

## On Energy Matrices for the Independent Particle Model

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A method which makes use of Fourier transforms of two-body interactions for the calculations of energy matrices in the independent particle model is proposed. The non-central interactions as well as central ones can be easily expanded into series of tensor products of spherical harmonics by this procedure. Furthermore, the radial integrals can be reduced to simple integrals which involve the Fourier transforms of the radial dependence of the interactions. For the harmonic oscillator wave functions, the procedure can be easily carried out and explicit formulas for the integrals are obtained. Useful tables for the calculations of the integrals for the central, tensor and spin-orbit interactions are given.

### § 1. Introduction

The matrix elements of two-body interactions are necessary in the investigation of nuclear properties by means of the independent particle model. The calculations of these matrix elements are usually carried out by expanding the interactions into series of Legendre polynomials.<sup>1)</sup> For the central interaction, it is well known that this procedure is quite easy if one applies the methods of tensor operator proposed by Racah.<sup>2)</sup> For the non-central interactions, the situations are somewhat complicated and the interactions have been discussed by Talmi,<sup>3)</sup> Hope and others.<sup>4)</sup>

In the next two sections of this paper, it is shown that the two-body interactions can be easily expanded into series of the products of spherical harmonics by considering Fourier transforms of the interactions, and the matrix elements can be obtained by straightforward application of the method of tensor operators. This procedure is much simpler and more systematic than those proposed so far for the treatment of the non-central interactions.

The radial integrals which appear in this expansion involve the variables  $r_1$  and  $r_2$ , the distances of the two particles from the origin, in separated forms in the integrands, because the Fourier transform is considered. Therefore, the

integrations over  $r_1$  and  $r_2$  are manageable and the integrals can be expressed by means of simple ones. However, it is difficult to carry out the integrations over  $r_1$  and  $r_2$  analytically for the wave functions with arbitrary radial dependence.

In order to avoid this difficulty, we assume three-dimensional isotopic harmonic oscillator wave functions for one-particle wave functions and consider the radial integrals in the last few sections of this paper. Then, the radial integrals can be obtained as linear combinations of simple integrals. The coefficients are expressed in terms of the expansion coefficients of the product of two associated Laguerre polynomials into power series. Simple recurrence formulas between the latter coefficients are obtained and they are useful for the evaluation of the radial integrals. The simple integrals into which the radial integrals are reduced have linear relations with the Talmi integrals which have been introduced as the integrals over relative coordinates after the separation of the center-of-mass motion of two particles in the harmonic oscillator potential.<sup>5)</sup> By making use of the relations, the expansion coefficients of the radial integrals into the Talmi integrals, which have been given by several authors in some cases for the central interactions,<sup>6)</sup> are easily obtained. Although the method which expands the two particle wave function into products of the wave functions of the relative and the center-of-mass motions and calculates the matrix elements of the interaction directly has been proposed,<sup>7)</sup> our procedure seems to be simpler than that for the calculations of the energy matrices of individual configurations.

## § 2. The central and tensor interactions

Two-particle matrix elements of the interactions are exclusively considered in this paper, since it is well known that matrix elements of the two-body interactions for many-particle configurations can be reduced to the two-particle ones.<sup>1),8)</sup> Let us first decompose the tensor interaction into spin and ordinary space parts, as an example. This interaction is defined as  $S_{12}V(r)$ , where  $S_{12} = (\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_2 \cdot \mathbf{r})/r^2 - 1/3 \cdot (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$  and  $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$  ( $r = |\mathbf{r}|$ ). It is easy to write the  $S_{12}$  as a scalar product of tensor operators of second rank which operate spin and ordinary spaces, respectively:<sup>3)</sup>

$$S_{12}V(r) = (2/3)^{1/2} ([\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2]^{(2)} \cdot V(r) \mathbf{C}^{(2)}(\boldsymbol{\Omega})), \quad (1)$$

where  $\boldsymbol{\Omega}$  denotes the direction of the vector  $\mathbf{r}$  and  $C_q^\kappa(\boldsymbol{\Omega}) = [4\pi/(2\kappa+1)]^{1/2} Y_{\kappa q}(\boldsymbol{\Omega})$  are the unnormalized spherical harmonics.\* It is seen from (1) that the spatial part of the tensor interaction is taken to be  $V(r)\mathbf{C}^{(2)}(\boldsymbol{\Omega})$ . In this section, we discuss the interactions the spatial parts of which has the form of  $V(r)\mathbf{C}^{(\kappa)}(\boldsymbol{\Omega})$ ,  $\kappa$  being zero or even positive integers. If  $\kappa$  equals zero, the interaction is central, since

\* For the notation, see reference 9). The formulas used in this paper are also contained in it, unless otherwise stated.

$C^{(0)}=1$ , and if  $\kappa$  equals two, the interaction is tensor. The spin parts are simple to be handled and only the spatial parts have to be treated in detail.

In order to separate the variables  $\mathbf{r}_1$  and  $\mathbf{r}_2$  in the spatial part of the interaction, we introduce its Fourier transform  $\mathbf{v}^{(\kappa)}(\mathbf{p})$  :

$$\mathbf{v}^{(\kappa)}(\mathbf{p}) = (2\pi)^{-3} \int V(r) C^{(\kappa)}(\Omega) \exp(i\mathbf{p} \cdot \mathbf{r}) d\mathbf{r}. \tag{2}$$

By making use of the well-known formula

$$\exp(i\mathbf{p} \cdot \mathbf{r}) = \sum_k i^k (2k+1) j_k(pr) (C^{(k)}(\Omega) \cdot C^{(k)}(\Omega_p)), \tag{3}$$

where  $j_k(pr)$  are the spherical Bessel functions and  $\Omega_p$  denotes the direction of vector  $\mathbf{p}$ , and the orthonormality relation of the spherical harmonics,  $\mathbf{v}^{(\kappa)}(\mathbf{p})$  becomes

$$\mathbf{v}^{(\kappa)}(\mathbf{p}) = (4\pi)^{-1} i^\kappa v_\kappa(p) C^{(\kappa)}(\Omega_p), \tag{4}$$

where

$$v_\kappa(p) = \frac{2}{\pi} \int_0^\infty V(r) j_\kappa(pr) r^2 dr. \tag{5}$$

Then, the spatial part of the interaction is expressed by the Fourier inverse transform as

$$V(r) C^{(\kappa)}(\Omega) = (4\pi)^{-1} i^\kappa \int v_\kappa(p) C^{(\kappa)}(\Omega_p) \exp(-i\mathbf{p} \cdot (\mathbf{r}_2 - \mathbf{r}_1)) d\mathbf{p}.$$

In this form of  $V(r) C^{(\kappa)}(\Omega)$ , the variables  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are separated and the integration over  $\Omega_p$  can be carried out by applying (3) for  $\exp(i\mathbf{p} \cdot \mathbf{r}_1)$  and  $\exp(-i\mathbf{p} \cdot \mathbf{r}_2)$ , respectively. Taking into account the symmetry relation of the Clebsch-Gordan coefficients, we have the result :

$$V(r) C^{(\kappa)}(\Omega) = \sum_{k_1, k_2} i^{k_1 - k_2 + \kappa} (2k_1 + 1) (2k_2 + 1) / (2\kappa + 1) \times (k_1 0 k_2 0 | \kappa 0) v^{(k_1, k_2; \kappa)}(r_1, r_2) [C_1^{(k_1)} \times C_2^{(k_2)}]^{(\kappa)}, \tag{6}$$

where  $C_i^{(k)}$  means  $C^{(k)}(\Omega_i)$  and

$$v^{(k_1, k_2; \kappa)}(r_1, r_2) = \int_0^\infty j_{k_1}(pr_1) j_{k_2}(pr_2) v_\kappa(p) p^2 dp. \tag{7}$$

