+l' is even for all types of forces, so p remains an integer.

## 3. The Diagonal Matrix Elements for Nuclear Forces

With the help of the coefficient  $B(nl, n'l', \phi)$  and the transformation brackets (10), we can give the matrix elements for nuclear forces directly in terms of Talmi integrals. We outline the procedure here only for the diagonal two particle matrix elements, but from the discussion in I, it is clear that the results can be generalized to any type of matrix element.

#### 3.1. CENTRAL FORCES

Let us consider the diagonal matrix element for a central force V(r), where r is the relative coordinate between two nucleons in a state  $|n_1 l_1, n_2 l_2, \lambda \mu\rangle$  given by (4). It was shown in I, eq. (19), that

$$\langle n_1 l_1, n_2 l_2, \lambda \mu | V(r) | n_1 l_1, n_2 l_2, \lambda \mu \rangle$$

$$= \sum_{n \mid N \mid} \{ [\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda \rangle]^2 \langle nl | | V(r) | | nl \rangle \delta_{\rho \varepsilon} \}, \quad (24)$$

where we introduce the Kronecker delta  $\delta_{o\varepsilon}$ ,

$$\rho = 2n_1 + l_1 + 2n_2 + l_2, \qquad \varepsilon = 2n + l + 2N + L,$$
(25)

to indicate explicitly that the transformation brackets vanish if  $\rho \neq \varepsilon$ , i.e. unless the energy conservation rule (8) is satisfied. From (24, 25) it is clear that none of the integers nlNL can exceed  $\rho$ .

From (19) we can write

$$\langle nl||V(r)||nl\rangle = \sum_{p=0}^{\rho} [B(nl, nl, p)f(l, p, 2n+l)I_p], \qquad (26)$$

where we again introduce the step function f(a, x, b) of (16) so that the summation can be extended from 0 to  $\rho$ , as from (25) it is clear that  $0 \le l \le 2n + l \le \rho$ . Substituting (26) in (24), and interchanging the summation order, we obtain

$$\langle n_1 l_1, n_2 l_2, \lambda \mu | V(r) | n_1 l_1, n_2 l_2, \lambda \mu \rangle = \sum_{p=0}^{\rho} C_c(n_1 l_1, n_2 l_2, \lambda, \rho) I_p,$$
 (27)

where

$$C_{c}(n_{1}l_{1}, n_{2}l_{2}, \lambda, p) = \sum_{nlNL=0}^{\rho} \{ [\langle nl, NL, \lambda | n_{1}l_{1}, n_{2}l_{2}, \lambda \rangle]^{2} \times B(nl, nl, p) \delta_{\rho\varepsilon} f(l, p, 2n+l) \}.$$
(28)

The matrix element (27) is then given directly in terms of Talmi integrals  $I_p$ , whose coefficients  $C_c$  are determined by (28) in terms of the transformation brackets (10) and the coefficients (23). An illustrative example is given in the next section.

#### 3.2. SPIN ORBIT COUPLING FORCES

As shown  $^{1,5}$ ) in I, for a spin orbit coupling force in LS coupling, it is enough to consider the reduced matrix element V(r)1 where r and 1 are the relative coordinate and angular momentum respectively. Following a procedure entirely similar to the previous subsection, we obtain

$$\langle n_1 l_1, n_2 l_2, \lambda | |V(r)\mathbf{l}| |n_1 l_1, n_2 l_2, \lambda \rangle = \sum_{p=0}^{\rho} C_{LS}(n_1 l_1, n_2 l_2, \lambda, p) I_p$$
 (29)

where, W being a Racah coefficient,

$$C_{LS}(n_1 l_1, n_2 l_2, \lambda, p) = \sum_{nlNL=0}^{\rho} \{ [l(l+1)(2l+1)(2\lambda+1)^2]^{\frac{1}{2}} \times (-1)^{L+1-l-\lambda} W(ll\lambda\lambda; 1L) [\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda \rangle]^2 \times B(nl, nl, p) \delta_{os} f(l, p, 2n+l) \}.$$
(30)