In (6), the summations over  $k_1$  and  $k_2$  are restricted by  $|k_1 - k_2| \leq \kappa \leq k_1 + k_2$  and  $k_1 + k_2 + \kappa = \text{even}$  from the properties of the Clebsch-Gordan coefficients. The formula (6) is useful for the calculation of the reduced matrix elements. They are easily obtained by means of the method of tensor operators<sup>2),9)</sup> as

$$(l_1 l_2 L \| V(r) C^{(\kappa)}(\Omega) \| l'_1 l'_2 L') = \sum_{k_1, k_2} i^{k_1 - k_2 + \kappa} (2k_1 + 1) (2k_2 + 1) / (2\kappa + 1) \cdot (k_1 0 k_2 0 | \kappa 0) \times [(2L + 1) (2L' + 1) (2\kappa + 1)]^{1/2} (l_1 \| C^{(k_1)} \| l'_1) (l_2 \| C^{(k_2)} \| l'_2) \times X \begin{pmatrix} l_1 & l_2 & L \\ l'_1 & l'_2 & L' \\ k_1 & k_2 & \kappa \end{pmatrix} R^{(k_1, k_2; \kappa)}(l_1 l_2; l'_1 l'_2), \tag{8}$$

where  $R^{(k_1, k_2; \kappa)}(l_1 l_2; l'_1 l'_2)$  are radial integrals:

$$R^{(k_1, k_2; \kappa)}(l_1 l_2; l'_1 l'_2) = \int_0^\infty \int_0^\infty R_{l_1}(r_1) R_{l_2}(r_2) v^{(k_1, k_2; \kappa)}(r_1, r_2) R_{l'_1}(r_1) R_{l'_2}(r_2) r_1^2 dr_1 r_2^2 dr_2, \quad (9)$$

$R_l(r)$  being the radial functions of the one-particle wave functions. (In this section, the principal quantum numbers  $n$  are omitted for the sake of simplicity.)

For the central interaction  $\kappa=0$ , (6) gives, by putting  $k_1=k_2=k$ ,

$$V(r) = \sum_k (2k+1) v^{(k)}(r_1, r_2) P_k(\cos \omega), \quad (10)$$

where  $\omega$  is the angle between the two radii vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$  (Fig. 1).  $P_k(\cos \omega)$  are the Legendre polynomials, and  $v^{(k)}(r_1, r_2)$  means  $v^{(k, k; 0)}(r_1, r_2)$ . By inserting the  $v_0(p)$  of (5) into (7) and making use of a formula of the Bessel functions:<sup>10)</sup>

$$\frac{2}{\pi} \int_0^\infty j_k(pr_1) j_k(pr_2) j_0(pr) p^2 dp = P_k(\cos \omega) / (2r_1 r_2 r), \quad (11)$$

it is given by

$$v^{(k)}(r_1, r_2) = \frac{1}{2} \int_{-1}^1 V(r) P_k(\cos \omega) d(\cos \omega). \quad (12)$$

The matrix element is reduced from (8) to

$$\begin{aligned} & (l_1 l_2 LM | V(r) | l'_1 l'_2 LM) \\ &= \sum_k (-)^{l_1+l'_2-L} (l_1 \| C^{(k)} \| l'_1) (l_2 \| C^{(k)} \| l'_2) W(l_1 l_2 l'_1 l'_2; Lk) (2k+1) R^{(k)}(l_1 l_2; l'_1 l'_2), \end{aligned} \quad (13)$$

which agrees with the well-known formula given by Racah.<sup>2)</sup>

For the tensor interaction given by (1), the matrix elements are easily obtained in the  $LS$ -coupling as

$$\begin{aligned} & (l_1 l_2 SLJM | S_{12} V(r) | l'_1 l'_2 S' L' JM) = (2/3)^{1/2} (S \| [\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2]^{(2)} \| S') \\ & \times (l_1 l_2 L \| V(r) C^{(2)}(\Omega) \| l'_1 l'_2 L') (-)^{S+L'-J} W(SLS'L'; J2), \end{aligned} \quad (14)$$

where  $(S \| [\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2]^{(2)} \| S') = 2 \cdot 5^{1/2} \delta_{S,1} \delta_{S',1}$  and the reduced matrix elements for the spatial part are given by putting  $\kappa=2$  in (8). The summations over  $k_1$  and  $k_2$  are restricted by  $|k_1 - k_2| \leq 2 \leq k_1 + k_2$  and  $k_1 + k_2 = \text{even}$ . If the matrix elements of the tensor interaction in  $jj$ -coupling is to be calculated, the interaction may be transformed from (1) and (6) by changing the coupling schemes of the tensor operators as

$$\begin{aligned} S_{12} V(r) &= (2/3)^{1/2} \sum_{k_1, k_2, K} i^{k_1+k_2} (2k_1+1) (2k_2+1) (k_1 0 k_2 0 | 20) \\ & \times W(k_1 1 k_2 1; K2) v^{(k_1, k_2; 2)}(r_1, r_2) ([\boldsymbol{\sigma}_1 \times \mathbf{C}_1^{(k_1)}]^{(K)} \cdot [\boldsymbol{\sigma}_2 \times \mathbf{C}_2^{(k_2)}]^{(K)}). \end{aligned} \quad (15)$$

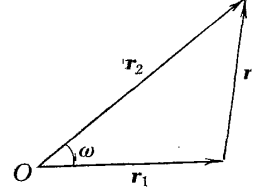


Fig. 1

For  $\kappa=2$ , the radial dependences  $v^{(k_1, k_2; 2)}(r_1, r_2)$  of the interaction can be written in somewhat different forms. Carrying out partial integrations in (7) after putting  $j_2(\rho) = \rho^2(\rho^{-1}d/d\rho)^2 j_0(\rho)$ , and applying the recurrence formulas for the Bessel functions, they are given by

$$v^{(k, k; 2)}(r_1, r_2) = r_1 r_2 \{ (2k+3)w^{(k-1)}(r_1, r_2) + (2k-1)w^{(k+1)}(r_1, r_2) \} / (2k+1) - (r_1^2 + r_2^2)w^{(k)}(r_1, r_2), \tag{16a}$$

and

$$v^{(k, k+2; 2)}(r_1, r_2) = r_2^2 w^{(k)}(r_1, r_2) - 2r_1 r_2 w^{(k+1)}(r_1, r_2) + r_1^2 w^{(k+2)}(r_1, r_2). \tag{16b}$$

Naturally,  $v^{(k_1, k_2; \kappa)}(r_1, r_2) = v^{(k_2, k_1; \kappa)}(r_2, r_1)$  from the definition (7). Here, the  $w^{(k)}(r_1, r_2)$  is defined by

$$w^{(k)}(r_1, r_2) = \frac{1}{2} \int_{-1}^1 V(r)/r^2 \cdot P_k(\cos \omega) d(\cos \omega),$$

corresponding to (12) for the central interaction.

### § 3. The spin-orbit interactions

Since the two-body spin-orbit interactions explicitly contain the momentum operators  $\mathbf{p}_1$  and  $\mathbf{p}_2$  of the interacting particles, the treatment in the preceding section must be modified. While there are some types of the spin-orbit interactions, we confine ourselves to the Case-Pais type<sup>11)</sup> in the following consideration and the procedure given here can be applied also to the other types with slight changes. The interaction is given by

$$V_{LS} = V(r) ((\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot [(\mathbf{r}_2 - \mathbf{r}_1) \times (\mathbf{p}_2 - \mathbf{p}_1)]), \tag{17}$$

where the square bracket without superfix denotes a vector product.

Let us separate the variables  $\mathbf{r}_1$  and  $\mathbf{r}_2$  in the spatial part of (17) as in the preceding section. Since  $\mathbf{r}_2 - \mathbf{r}_1 = \mathbf{r} = r\mathbf{C}^{(1)}(\Omega)$ , by making use of (6) for  $rV(r)\mathbf{C}^{(1)}(\Omega)$ , and changing the coupling schemes of the tensor operators, we have

$$V(r)[(\mathbf{r}_2 - \mathbf{r}_1) \times (\mathbf{p}_2 - \mathbf{p}_1)] = \sum_{k_1, k_2, K} i^{k_1 - k_2} (2k_1 + 1)(2k_2 + 1)[2(2K + 1)/3]^{1/2} \times (k_1 0 k_2 0 | 10) W(k_1 1 k_2 1; K 1) u^{(k_1, k_2; 1)}(r_1, r_2) \times \{ (-)^{1+k_1-K} [[\mathbf{C}_1^{(k_1)} \times \mathbf{p}_1]^{(K)} \times \mathbf{C}_2^{(k_2)}]^{(1)} + [\mathbf{C}_1^{(k_1)} \times [\mathbf{C}_2^{(k_2)} \times \mathbf{p}_2]^{(K)}]^{(1)} \}, \tag{18}$$

where

$$u^{(k_1, k_2; 1)}(r_1, r_2) = \frac{2}{\pi} \int_0^\infty j_{k_1}(pr_1) j_{k_2}(pr_2) p^2 dp \int_0^\infty r V(r) j_1(pr) r^2 dr. \tag{19}$$

The summations over  $k_1, k_2$  and  $K$  in (18) are restricted by the conditions:  $k_1 + k_2 = \text{odd}$ ,  $|k_1 - k_2| \leq 1 \leq k_1 + k_2$ ,  $|k_1 - 1| \leq K \leq k_1 + 1$  and  $|k_2 - 1| \leq K \leq k_2 + 1$ . Therefore,  $K$  equals either  $k_1$  or  $k_2$ , and (18) can be rewritten as

$$\begin{aligned}
V(r)[(\mathbf{r}_2 - \mathbf{r}_1) \times (\mathbf{p}_2 - \mathbf{p}_1)] = & \sum_{k, k'} i^{k+k'} (2k+1) (2k'+1) 2^{1/2} (k' 0 1 0 | k 0) W(k 1 k 1; k' 1) \\
& \times (\{u^{(k, k'; 1)}(r_1, r_2) [[\mathbf{C}_1^{(k)} \times \mathbf{p}_1]^{(k)} \times \mathbf{C}_2^{(k')}]^{(1)} + u^{(k', k; 1)}(r_1, r_2) [\mathbf{C}_1^{(k')} \times [\mathbf{C}_2^{(k)} \times \mathbf{p}_2]^{(k)}]^{(1)}\} \\
& + \{u^{(k', k; 1)}(r_1, r_2) [[\mathbf{C}_1^{(k')} \times \mathbf{p}_1]^{(k')} \times \mathbf{C}_2^{(k)}]^{(1)} - u^{(k, k'; 1)}(r_1, r_2) [\mathbf{C}_1^{(k)} \times [\mathbf{C}_2^{(k')} \times \mathbf{p}_2]^{(k')}]^{(1)}\}),
\end{aligned} \tag{18}'$$

where  $k' = k \pm 1$ . The radial parts of the interaction  $u^{(k, k'; 1)}(r_1, r_2)$  can be expressed in terms of those of the central interaction  $v^{(k)}(r_1, r_2)$ . They are obtained from (19) by making use of  $j_1(\rho) = -dj_0(\rho)/d\rho$  in a similar way to the derivation of (16).

$$u^{(k', k; 1)}(r_1, r_2) = i^{k-k'+1} \{r_1 v^{(k)}(r_1, r_2) - r_2 v^{(k')}(r_1, r_2)\}, \quad (k' = k \pm 1) \tag{20}$$

and  $u^{(k, k'; 1)}(r_1, r_2) = u^{(k', k; 1)}(r_2, r_1)$ , where  $v^{(k)}(r_1, r_2)$  is defined by (12).

Since the operator  $[\mathbf{C}_i^{(k)} \times \mathbf{p}_i]^{(K)}$  cannot be easily handled for the calculations of matrix elements, we rewrite it so as to separate  $(\mathbf{r}_i \cdot \mathbf{p}_i) = i^{-1} r_i d/dr_i$ . On observing that  $\mathbf{p}_i = r_i^{-2} \{\mathbf{r}_i (\mathbf{r}_i \cdot \mathbf{p}_i) - [\mathbf{r}_i \times \mathbf{L}_i]\}$  ( $\mathbf{L}_i$  are the orbital angular momenta), it can be expressed as

$$i r_i [\mathbf{C}_i^{(k)} \times \mathbf{p}_i]^{(K)} = (k 0 1 0 | K 0) \mathbf{C}_i^{(K)} r_i \partial / \partial r_i - \mathbf{D}_i^{(k, K)}, \tag{21}$$

where  $\mathbf{D}_i^{(k, K)}$  do not involve differential operator and it is defined as

$$\mathbf{D}_i^{(k, K)} = 2^{1/2} [\mathbf{C}_i^{(k)} \times [\mathbf{C}_i^{(1)} \times \mathbf{L}_i]^{(1)}]^{(K)}.$$

Simpler forms of  $\mathbf{D}_i^{(k, K)}$  can be obtained by changing the coupling schemes of the tensor operators:

$$\mathbf{D}_i^{(k, k)} = [(2k-1)/(k+1)]^{1/2} [\mathbf{C}_i^{(k-1)} \times \mathbf{L}_i]^{(k)} = [(2k+3)/k]^{1/2} [\mathbf{C}_i^{(k+1)} \times \mathbf{L}_i]^{(k)}, \tag{22a}$$

and

$$[(2k-1)/(k+1)]^{1/2} \mathbf{D}_i^{(k-1, k)} = [(2k+3)/k]^{1/2} \mathbf{D}_i^{(k+1, k)} = [\mathbf{C}_i^{(k)} \times \mathbf{L}_i]^{(k)}. \tag{22b}$$