#### 3.3. TENSOR FORCES

As shown 1,5) in I, for a tensor force in LS coupling, it is enough to consider the reduced matrix element of the potential  $V(r)Y_{2\mu}(\theta, \varphi)$ , where  $(r, \theta, \varphi)$  are the polar components of the relative coordinate. As this potential does not commute with 1, we have that for diagonal matrix elements there are coefficients  $B(nl, n'l', \phi)$  with  $n' \neq n, l' \neq l$  but satisfying the relation

$$2n'+l'=2n+l, l'=l\pm 2, l.$$
 (31)

Following the same procedure as in previous subsections, we have

$$\langle n_1 l_1, n_2 l_2, \lambda || V(r) Y_2(\theta, \varphi) || n_1 l_1, n_2 l_2, \lambda \rangle = \sum_{p=0}^{\rho} C_T(n_1 l_1, n_2 l_2, \lambda, \phi) I_p$$
 (32)

where

$$C_{T}(n_{1}l_{1}, n_{2}l_{2}, \lambda, p) = \sum_{nlNL=0}^{\rho} \sum_{n'=0}^{\rho} \sum_{l'=|l-2|}^{l+2} \{\frac{1}{2}[1+(-1)^{l-l'}] \times \langle nl, NL, \lambda | n_{1}l_{1}, n_{2}l_{2}, \lambda \rangle \langle n'l', NL, \lambda | n_{1}l_{1}, n_{2}l_{2}, \lambda \rangle (-1)^{L-\lambda-l'} \times [(2\lambda+1)^{2}(2l+1)(5/4\pi)]^{\frac{1}{2}} \langle l200|l'0 \rangle W(ll'\lambda\lambda; 2L) \times B(nl, n'l', p) \delta_{n', n+\frac{1}{2}l-\frac{1}{2}l'} \delta_{\rho\varepsilon} f(\frac{1}{2}l+\frac{1}{2}l', p, \frac{1}{2}l+\frac{1}{2}l'+n+n') \}.$$
(33)

For the diagonal matrix elements for the three types of forces, we need therefore the coefficients

$$B(nl, nl, p), B(nl, n-1l+2, p)$$
 and  $B(nl, n+1l-2, p)$ .

But from the definition (9), (19) of B(nl, n'l', p) we see that

$$B(nl, n+1l-2, p) = B(n+1l-2, nl, p) = [B(n'l', n'-1l'+2, p)]_{n'=n}$$
(34)

so that actually we only need to tabulate the coefficients B(nl, nl, p) and

B(nl, n-1l+2, p). These coefficients are given at the end of this paper in tables 2 and 3 for all values of n, l, p such that  $\dagger$ 

$$2n+l \le 12, \quad \frac{1}{2}(l+l') \le p \le 2n+l.$$
 (35)

These values of the parameters will correspond to all levels of interest in nuclear shell theory, for a system of two particles in the i-shell or lower, as then

$$2n_1 + l_1 \le 6$$
,  $2n_2 + l_2 \le 6$ , and  $\rho \le 12$ . (36)

For convenient use, the tables are arranged in order of increasing p and there is a blank line between the sets of values corresponding to different p's. For a fixed p the tables are arranged in order of increasing l first and then of increasing n.

## 4. An Example: the (0p)(0d) Configuration

To illustrate the systematic procedure to be followed when we want to express the matrix elements in terms of Talmi integrals, we take the simple configuration (0p)(0d) i.e.  $n_1=0$ ,  $l_1=1$ ,  $n_2=0$ ,  $l_2=2$ , and then discuss the matrix element for a central force when the total angular momentum  $\lambda=1$ , i.e.

$$\langle 01, 02, 1||V(r)||01, 02, 1\rangle = \sum_{p=0}^{3} C_{e}(01, 02, 1, p)I_{p}$$
 (37)

The values of nlNL compatible with  $\rho=3$ ,  $\lambda=1$ , are given in table 1. For each set of values nlNL there is a corresponding set of p's that from (26) satisfies the inequality

$$l \le p \le 2n + l. \tag{38}$$

In table 1, in the column marked p, we give the values of p that satisfy (38) corresponding to the n, l in the same row. We see, for example, that p=0 appears in the first and fifth rows of the table, and therefore from (28) we have

$$C_{o}(01, 02, 1, 0) = [\langle 00, 11, 1|01, 02, 1\rangle]^{2} B(00, 00, 0) + [\langle 10, 01, 1|01, 02, 1\rangle]^{2} B(10, 10, 0).$$
(39)

From table 1 and table 2 we immediately obtain ††

$$C_c(01, 02, 1, 0) = \frac{7}{12}.$$
 (40)

<sup>†</sup> The lower bound of p is l+1 if l'=l+2 and l if l'=l.

<sup>††</sup> The coefficients  $C_e$  are clearly rational numbers, so in simple cases such as this example, the decimal fraction can be replaced by the corresponding simple fraction.

TABLE 2

	т	<del></del>			т	<del></del>	
n	l	Þ	B(nl, nl, p)	n	ı	Þ	B(nl, nl, p)
0	0	0	1.000 000 0	2	2	3	-31,500 001
l 1	0	0	1.500 000 0	3	2	3	-86.625 000
2	0	0	1.875 000 0	4	2	3	-187.687 51
3	0	0	2.187 500 0	5	2	3	-351.91408
4	0	0	2.460 937 4	0	3	3	1.000 000 0
5	0	0	2.707 031 2	1	3	3	4.500 000 1
6	о (	0	2.932 617 1	2	3	3	12.375 000
1	ŀ			3	3	3	26.812 500
1	0	1	$-3.000\ 000\ 1$	4	3	3	50.273 440
2	0	1	$-7.500\ 000\ 0$	[[		ĺ	
3	0	1	-13.125000	2	0	4	7.875 000 0
4	0	1	19.687 499	3	0	4	122.062 50
5	0	1	27.070 313	4	0	4	613.265 60
6	0	1	$-35.191\ 406$	5	0	4	1 976.132 8
0	1	1	1.000 000 0	6	0	4	4 970.786 1
1	1	1	2.500 000 0	2	1	4	-31.500000
2	1	1	4.375 000 1	3	1	4	-225.749 98
3	1	1	$6.562\ 500\ 0$	4	1	4	-851.812 50
4	1	1	9.023 437 8	5	1	4	-2 346.093 8
5	1	1	11.730 469	1	2	4	4.500 000 1
				2	2	4	56.250 003
1	0	2	2.500 000 1	3	2	4	<b>253</b> .687 50
2	0	2	16.250 002	4	2	4	764.156 22
3	0	2	45.937 501	5	2	4	1 834.980 6
4	0	2	95.156 252	1	3	4	-9.000 000 6
5	0	2	166.9 <b>33</b> 60	2	3	4	49.500 000
6	0	2	263.935 56	3	3	4	-160.87500
1	1	2	-5.000 000 0	4	3	4	-402.18752
2	1	2	$-17.500\ 000$	0	4	4	0.999 999 99
3	1	2	-39.375000	1	4	4	5.500 000 2
4	1	2	-72.187499	2	4	4	17.875 000
5	1	2	-117.304 69	3	4	4	44.687 504
0	2	2	1.000 000 0	4	4	4	94.960 939
1	2	2	3.500 000 0		_		
2	2	2	7.875 000 0	3	0	5	-86.625004
3	2	2	14.437 500	4	0	5	-851.812 50
4	2	2	23.460 938	5	0	5	-4 074.984 8
5	2	2	35.191 409	6	0	5	-13 583.883
2	0	3	17 500 000	2	1	5	12.375 000
3	0	3	$-17.500\ 000$ $-96.250\ 004$	3 4	1	5	253.687 50
4	0	3	$-96.250\ 004$ $-295.312\ 49$	5	1 1	5 5	1 572.140 6
5	0	3	-295.31249 $-685.78126$	2	1 -2	5 5	$egin{array}{cccccccccccccccccccccccccccccccccccc$
6	0	3	-085.78126 $-1349.0039$		_		
1	1	3	3.500 000 0	3 4	2 2	5 5	-437.25002 $-1957.3125$
2	1	3	33.250 000	5	2	5 5	-1957.3125 $-6233.9064$
3	1	3	122.062 51	1	3	5	- 6 233.906 4 5.500 000 2
4	î	3	310.406 24	2	3	5	85.249 998
5	1	3	645.175 79	3	3	5	455.812 49
1	2	3	-7.000 000 1	4	3	5	1 586.406 3
-	_	-		i i	4	5	-11.000000
	1	j		2	4	5	-71.499998
				<u> </u>			