The spatial part of the interaction is thus given by introducing (20), (21) and (22) into (18)' and by manipulation with respect to the Clebsch-Gordan and the Racah coefficients involved as

$$\begin{aligned}
V(r)[(\mathbf{r}_2 - \mathbf{r}_1) \times (\mathbf{p}_2 - \mathbf{p}_1)] = & \sum_k (-)^k (2k+1) \sum_{k' = k \pm 1} [(2k'+1)/3]^{1/2} \{ (v^{(k)} - v^{(k')} r_2/r_1) [[\mathbf{C}_1^{(k)} \times \mathbf{L}_1]^{(k')} \times \mathbf{C}_2^{(k)}]^{(1)} \\
& + (v^{(k)} - v^{(k')} r_1/r_2) [\mathbf{C}_1^{(k)} \times [\mathbf{C}_2^{(k)} \times \mathbf{L}_2]^{(k')}]^{(1)} \} \\
& + \sum_k (-)^k [(2k+1)/3]^{1/2} \{ -(k+1) v^{(k-1)} r_2/r_1 + (2k+1) v^{(k)} - k v^{(k+1)} r_2/r_1 \} \\
& \times [[\mathbf{C}_1^{(k)} \times \mathbf{L}_1]^{(k)} \times \mathbf{C}_2^{(k)}]^{(1)} \\
& - \{ -(k+1) v^{(k-1)} r_1/r_2 + (2k+1) v^{(k)} - k v^{(k+1)} r_1/r_2 \} [\mathbf{C}_1^{(k)} \times [\mathbf{C}_2^{(k)} \times \mathbf{L}_2]^{(k)}]^{(1)} \\
& + \sum_k (-)^k [k(k+1) (2k+1)/3]^{1/2} \{ v^{(k-1)} - v^{(k+1)} \} (r_2 \partial / \partial r_1 - r_1 \partial / \partial r_2) [\mathbf{C}_1^{(k)} \times \mathbf{C}_2^{(k)}]^{(1)},
\end{aligned} \tag{23}$$

where  $v^{(k)}$  means  $v^{(k)}(r_1, r_2)$ . This expression is rather complicated at first sight,

but the reduced matrix elements  $(l||[C^{(k')} \times L]^{(k)}||l')$  is very simple and the angular parts of the matrix elements are easily calculated. Corresponding to  $(l||C^{(k)}||l') = (2l'+1)^{1/2}(l'0k0|l0)$ , the reduced matrix elements of  $[C^{(k')} \times L]^{(k)}$  is obtained as

$$(l||[C^{(k')} \times L]^{(k)}||l') = [2l'(l'+1)(2l'+1)]^{1/2}(k'011|k1)(l'1k-1|l0). \tag{22}$$

$(k' = k, k \pm 1)$

Especially for  $l^2$  configurations, the contributions from the second and third sums over  $k$  in (23) vanish as can readily be seen, and the calculations of the matrix elements become very simple.

#### § 4. Radial integrals in terms of the harmonic oscillator wave functions

The radial integrals which are necessary in the evaluation of the interaction matrix elements can be obtained from (7) and (9). Inserting (7) into (9), they are

$$R^{(k_1, k_2; \kappa)}(n_1 l_1, n_2 l_2; n_1' l_1', n_2' l_2') = \int_0^\infty v_\kappa(p) p^2 dp \times \int_0^\infty R_{n_1 l_1}(r_1) R_{n_1' l_1'}(r_1) j_{k_1}(pr_1) r_1^2 dr_1 \int_0^\infty R_{n_2 l_2}(r_2) R_{n_2' l_2'}(r_2) j_{k_2}(pr_2) r_2^2 dr_2,$$

where principal quantum numbers  $n$  are explicitly introduced and the expression for  $v_\kappa(p)$  is given by (5). If the integrations over  $r_1$  and  $r_2$  can be carried out, the radial integrals will be obtained as simple integrals over  $p$ . However, it seems difficult to carry out the integrations analytically over  $r_1$  and  $r_2$  for single particle wave functions with arbitrary radial dependence, and we confine ourselves to the harmonic oscillator wave functions which are used quite often for the analysis of the nuclear spectroscopy.

The wave functions of three-dimensional isotropic harmonic oscillator are given as<sup>5)</sup>

$$R_{nl}(r) = N_{nl} \exp(-\nu r^2/2) r^l v_{n,l}(\nu r^2), \tag{24}$$

where  $\nu = m\omega/\hbar$ ,  $\hbar\omega$  is energy quantum, and  $m$  is mass.  $N_{nl}$  is the normalization constant:

$$N_{nl}^2 = \frac{(2l+2n+1)!!}{2^n n! [(2l+1)!!]^2} (2\nu)^{l+3/2} \left(\frac{2}{\pi}\right)^{1/2}. \tag{25}$$

And  $v_{n,l}(\rho)$  is the associated Laguerre polynomial:

$$v_{n,l}(\rho) = \sum_\mu \binom{n}{\mu} \frac{(2l+1)!!}{(2l+2\mu+1)!!} (-2\rho)^\mu. \tag{26}$$

In order to carry out the integration  $\int_0^\infty R_{nl}(r) R_{n'l'}(r) j_k(pr) r^2 dr$  with the har-

monic oscillator wave functions (24), we expand the product of the two associated Laguerre polynomials into power series and define the expansion coefficients  $a_m(nl, n'l')$  by

$$v_{n,i}(\rho)v_{n',i'}(\rho) = \frac{(2l+1)!!(2l'+1)!!}{(2l+2n+1)!!(2l'+2n'+1)!!} \sum_{s=0}^{n+n'} a_{l+l'+2s}(nl, n'l')(2\rho)^s. \quad (27)$$

Then, the product of two harmonic oscillator wave function is written down as

$$R_{nl}(r)R_{n'l'}(r) = M(nl, n'l')^{-1/2} (2/\pi)^{1/2} \exp(-\nu r^2) \sum_m a_m(nl, n'l') (2\nu)^{(m+3)/2} r^m, \quad (28)$$

where  $m=l+l'+2s$  ( $s=0, 1, \dots, n+n'$ ) and

$$M(nl, n'l') = 2^{n+n'} n! n'! (2l+2n+1)!! (2l'+2n'+1)!! \quad (29)$$

Thus, by making use of a formula of the integral involving the Bessel function<sup>12)</sup>

$$\int_0^\infty \exp(-\nu r^2) j_k(pr) r^{m+2} dr = \frac{(m+k+1)!!}{(2k+1)!!} \left(\frac{\pi}{2}\right)^{1/2} (2\nu)^{-(m+3)/2} \exp\left(-\frac{p^2}{4\nu}\right) \left(\frac{p^2}{2\nu}\right)^{k/2} v_{(m-k)/2, k}\left(\frac{p^2}{4\nu}\right), \quad (30)$$

where  $m-k = \text{even} \geq 0$  and  $v_{n,i}(\rho)$  is defined by (26), the integration can be easily carried out.

$$\int_0^\infty R_{nl}(r)R_{n'l'}(r)j_k(pr)r^2 dr = M(nl, n'l')^{-1/2} \sum_m a_m(nl, n'l') \times (m+k+1)!!/(2k+1)!! \cdot \exp(-p^2/4\nu) (p^2/2\nu)^{k/2} v_{(m-k)/2, k}(p^2/4\nu). \quad (31)^*$$

Actually,  $(m-k)/2 = (l+l'-k)/2 + s$  are non-negative integers, since there are factors of the type  $(l||C^{(k)}||l')$  in (8) which give the conditions  $|l-l'| \leq k \leq l+l'$  and  $l+l'-k$  is even. Then, the radial integral is obtained by the application of (31) for the integrations over  $r_1$  and  $r_2$ :

$$R^{(k_1, k_2; \kappa)}(n_1 l_1, n_2 l_2; n_1' l_1', n_2' l_2') = (M_1 M_2)^{-1/2} \sum_{m_1, m_2} a_{m_1}(n_1 l_1, n_1' l_1') a_{m_2}(n_2 l_2, n_2' l_2') f^{(k_1, k_2; \kappa)}(m_1, m_2), \quad (32)$$

where the abbreviations  $M_i = M(n_i l_i, n_i' l_i')$  ( $i=1, 2$ ) are used, and by taking (27) into account again,  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  are given as

\* In (31), if one takes the limit  $p \rightarrow 0$ , the following expression is obtained.

$$\int_0^\infty R_{nl}(r)r^k R_{n'l'}(r)r^2 dr = (2\nu)^{-k/2} M(nl, n'l')^{-1/2} \sum_m (m+k+1)!! a_m(nl, n'l').$$