TABLE 2

n	l	Þ	B(nl, nl, p)	n	l	Þ	B(nl, nl, p)
3	4	5	-268.125 01	2	6	7	-127.500 00
4	4	5	-759.68752	3	6	7	-605.62498
0	5	5	0.999 999 98	0	7	7	1.000 000 0
1	5	5	6.499 999 8	1	7	7	8.500 000 0
2	5	5	24.375 002	2	7	7	40.374 999
3	5	5	69.062 499	-			
	Ì			4	0	8	94.960 936
3	0	6	26.812 500	5	0	8	4 320.722 7
4	0	6	764.156 21	6	0	8	49 177.895
5	0	6	6 016.054 8	4	1	8	<b>— 759.687 49</b>
6	0	6	27 879.972	5	1	8	-14054.218
3	1	6	- 160.875 00	3	2	8	69.062 498
4	1	6	1 957.312 5	4	2	8	2 935.156 3
5	1	6	-11 133.892	5	2	8	31 932.776
2	2	6	17.874 999	3	3	8	<b>— 414.375 00</b>
3	2	6	455.812 51	4	3	8	-6 975.312 9
4	2	6	<b>3 3</b> 58.265 5	2	4	8	31.874 998
5	2	6	14 875.352	3	4	8	1 131.562 5
2	3	6	-71.499998	4	4	8	10 982.266
3	3	6	<b></b> 750.749 99	2	5	8	- 127.500 00
4	3	6	-3887.8127	3	5	8	1 763.750 1
1	4	6	6.500 000 3	1	6	8	8.500 000 2
2	4	6	120.250 00	2	6	8	208.250 01
3	4	6	743.437 47	3	6	8	1 635.187 4
4	4	6	2 935.156 2	1	7	8	-16.999 999
1	5	6	$-13.000\ 001$	2	7	8	<b>— 161.499 99</b>
2	5	6	$-97.500\ 002$	0	8	8	0.999 999 99
3	5	6	<b>- 414.375 00</b>	1	8	8	9.499 999 7
0	6	6	1.000 000 1	2	8	8	49.875 004
1	6	6	7.500 000 7				
2	6	6	31.875 000	5	0	9	-1804.2578
3	6	6	100.937 50	6	0	9	-40595.799
				4	1	9	164.023 43
4	0	7	- 402.187 49	5	1	9	8 939.277 0
5	0	7	-6 233.906 7	4	2	9	-1 312.187 5
6	0	7	-42 983.790	5	2	9	$-28\ 212.033$
3	1	7	44.687 502	3	3	9	100.937 50
4	1	7	1 586.406 2	4	3	9	4 996.406 4
5	1	7	14 875.352	3	4	9	-605.62496
3	2	7	- 268.125 02	4	4	9	-11 607.813
4	2	7	-3887.8126	2	5	9	40.375 000
5	2	7	-25626.048	3	5	9	1 635.187 5
2	3	7	24.375 000	2	6	9	-161.50000
3	3	7	743.437 55	3	6	9	-2503.2498
4	3	7	6 346.640 8	1	7	9	9.499 999 7
2	4	7	-97.499999	2	7	9	261.249 99
3	4	7	-1186.2500	1	8	9	-19.00000
4	4	7	-6975.3128	2	8	9	-199.50000
1	5	7	7.500 000 4	0	9	9	0.999 999 97
2	5	7	161.250 02	1	9	9	10.500 000
3	5	7	1 131.562 6			İ	
1	6	7	$-15.000\ 001$				

5							l
	0	10	344.449 21	6	0	11	<b>-7 922.331 9</b>
6	0	10	22 905.872	5	1	11	609.410 12
5	1	10	3 444.492 3	5	2	11	<b>-6094.1014</b>
4	2	10	264.960 93	4	3	11	406.273 40
5	2	10	16 825.019	4	4	11	-3250.1873
4	3	10	-2 119.687 5	3	5	11	191.187 50
3	4	10	141.312 49	3	6	11	-1147.1250
4	4	10	7 984.156 2	2	7	11	60.375 000
3	5	10	<b> 847.874 98</b>	2	8	11	-241.500 00
2	6	10	49.875 002	1	9	11	11.500 000
3	6	10	2 269.312 5	1	10	11	-23.000 000
2	7	10	-199.50000	0	11	11	1.000 000 0
1	8	10	10.500 000	[]			
2	8	10	320.250 01	6	0	12	1 269.604 5
1	9	10	-21.000000	5	2	12	1 015.683 5
0	10	10	1.000 000 0	4	4	12	597.460 94
1	10	10	11.500 000	3	6	12	251.562 49
[				2	8	12	71.875 003
				1	10	12	12.500 001
				0	12	12	0.999 999 98