This expression is useful for the calculations of the matrix elements for the nuclear moments,  $\beta$  and  $\gamma$  transitions when the harmonic oscillator wave functions are used as one particle wave functions.



$$f^{(k_1, k_2; \kappa)}(m_1, m_2) \equiv (2\nu)^{\bar{m}+3} \frac{2}{\pi} \int_0^\infty \int_0^\infty v^{(k_1, k_2; \kappa)}(r_1, r_2) \times \exp\{-\nu(r_1^2 + r_2^2)\} r_1^{m_1+2} r_2^{m_2+2} dr_1 dr_2 = \sum_m a_{2m} \left( \frac{m_1 - k_1}{2} k_1, \frac{m_2 - k_2}{2} k_2 \right) J_m^{(\kappa)}. \quad (33)$$

The summation over  $m$  is restricted by  $m = \bar{k}, \bar{k} + 1, \dots, \bar{m}$ , where  $\bar{k} = (k_1 + k_2)/2$  and  $\bar{m} = (m_1 + m_2)/2$ .  $J_m^{(\kappa)}$  are simple integrals which involve the Fourier transform  $v_\kappa(p)$  of the radial dependence  $V(r)$  of the interaction

$$J_m^{(\kappa)} = (2\nu)^{-m} \int_0^\infty \exp(-p^2/2\nu) v_\kappa(p) p^{2m+2} dp. \quad (34)$$

By (32) and (33), the radial integrals which involve any quartets of quantum numbers  $nl$  (naturally  $l_1 + l_2 + l_1' + l_2' = \text{even}$  from the conservation of parity), can be expressed as linear combinations of simple integrals  $J_m^{(\kappa)}$  given by (34). The coefficients which appear in both (32) and (33) are defined by (27). The  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  has a close connection with  $R^{(k_1, k_2; \kappa)}(0l_1, 0l_2; 0l_1', 0l_2')$  which is given by (32) when

$$R^{(k_1, k_2; \kappa)}(0l_1, 0l_2; 0l_1', 0l_2') = [(2l_1 + 1)!! (2l_2 + 1)!! (2l_1' + 1)!! (2l_2' + 1)!!]^{-1/2} f^{(k_1, k_2; \kappa)}(l_1 + l_1', l_2 + l_2'). \quad (35)$$

The above expressions for the radial integrals hold for the central and tensor interactions which were discussed in § 2. For the spin-orbit interactions, one needs further considerations, since there appear two types of integrals, one of which contains the derivatives with respect to  $r_1$  or  $r_2$  and the other  $r_2/r_1$  or  $r_1/r_2$  in the integrand. The calculation of these integrals is given in the Appendix.

### § 5. The coefficients $a_m(nl, n'l')$

The coefficients  $a_m(nl, n'l')$  defined by (27) proved very useful in the calculation of the radial integrals in terms of the harmonic oscillator wave functions. In this section, the convenient formulas for the evaluation of the coefficients are derived and those for  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  are obtained.

It is evident from the definitions (26) and (27) that

$$a_{l+l'+2s}(nl, n'l') = (-)^s \sum_{(\mu + \mu' = s)} \binom{n}{\mu} \binom{n'}{\mu'} \frac{(2l + 2n + 1)!!}{(2l + 2\mu + 1)!!} \frac{(2l' + 2n' + 1)!!}{(2l' + 2\mu' + 1)!!}, \quad (36)*$$

In the case of  $l = l'$ , it may be written in another form which is useful in the application to the central interaction in the next section,

\* The coefficients  $a_m(nl, n'l')$  have the following relation to  $B(nl, n'l', p)$  defined by Brody, Jacob and Moshinski. (Nuclear Phys. 17 (1960), 16)

$$B(nl, n'l', p) = M(nl, n'l')^{-1/2} (2p + 1)!! a_{2p}(nl, n'l').$$

$$a_{2l+2s}(nl, n'l) = (-)^s \frac{(2l+2n+1)!! (2l+2n'+1)!!}{(2l+2s+1)!!} \times \sum_{\mu} \frac{2^{\mu} n! n'!}{\mu! (n-\mu)! (n'-\mu)! (2l+2\mu+1)!!} \binom{n+n'-2\mu}{s-2\mu}. \quad (37)$$

The coefficients are naturally symmetric with respect to the exchange of their arguments:

$$a_m(nl, n'l') = a_m(n'l', nl). \quad (38)$$

For some special values of  $n$  and  $n'$ , the simple expressions are obtained:

$$a_{l+l'+2s}(0l, 0l') = \delta_{s,0}, \quad (39)$$

and

$$a_{l+l'+2s}(0l, n'l') = (-)^s \binom{n'}{s} \frac{(2l'+2n'+1)!!}{(2l'+2s+1)!!}. \quad (40)$$

Table I.  $a_m(nl, n'l')$   $l+l'=\text{even}$

$nl \ n'l'$	$m=0$	2	4	6	8	10	12
00 00	1						
01 01	.	1					
02 00	.	1					
02 02	.	.	1				
10 00	3	-1					
02 02	.	3	-1				
10 10	9	-6	1				
03 01	.	.	1				
03 03	.	.	.	1			
11 01	.	5	-1				
03 03	.	.	5	-1			
11 11	.	25	-10	1			
04 00	.	.	1				
02 02	.	.	.	1			
10 10	.	.	3	-1			
04 04	.	.	.	.	1		
12 00	.	7	-1				
02 02	.	.	7	-1			
10 10	.	21	-10	1			
04 04	.	.	.	7	-1		
12 12	.	.	49	-14	1		
20 00	15	-10	1				
02 02	.	15	-10	1			
10 10	45	-45	13	-1			
04 04	.	.	15	-10	1		
12 12	.	105	-85	17	-1		
20 20	225	-300	130	-20	1		
05 01	.	.	.	1			
03 03	.	.	.	.	1		
11 11	.	.	.	5	-1		
05 05	.	.	.	.	.	1	

Table I. (Continued)  $a_m(nl, n'l')$   $l+l'=even$

$nl\ n'l'$	$m=0$	2	4	6	8	10	12
13 01	.	.	9	-1			
03	.	.	.	9	-1		
11	.	.	45	-14	1		
05	.	.	.	.	9	-1	
13	.	.	.	81	-18	1	
21 01	.	35	-14	1			
03	.	.	35	-14	1		
11	.	175	-105	19	-1		
05	.	.	.	35	-14	1	
13	.	.	315	-161	23	-1	
21	.	1225	-980	266	-28	1	
06 00	.	.	.	1			
02	.	.	.	.	1		
10	.	.	.	3	-1		
04	.	.	.	.	.	1	
12	.	.	.	.	7	-1	
20	.	.	.	15	-10	1	
06	.	.	.	.	.	.	1
14 00	.	.	11	-1			
02	.	.	.	11	-1		
10	.	.	33	-14	1		
04	.	.	.	.	11	-1	
12	.	.	.	77	-18	1	
20	.	.	165	-125	21	-1	
06	.	.	.	.	.	11	-1
14	.	.	.	.	121	-22	1
22 00	.	63	-18	1			
02	.	.	63	-18	1		
10	.	189	-117	21	-1		
04	.	.	.	63	-18	1	
12	.	.	441	-189	25	-1	
20	.	945	-900	258	-28	1	
06	.	.	.	.	63	-18	1
14	.	.	.	693	-261	29	-1
22	.	.	3969	-2268	450	-36	1
30 00	105	-105	21	-1			
02	.	105	-105	21	-1		
10	315	-420	168	-24	1		
04	.	.	105	-105	21	-1	
12	.	735	-840	252	-28	1	
20	1575	-2625	1470	-330	31	-1	
06	.	.	.	105	-105	21	-1
14	.	.	1155	-1260	336	-32	1
22	.	6615	-8505	3318	-546	39	-1
30	11025	-22050	15435	-4620	651	-42	1

Actually, we used (39) in obtaining (35). Furthermore, the following recurrence formulas hold between the coefficients\*

\* The recurrence formulas between the coefficients  $a_m(nl, n'l')$  are easily derived from those between the associated Laguerre polynomials:

$$(2n+2l+1)v_{n,l}(\rho) = (2l+1)v_{n,l-1}(\rho) + 2nv_{n-1,l}(\rho),$$

$$2\rho v_{n,l}(\rho) = (2l+1)\{v_{n,l-1}(\rho) - v_{n+1,l-1}(\rho)\},$$

and the definition of the coefficients (27).