TABLE 2

In a similar fashion we obtain

$$C_{\mathfrak{o}}(01, 02, 1, 1) = -\frac{1}{12}, \quad C_{\mathfrak{o}}(01, 02, 1, 2) = -\frac{1}{12},$$

$$C_{\mathfrak{o}}(01, 02, 1, 3) = \frac{7}{12}. \tag{41}$$

Thus the matrix element (37) can be written in terms of Talmi integrals as

$$\langle 01, 02, 1||V(r)||01, 02, 1\rangle = \frac{1}{12}(7I_0 - I_1 - I_2 + 7I_3)$$
 (42)

We can now give the general procedure for the calculation of the matrix elements:

- 1. Given a definite state  $|n_1l_1, n_2l_2, \lambda\mu\rangle$  we look in the table 2) of the transformation brackets to get all values of nlNL compatible with (8) and (11). These values are immediately available, as shown in table 1.
- 2. For each set nlNL we determine all values of p compatible with the inequality (38).
- 3. We then take the brackets corresponding to a definite p, square them and multiply by the corresponding B's of table 2, and add them to obtain the coefficients  $C_c(n_1l_1, n_2l_2, \lambda, p)$ . For spin orbit coupling and tensor forces, one follows a similar procedure as indicated in Section 3.

The analysis outlined above is particularly suitable for machine computation. It is planned to give tables of coefficients C at some future date.

TABLE 3

n	ı	Þ	B(nl, n-1 l+2, p)	n	ı	Þ	B(nl, n-1 l+2, p)
1	0	1	0.948 683 34	2	3	4	8.112 490 1
2	0	1	1.984 313 6	3	3	4	23.124 156
3	0	1	3.214 955 2	4	3	4	53.298 544
4	0	1	4.617 128 0		_		
5	0	1	6.172 981 2	3	0	5	65.676 943
6	0	1	7.869 037 8	4	o	5	613.638 33
ľ		-		5	0	5	2 843.415 3
1	0	2	-1.581 138 8	6	o	5	9 272.493 8
2	0	2	$-8.031\ 745\ 1$	2	1	5	-8.2499998
3	Ŏ	2	-20.667570	3	ī	5	-149.27920
4	ŏ	2	-40.674 700	4	i	5	-864.191 85
5	ő	2	-69.078 598	5	î	5	-3 163.860 4
6	o	2	-106.794.08	2	2	5	24.045 529
1	ì	2	1.336 306 2	3	2	5	185.891 58
2	1	2	3.750 000 0	4	2	5	769.122 29
3	1	2	7.616 286 4	5	2	5	2 323.892 0
4	1	2	13.145 910	1	3	5	$-2.345\ 207\ 9$
5	1	2	20.524 045	2	3	5	-26.694946
1 "	1	2	20.324 043	3	3	5	-123.921.76
2	0	3	11.244 443	4	3	5	-395.866 95
3	0	3	56.440 324	1	4	5	2.157 277 5
4	0	3	164.677 56	2	4	5	10.650 704
5	0	3	370.378 87	3	4	5	34.717 049
6	0	3	712.585 09	4	4	5	90.058 236
1 1	1	3	-1.8708287	*	4	3	90.038 230
$\begin{array}{c c} & 1 \\ & 2 \end{array}$	1	3		9			$-21.892\ 314$
	1	i I	-13.416 667	3	0	6	
3		3	-43.835 958	4	0	6	-591.652 01
4	l	3	-104.290 89	5	0	6	-4 510.979 <b>3</b>
5	1	3	-207.520 90	6	0	6	-20 451.255
1	2	3	1.649 915 9	3	1	6	107.812 76
2	2	3	5.804 093 2	4	1	6	1 224.322 4
3	2	3	14.167 616	5	1	6	6 661.648 8
4	2	3	28.555 744	2	2	6	-10.779 030
5	2	3	50.982 201	3	2	6	-238.825.55
	_		* 0** 0 * 0 * 0	4	2	6	-1 624.414 0
2	0	4	-5.9529404	5	2	6	-6 822.875 7
3	0	4	83.588 838	2	3	6	31.548 572
4	0	4	-399.171 70	3	3	6	286.739 53
5	0	4	-1 245.819 8	4	3	6	1 360.889 6
6	0	4	-3065.3480	1	4	6	-2.549 509 8
2	1	4	17.250 000	2	4	6	-34.405004
3	1	4	109.951 47	3	4	6	-183.263 94
4	1	4	387.923 84	4	4	6	$-659.881\ 25$
5	1	4	1 022.470 6	1	5	6	2.373 464 5
1	2	4	$-2.121\ 320\ 3$	2	5	6	13.400 094
2	2	4	-19.673615	3	5	6	49.159 048
3	2	4	-77.829 89 <b>3</b>		_	_	999 697 77
4	2	4	-216.94950	4	0	7	328.695.55
5	2	4	-494.59357	5	0	7	4 932.506 0
1	3	4	1.918 806 4	6	0	7	33 271.041