Table II.  $a_m(nl, n'l')$   $l+l'=\text{odd}$ 

$nl$ $n'l'$	$m=1$	3	5	7	9	11
01 00	1					
02 01	.	1				
10 01	3	-1				
03 00	.	1				
02	.	.	1			
10	.	3	-1			
11 00	5	-1				
02	.	5	-1			
10	15	-8	1			
04 01	.	.	1			
03	.	.	.	1		
11	.	.	5	-1		
12 01	.	7	-1			
03	.	.	7	-1		
11	.	35	-12	1		
20 01	15	-10	1			
03	.	15	-10	1		
11	76	-65	15	-1		
05 00	.	.	1			
02	.	.	.	1		
10	.	.	3	-1		
04	.	.	.	.	1	
12	.	.	.	7	-1	
20	.	.	15	-10	1	
13 00	.	9	-1			
02	.	.	9	-1		
10	.	27	-12	1		
04	.	.	.	9	-1	
12	.	.	63	-16	1	
20	.	135	-105	19	-1	
21 00	35	-14	1			
02	.	35	-14	1		
10	105	-77	17	-1		
04	.	.	35	-14	1	
12	.	245	-133	21	-1	
20	525	-560	190	-24	1	
06 01	.	.	.	1		
03	.	.	.	.	1	
11	.	.	.	5	-1	
05	.	.	.	.	.	1
13	.	.	.	.	9	-1
21	.	.	.	35	-14	1
14 01	.	.	11	-1		
03	.	.	.	11	-1	
11	.	.	55	-16	1	
05	.	.	.	.	11	-1
13	.	.	.	99	-20	1
21	.	.	385	-189	25	-1
22 01	.	63	-18	1		
03	.	.	63	-18	1	
11	.	315	-153	23	-1	
05	.	.	.	63	-18	1
13	.	.	567	-225	27	-1
21	.	2205	-1512	350	-32	1

Table II. (Continued)  $a_m(nl, n'l')$   $l+l'=\text{odd}$

$nl\ n'l'$	$m=1$	3	5	7	9	11
30 01	105	-105	21	-1		
03	.	105	-105	21	-1	
11	525	-630	210	-26	1	
05	.	.	105	-105	21	-1
13	.	945	-1050	294	-30	1
21	3675	-5145	2310	-434	35	-1

$$a_m(nl, n'l') = 2na_m(n-1l, n'l') + a_{m-1}(nl-1, n'l'), \tag{41a}$$

and

$$a_m(nl, n'l') = (2l+3)a_{m+1}(n-1l+1, n'l') - a_m(n-1l+2, n'l'). \tag{41b}$$

These recurrence formulas are quite useful in obtaining the values of the  $a_m(nl, n'l')$  starting from (39) or (40), although it is not difficult to calculate them by the direct application of (36) or (37).

In Tables I and II, the values of the coefficients  $a_m(nl, n'l')$ , which are necessary for the evaluation in (32), are listed for  $l+l'$  even and odd, respectively.

The properties of the  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  can also be obtained from those of the  $a_m(nl, n'l')$  by (33). First of all, from (38), the symmetry property of the  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  with respect to the exchange of their arguments is

$$f^{(k_1, k_2; \kappa)}(m_1, m_2) = f^{(k_2, k_1; \kappa)}(m_2, m_1). \tag{38}'$$

For the special cases of  $m_1=k_1$  and  $m_2=k_2$ , we have, corresponding to (39),

$$f^{(m_1, m_2; \kappa)}(m_1, m_2) = J_m^{(\kappa)}, \tag{39}'$$

and, for  $m_1=k_1$ ,

$$f^{(m_1, k_2; \kappa)}(m_1, m_2) = \sum_{\mu} (-)^{\mu} \binom{(m_2-k_2)/2}{\mu} \frac{(m_2+k_2+1)!!}{(2k_2+2\mu+1)!!} J_{m+\mu}^{(\kappa)}. \tag{42}$$

Four recurrence formulas for the  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  are obtained from those between the coefficients  $a_m(nl, n'l')$  with common suffices  $m$ , which are derived from (41a) and (41b). Those formulas are, for example,

$$\begin{aligned} f^{(k_1, k_2; \kappa)}(m_1, m_2) &= (m_1+k_1+1)f^{(k_1, k_2; \kappa)}(m_1-2, m_2) - f^{(k_1+1, k_2+1; \kappa)}(m_1-1, m_2+1) \\ &\quad + (m_2-k_2)f^{(k_1+1, k_2+1; \kappa)}(m_1-1, m_2-1), \\ f^{(k_1, k_2; \kappa)}(m_1, m_2) &= (m_1+k_1+1)f^{(k_1, k_2; \kappa)}(m_1-2, m_2) \\ &\quad + (m_1-k_1-2)f^{(k_1+2, k_2; \kappa)}(m_1-2, m_2) - f^{(k_1+2, k_2; \kappa)}(m_1, m_2), \end{aligned} \tag{43}$$

which hold irrespective of the values of  $\kappa$ .

### § 6. The integrals $J_m^{(\kappa)}$

As was shown in § 4, any radial integral can be expanded into a linear combination of the simple integrals  $J_m^{(\kappa)}$ , if we assume the harmonic oscillator

wave function for the radial wave function.  $J_m^{(\kappa)}$  was defined by (34) and it is an integral containing the Fourier transform  $v_\kappa(p)$  of the interaction.

Without the knowledge of the radial dependence of interaction  $V(r)$ , we can obtain the relation between the  $J_m^{(\kappa)}$  and the Talmi integral  $I_l$ , where  $I_l$  is defined as<sup>5)</sup>

$$I_l = \int_0^\infty V(\sqrt{2}r) R_{0l}^2(r) r^2 dr. \quad (44)$$

$I_l$  may be written more explicitly by employing (24) and changing the integration variable

$$I_l = \left(\frac{2}{\pi}\right)^{1/2} \frac{\nu^{l+3/2}}{(2l+1)!!} \int_0^\infty V(r) \exp\left(-\frac{\nu r^2}{2}\right) r^{2l+2} dr. \quad (44)'$$

On the other hand, the  $J_m^{(\kappa)}$  may be expressed in terms of  $V(r)$ , by the introduction of the Fourier inverse transform (5) and carrying out the integration over  $p$  by (30)

$$J_m^{(\kappa)} = \frac{\nu^{(\kappa+3)/2}}{2^m} \frac{(2m+\kappa+1)!!}{(2\kappa+1)!!} \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty V(r) \exp\left(-\frac{\nu r^2}{2}\right) v_{m-\kappa/2, \kappa} \left(\frac{\nu r^2}{2}\right) r^{\kappa+2} dr.$$