TABLE 3

		,		LE 3			
n	ı	Þ	B(nl, n-1 l+2, p)	n	l	Þ	B(nl, n-1 l+2, p)
3	1	7	-33.003 905	2	6	9	57.755 410
4	1	7	-1091.1105	3	6	9	760.425 04
5	ī	7	-9 783.128 0	i	7	9	-3.082 207 1
3	2	7	162.835 59	2	7	9	-61.155563
4	2	7	2 177.282 8	1	8	9	2.931 763 6
5	2	7	13 603.484	2	8	9	22.780 199
2	3	7	-13.520817				
3	3	7	-354.57041	5	0	10	-302.10195
4	3	7	-2770.4791	6	0	10	-19640.402
2	4	7	39.698 080	5	ı	10	$2\ 704.246\ 2$
3	4	7	414.748 08	4	2	10	-193.50011
4	4	7	2 220.634 0	5	2	10	-11623.941
1	5	7	$-2.738\ 612\ 8$	4	3	10	1 345.036 5
2	5	7	-42.746905	3	4	10	<b>- 83</b> .952 135
3	5	7	-256.917 21	4	4	10	-4298.2337
1	6	7	2.572 478 9	3	5	10	415.738 74
2	6	7	16.345 871	2	6	10	$-22.884\ 219$
3	6	7	66.648 271	3	6	10	-879.757 15
				2	7	10	67.592989
4	0	8	-80.982 960	1	8	10	$-3.240\ 370\ 2$
5	0	8	-3564.6518	2	8	10	-71.155540
6	0	8	<b>39</b> 686.181	1	9	10	3.096 281 1
4	1	8	562.087 23	! !			
5	1	8	9 938.613 2	6	0	11	6 949.680 9
3	2	8	-46.918729	5	1	11	$-497.581\ 27$
4	2	8	1 834.613 8	5	2	11	4 455.844 2
5	2	8	-18 911.085	4	3	11	$-278.701\ 25$
3	3	8	231.834 49	4	4	11	1 938.419 1
4	3	8	3 567.358 2	3	5	11	-107.43809
2	4	8	$-16.460\ 178$	3	6	11	532.484 60
3	4	8	-498.66304	2	7	11	-26.349 809
4	4	8	-4 400.787 9	2	8	11	77.932 257
2	5	8	48.446 492	1	9	11	$-3.391\ 164\ 8$
3	5	8	571.996 36	1	10	11	3.252 691 1
1	6	8	-2.9154759	) ]			
2	6	8	-51.675895	6	0	12	$-1\ 135.568\ 8$
3	6	8	$-345.869\ 45$	5	2	12	-778.99370
1	7	8	2.757 764 3	4	4	12	-387.68385
2	7	8	19.475 947	3	6	12	-134.46582
<b> </b> _	_ j			2	8	12	-29.973948
5	0	9	1 539.281 4	1	10	12	-3.5355338
6	0	9	33 870.982				
4	1	9	- 128.670 57				
5	1	9	-6696.2288				
4	2	9	893.786 22	)			
5	2	9	18 196.521				
3	3	9	-63.838 480				
4	3	9	-2882.2213		'		
3	4	9	315.819 94				
4 2	4 5	9	$5496.8270 \\ -19.584752$				
3	5	9	-19.584752 $-673.10080$	] .[			
"		9	- 013.100 00		'		
<u> </u>				<u>'</u>			