Then, expanding  $v_{m-\kappa/2, \kappa}(\nu r^2/2)$  into a series of  $r^2$  by (26), it is easy to obtain the relation between  $J_m^{(\kappa)}$  and  $I_l$ :

$$J_m^{(\kappa)} = \frac{(2m+\kappa+1)!!}{2^m} \sum_l (-)^l \binom{m-\kappa/2}{l} \frac{(2l+\kappa+1)!!}{(2l+2\kappa+1)!!} I_{l+\kappa/2}. \quad (45)$$

For the central interaction ( $\kappa=0$ ), the above relation is simplified:

$$J_m^{(0)} = \frac{(2m+1)!!}{2^m} \sum_l (-)^l \binom{m}{l} I_l. \quad (46)$$

In this case,  $I_l$  may also be expressed in terms of  $J_m^{(0)}$  from (46)

$$I_l = \sum_m (-)^m \binom{l}{m} \frac{2^m}{(2m+1)!!} J_m^{(0)}.$$

For the tensor interaction ( $\kappa=2$ ), the relation is given by

$$J_m^{(2)} = \frac{(2m+3)!!}{2^m} \sum_l (-)^l \binom{m-1}{l} \frac{1}{2l+5} I_{l+1}. \quad (47)$$

It is apparent that the radial integral of the tensor interaction does not involve  $I_0$ . From (46) and (47), the relation between the  $J_m^{(2)}$  and  $J_m^{(0)}$  may be obtained:

$$J_m^{(2)} = \frac{3}{2} \sum_{m'=0}^{m-1} \frac{(m-1)!}{m'!} J_{m'}^{(0)} - J_m^{(0)}. \quad (48)$$

The radial integral  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  may be expanded in terms of  $I_l$  instead of  $J_m^{(\kappa)}$  in (33). By the relation (45) between  $J_m^{(\kappa)}$  and  $I_l$  it becomes

$$f^{(k_1, k_2; \kappa)}(m_1, m_2) = \sum_l (-)^l \frac{(2l + \kappa + 1)!!}{(2l + 2\kappa + 1)!!} \sum_m \frac{(2m + \kappa + 1)!!}{2^m} \binom{m - \kappa/2}{l} \times a_{2m} \left( \frac{m_1 - k_1}{2} k_1, \frac{m_2 - k_2}{2} k_2 \right) I_{l + \kappa/2}. \tag{49}$$

For the central interaction, by putting  $k_1 = k_2 = k$  and inserting (37) into (49), we have

$$f^{(k)}(m_1, m_2) \equiv f^{(k, k; 0)}(m_1, m_2) = (m_1 + k + 1)!! (m_2 + k + 1)!! \sum_l (-)^l \sum_m (-)^{m-k} \times \frac{1}{2^m} \binom{m}{l} \sum_{\mu} \frac{2^{\mu} [(m_1 - k)/2]! [(m_2 - k)/2]!}{\mu! [(m_1 - k)/2 - \mu]! [(m_2 - k)/2 - \mu]! (2k + 2\mu + 1)!!} \binom{\bar{m} - k - 2\mu}{m - k - 2\mu} I_l. \tag{50}$$

This form of the expansion has been obtained by Ford and Konopinski<sup>6)</sup> from the consideration of Gaussian type interaction. If  $I_l$  is proportional to  $z^l$  ( $z$  is a variable), the summations over  $l$  and  $m$  in (50) can be carried out by putting  $I_l \sim z^l$ :

$$f^{(k)}(m_1, m_2 | z) \sim \frac{(m_1 + k + 1)!! (m_2 + k + 1)!!}{(2k + 1)!!} \left( \frac{1 + z}{2} \right)^{\bar{m}} \left( \frac{1 - z}{1 + z} \right)^k \times {}_2F_1 \left( (k - m_1)/2, (k - m_2)/2; k + \frac{3}{2}; \left( \frac{1 - z}{1 + z} \right)^2 \right), \tag{51}$$

where  ${}_2F_1(\alpha, \beta; \gamma; x)$  is a hypergeometric function. Some other forms of  $f^{(k)}(m_1, m_2 | z)$  can be obtained by the transformation of the hypergeometric function and those of  $f^{(k)}(m_1, m_2)$  can also be derived by expanding them into power series of  $z$ .

Now we calculate the explicit formulas for the integral  $J_m^{(0)}$  and  $I_l$  from (5), (34) and (45) for some radial dependences which are used for the phenomenological analysis in the nuclear spectroscopy. The simplest cases are the short- and long-range limits of the radial dependences. In these cases, the values of  $J_m^{(0)}$ ,  $J_m^{(2)}$ ,  $I_l$  and  $f^{(k)}(m_1, m_2)$  are listed in Table III.

Table III. The short- and long-range limits

	short-range limit	long-range limit
$V(r)$	$\delta(r)/r^2$	1
$J_m^{(0)}$	$(2m + 1)!! / 2^m \cdot (2\nu^3/\pi)^{1/2}$	$\delta_{m, 0}$
$J_m^{(2)}$	0	$3/2 \cdot (m - 1)!$
$I_l$	$\delta_{l, 0} (2\nu^3/\pi)^{1/2}$	1
$f^{(k)}(m_1, m_2)$	$(2\bar{m} + 1)!! / 2^{\bar{m}} \cdot (2\nu^3/\pi)^{1/2}$	$(m_1 + 1)!! (m_2 + 1)!! \delta_{k, 0}$

The values of  $f^{(k)}(m_1, m_2)$  may also be obtainable from (51) by putting  $z=0$  and 1 for the short- and long-range limits, respectively. For the interactions with finite range, we consider Gaussian and Yukawa potentials.

i) Gaussian potential:  $V(r) = \exp(-r^2/r_0^2)$  ( $r_0$ =force range)

$$J_m^{(0)} = (2m+1)!!/2^m \cdot \lambda^3 (1+\lambda^2)^{-(m+3/2)}, \quad (52)$$

and

$$I_l = [\lambda^2/(1+\lambda^2)]^{l+3/2}, \quad (53)$$

where  $\lambda = r_0(\nu/2)^{1/2}$  is the non-dimensional range parameter. Hence, by assuming  $z = \lambda^2/(1+\lambda^2)$ , (51) can be used for the radial integrals.<sup>6)</sup>

ii) Yukawa potential:  $V(r) = \exp(-r/r_0)/(r/r_0)$

We introduce the parameters  $\mu = 1/(2\lambda)$  and  $\beta = p(2\nu)^{-1/2}$ . Then, from (5) and (34), we obtain

$$J_m^{(0)} = \frac{2}{\pi\mu} \int_0^\infty \exp(-\beta^2) \frac{\beta^{2m+2}}{\beta^2 + \mu^2} d\beta.$$

For these integrals, we get a recurrence formula

$$J_m^{(0)} = (2m-1)!!/2^m \cdot \mu^{-1} \pi^{-1/2} - \mu^2 J_{m-1}^{(0)}, \quad (m \geq 0)$$

and for  $m = -1$ ,

$$J_{-1}^{(0)} = \mu^{-2} \{1 - \Phi(\mu)\} \exp(\mu^2),$$

where  $\Phi(\mu) = 2/\pi^{1/2} \cdot \int_0^\mu \exp(-t^2) dt$  is an error function. From these relations, the expression for  $J_m^{(0)}$  may be obtained:

$$J_m^{(0)} = \frac{1}{\mu\sqrt{\pi}} \sum_{n=0}^m \frac{(2m-2n-1)!!}{2^{m-n}} (-\mu^2)^n - (-\mu^2)^m \{1 - \Phi(\mu)\} \exp(\mu^2), \quad (54)$$

although the direct application of the above recurrence formula and the initial value seems more practical in the numerical calculation of  $J_m^{(0)}$ . The expression for  $I_l$  can be written down by making use of (46) and  $J_m^{(2)}$  are obtainable from (48).

### § 7. An example: The (0d) (1s) configuration

In order to illustrate the systematic procedure to be followed when we want to calculate the matrix elements, we take the simple configuration (0d) (1s). The radial integrals, which are necessary for both the central and the tensor interactions, are reduced to the  $f^{(k_1, k_2; \kappa)}(m_1, m_2)$  by (32).

$$R^{(k_1, k_2; \kappa)}(0d1s; 0d1s) = \{9f^{(k_1, k_2; \kappa)}(4, 0) - 6f^{(k_1, k_2; \kappa)}(4, 2) + f^{(k_1, k_2; \kappa)}(4, 4)\}/90,$$

and

$$\begin{aligned} R^{(k_1, k_2; \kappa)}(0d1s; 1s0d) \\ = \{9f^{(k_1, k_2; \kappa)}(2, 2) - 3f^{(k_1, k_2; \kappa)}(4, 2) - 3f^{(k_1, k_2; \kappa)}(2, 4) + f^{(k_1, k_2; \kappa)}(4, 4)\}/90. \end{aligned}$$



Therefore, for the central interaction, the direct integral  $F^0(0d, 1s)$  and the exchange integral  $G^2(0d, 1s)$  are given by (33) and Table I as follows :

$$F^0(0d, 1s) = R^{(0,0;0)}(0d1s; 0d1s) = \{9(15J_0 - 10J_1 + J_2) - 6(45J_0 - 45J_1 + 13J_2 - J_3) + (225J_0 - 300J_1 + 130J_2 - 20J_3 + J_4)\} / 90,$$

and

$$G^2(0d, 1s) = 5R^{(2,2;0)}(0d1s; 1s0d) = 5\{9J_2 - 6(7J_2 - J_3) + (49J_2 - 14J_3 + J_4)\} / 90,$$

where we write  $J_m$  instead of  $J_m^{(0)}$ .

For the tensor interaction, the direct integral  $R^{(2,0;2)}(0d1s; 0d1s)$  and the exchange integral  $R^{(2,2;2)}(0d1s, 1s0d)$  are given in the same way as follows :

$$R^{(2,0;2)}(0d1s; 0d1s) = \{9(7J_1^{(2)} - J_2^{(2)}) - 6(21J_1^{(2)} - 10J_2^{(2)} + J_3^{(2)}) + (105J_1^{(2)} - 85J_2^{(2)} + 17J_3^{(2)} - J_4^{(2)})\} / 90,$$

and

$$R^{(2,2;2)}(0d1s; 1s0d) = \{9J_2^{(2)} - 6(7J_2^{(2)} - J_3^{(2)}) + (49J_2^{(2)} - 14J_3^{(2)} + J_4^{(2)})\} / 90.$$

The relations between  $J_m^{(2)}$  and  $J_m^{(0)}$  (which are denoted as  $J_m$  in this section) are given by (48) :

$$\begin{aligned} J_1^{(2)} &= 3/2 \cdot J_0 - J_1, \\ J_2^{(2)} &= 3/2(J_0 + J_1) - J_2, \\ J_3^{(2)} &= 3/2(2J_0 + 2J_1 + J_2) - J_3, \\ J_4^{(2)} &= 3/2(6J_0 + 6J_1 + 3J_2 + J_3) - J_4. \end{aligned}$$

In the above expression,  $J_m$  may be rewritten in terms of the Talmi integral  $I_i$  by the use of (46).

### Appendix

#### The radial integrals for the spin-orbit interaction

For the calculation of the matrix elements of the spin-orbit interaction, it is seen from (23) that the radial integrals which involve  $v^{(k)}(r_1, r_2)$ ,  $v^{(k')}(r_1, r_2)r_2/r_1$  and  $\{v^{(k-1)}(r_1, r_2) - v^{(k+1)}(r_1, r_2)\}(r_2\partial/\partial r_1 - r_1\partial/\partial r_2)$  are necessary. The first integral is given in (32) as

$$\begin{aligned} &\int_0^\infty \int_0^\infty R_{n_1 l_1}(r_1) R_{n_2 l_2}(r_2) v^{(k)}(r_1, r_2) R_{n_1' l_1'}(r_1) R_{n_2' l_2'}(r_2) r_1^2 dr_1 r_2^2 dr_2 \\ &= (M_1 M_2)^{-1/2} \sum_{m_1, m_2} a_{m_1}(n_1 l_1, n_1' l_1') a_{m_2}(n_2 l_2, n_2' l_2') f^{(k)}(m_1, m_2), \end{aligned}$$

where  $M_i$ ,  $a_{m_i}(n_i l_i, n_i' l_i')$  ( $i=1, 2$ ) and  $f^{(k)}(m_1, m_2)$  are defined by (29), (27) and (33), respectively. The second integral is also simple and it can be easily calculated in quite a similar way to the first one.

$$\int_0^\infty \int_0^\infty R_{n_1 l_1}(r_1) R_{n_2 l_2}(r_2) v^{(k')} (r_1, r_2) r_2 / r_1 R_{n_1' l_1'}(r_1) R_{n_2' l_2'}(r_2) r_1^2 dr_1 r_2^2 dr_2$$

$$= (M_1 M_2)^{-1/2} \sum_{m_1, m_2} a_{m_1}(n_1 l_1, n_1' l_1') a_{m_2}(n_2 l_2, n_2' l_2') f^{(k')} (m_1 - 1, m_2 + 1).$$

The calculation of the third integral which involve differentiations with respect to  $r_1$  and  $r_2$  is a little more tedious. By taking into account

$$(d/dr - l/r) R_{nl}(r) = -(\nu/2)^{1/2} \{ (2L + 2n + 3)^{1/2} R_{n, l+1}(r) + (2n)^{1/2} R_{n-1, l+1}(r) \},$$

and calculating by the similar procedure as above, we have

$$\int_0^\infty \int_0^\infty R_{n_1 l_1}(r_1) R_{n_2 l_2}(r_2) v^{(k')} (r_1, r_2) \{ (r_2 \partial / \partial r_1 - r_1 \partial / \partial r_2) \\ \times R_{n_1' l_1'}(r_1) R_{n_2' l_2'}(r_2) \} r_1^2 dr_1 r_2^2 dr_2$$

$$= (M_1 M_2)^{-1/2} \sum_{m_1, m_2} [ \{ l_1' a_{m_1}(n_1 l_1, n_1' l_1') - a_{m_1-1}(n_1 l_1, n_1' l_1' + 1) \} \\ \times a_{m_2}(n_2 l_2, n_2' l_2') f^{(k')} (m_1 - 1, m_2 + 1) \\ - a_{m_1}(n_1 l_1, n_1' l_1') \{ l_2' a_{m_2}(n_2 l_2, n_2' l_2') \\ - a_{m_2-1}(n_2 l_2, n_2' l_2' + 1) \} f^{(k')} (m_1 + 1, m_2 - 1) ].$$

**Note added in proof:** Tables I and II are sufficient in the evaluation of (32) up to the  $N=6$  shell, but, in the evaluation of (33), they are not enough for the shells higher than  $N=3$ . Tables which can be applied up to the  $N=6$  shell for the evaluation of (33) will be published in the Bulletin of the Tokyo Institute of Technology.

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