# 5. Transformation Brackets and the Relation between Slater Coefficients and Talmi Integrals

The usual method of calculating matrix elements for nuclear forces is based on the reduction of the matrix elements to Slater coefficients  $^{3, 6, 7}$ ). For the sake of comparison we shall derive in this section a relation between Slater coefficients and Talmi integrals, using the coefficients  $C_c(n_1l_1, n_2l_2, \lambda, p)$  discussed in the previous sections.

Using the well known methods of Racah, we can write the matrix elements for a central force

$$\begin{split} \langle n_1 l_1, \, n_2 l_2, \, \lambda \mu | V(|\mathbf{r}_1 - \mathbf{r}_2|) | n_1 l_1, \, n_2 l_2, \, \lambda \mu \rangle \\ &= \sum_k \left\{ F^k(n_1 l_1, \, n_2 l_2) (-1)^{\lambda} \, \frac{(2l_1 + 1) (2l_2 + 1)}{2k + 1} \right. \\ & \left. W(l_1 l_1 l_2 l_2; \, k\lambda) \, \langle l_1 l_1 \, 00 | k0 \rangle \, \langle l_2 l_2 00 | k0 \rangle \right\}, \end{split}$$

where  $W(l_1 l_1 l_2 l_2; k\lambda)$  is a Racah coefficient<sup>8</sup>) and  $F^k$  stands for the Slater coefficient

$$\begin{split} F^{k}(n_{1}l_{1}, n_{2}l_{2}) &= \frac{1}{2}(2k+1) \int_{0}^{\infty} \int_{0}^{\infty} \int_{-1}^{1} R_{n_{1}l_{1}}^{2}(r_{1}) R_{n_{2}l_{2}}^{2}(r_{2}) V(|\mathbf{r}_{1}-\mathbf{r}_{2}|) P_{k}(\cos \omega) r_{1}^{2} dr_{1} r_{2}^{2} dr_{2} d\cos \omega \end{split}$$

$$(44)$$

where  $\omega$  is the angle between  $\mathbf{r}_1$  and  $\mathbf{r}_2$ .

Comparing (43) with (27), and using the orthogonality relation 8) for Racah coefficients, we obtain

$$F^{k}(n_{1}l_{1}, n_{2}l_{2}) = (2k+1)^{2}[(2l_{1}+1)(2l_{2}+1)\langle l_{1}l_{1}00|k0\rangle\langle l_{2}l_{2}00|k0\rangle]^{-1}$$

$$\sum_{\lambda} \{(2\lambda+1)(-1)^{\lambda}W(l_{1}l_{1}l_{2}l_{2}; k\lambda)\sum_{p=0}^{\rho} [C_{c}(n_{1}l_{1}, n_{2}l_{2}, \lambda, \rho)I_{p}]\}.$$

$$(45)$$

In (45) we have a closed expression for the Slater coefficients in terms of Talmi integrals.

In using tables 2 and 3, it is to be noted that though all values are given to eight significant digits, the last of these may be out by several units, due to the accumulation of rounding-off errors in the calculations. Thus B(04, 04, 4) in table 2 can be taken as equal to 1.

Within the limits of rounding-off errors, all values in tables 2 and 3 obey the sum rules

$$\sum_{p} (p + \frac{3}{2}) B(nl, n - 1 l + 2, p) = -2\sqrt{n(n + l + \frac{3}{2})}, \quad \sum_{p} B(nl, nl, p) = 1, (46)$$

which are easily obtained from the definition (14) together with (9) and (13).

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The tabulation of the coefficients B(nl, n'l', p), as well as the tabulation of the transformation brackets, was done with the 650 IBM machine at the University of Mexico. We are indebted to Ing. S. Beltran for making available the machine for the present calculations and to Raúl Ortega for help in carrying them out.

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Note added in proof: The transformation brackets have also been discussed recently by R. D. Lawson and M. Goeppert-Mayer, Phys. Rev. 117 (1960) 174;

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