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TRANSFORMATION BRACKETS BETWEEN CARTESIAN AND ANGULAR MOMENTUM HARMONIC OSCILLATOR BASIS FUNCTIONS WITH AND WITHOUT SPIN-ORBIT COUPLING TABLES FOR THE 2s-ld NUCLEAR SHELL.

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ABSTRACT

Orbital wave functions of a single particle in a harmonic oscillator potential are given in terms of spherical components of a creation vector operator acting on the ground state. The wave functions are given in different bases. Numerical coefficients for transforming from one basis to another are given in tabular form for principal quantum $\nu = 2$ *. Wave functions for spin-orbit coupling are also considered.*

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1. INTRODUCTION

The energy of a single particle in a harmonic oscillator well is

$$E = (\nu + \frac{3}{2})\ \hbar\omega$$

where ν is the principal quantum number. The orbital degeneracy of the ν shell is given by

$$\tau = \frac{1}{2}\ (\nu + 1)\ (\nu + 2)$$

The spin-orbital degeneracy is then simply 2τ.

We wish to obtain the coefficients involved in the τ-dimensional transformation

$$|n_1 n_2 n_3> \ = \sum_{lm} <\nu lm | n_1 n_2 n_3> \ | \nu lm>$$

where the state on the left may be either $|n_+ n_0 n_- >$ (eigenstate of H_+, H_0, H_-) or $|n_x n_y n_z>$ (eigenstate of H_x, H_y, H_z) and in each case

$$n_+ + n_0 + n_- = \nu = n_x + n_y + n_z$$

Likewise, we want to determine the coefficients of the $2\tau \times 2\tau$ transformation between spin-orbital wave functions

$$|n_1 n_2 n_3 \sigma> \ = \sum_{jl\mu} <\nu lj\mu | n_1 n_2 n_3 \sigma> \ | \nu lj\mu>$$

for both bases $\{n_+, n_0, n_-\}$ and $\{n_x, n_y, n_z\}$. The single-particle state $|\nu lj\mu>$ is the usual starting point wave function in j-j coupling scheme problems, μ being the projection of j.

STATE FUNCTIONS FOR AN ARBITRARY SHELL

For typographical convenience we shall denote by η_s the usual boson creation operators a_s^+ where $s = x, y, z$. The spherical components of this operator will then be

$$\eta_\pm = \mp \frac{1}{\sqrt{2}} (\eta_x \pm i\eta_y), \quad \eta_0 = \eta_z, \tag{2.1}$$

and the square of the creation vector-operator is

$$\eta^2 = \vec{\eta} \cdot \vec{\eta} = \eta_x^2 + \eta_y^2 + \eta_z^2 = \eta_0^2 - 2\eta_+\eta_- \tag{2.2}$$

The oscillator states $|\eta_+ \eta_0 \eta_- >$ have the usual expression

$$|\eta_+\eta_0\eta_-> = \frac{\eta_+^{n_+}\eta_0^{n_0}\eta_-^{n_-}\,|0>}{\sqrt{n_+!\,n_0!\,n_-!}} \tag{2.3}$$

The states $|\eta_x n_y n_z>$, by means the definitions (2.1), can be expressed in the following form:

$$|n_x n_y n_z< = \frac{\eta_x^{n_x}\eta_y^{n_y}\eta_z^{n_z}\,|0>}{\sqrt{n_x!\,n_y!\,n_z!}} = \frac{(\eta_- - \eta_+)^{n_+} i^{n_y} (\eta_+ + \eta_-)^{n_y}\eta_0^{n_z}\,|0>}{\sqrt{(n_x!\,n_y!\,n_z!\,2^{n_x+n_y}}}$$

$$= i^{n_y}\sqrt{\frac{n_x!\,n_y!}{n_z!\,2^{n_x+n_y}}}\sum_{\lambda=0}^{n_y}\sum_{\mu=0}^{n_z}\frac{(-)^{\mu}\eta_+^{\lambda+\mu}\,\eta_0^{n_z}\,\eta_-^{n_x+n_y-\lambda-\mu}\,|0>}{(n_x-\mu)!\,(n_y-\lambda)!\,\mu!\,\lambda!} \tag{2.4}$$

by the well-known binomial expansion theorem. Finally, the states $|\nu l m>$ have the explicit form[1]:

$$|\nu l m> = A_{\nu l}\,(\eta^2)^{\frac{\nu-l}{2}}\,\mathcal{Y}_{lm}(\vec{\eta})\,|0> \tag{2.5}$$

with $A_{\nu l} = (-)^{\frac{\nu-l}{2}} \sqrt{4\pi/(\nu+l+1)!!(\nu-l)!!}$, and $\mathcal{Y}_{lm}(\vec{r})$ being a solid spherical harmonic in the components of a vector $\vec{r}$. Now[2],

$$\mathcal{Y}_{lm}(\vec{r}) = N_{lm}(-)^m r^l \sin^m\theta\, e^{im\theta} \frac{d^{l+m}}{d(\cos\theta)^{l+m}} (\cos^2\theta - 1)^l \quad (2.7)$$

where N_{lm} is a normalization factor given by

$$N_{lm} = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \quad (2.8)$$

We can write $x + iy = r\sin\theta\, e^{i\phi}$, so the plus-component of the $\vec{r}$ vector is then $x_+ = -\frac{1}{\sqrt{2}} r \sin\theta\, e^{i\phi}$ and in (2.7) we can write

$$(-)^m r^l \sin^m\theta\, e^{im\phi} = \sqrt{2^m}\, x_+^m r^{l-m} \qquad (\text{for } m > 0) \quad (2.9)$$

Making this replacement and calculating the derivatives in (2.7), we have

$$\mathcal{Y}_{lm}(\vec{r}) = N_{lm}\sqrt{2^m}\, x_+^m \sum_{S=0}^{l} \frac{(-)^S l!(2l-2S)!}{(l-S)!S!(l-2S-m)!} (r^2)^S (r\cos\theta)^{l-2S-m} \quad (m \geq 0)$$
(2.10)

where furthermore we can put $r\cos\theta = X_0$ and $r^2 = (X_0^2 - 2X_+X_-)$, thus obtaining an expression for $\mathcal{Y}_{lm}(\vec{r})$ solely in terms of the $\vec{r}$ vector spherical components. Using this result in (2.5) and expanding the power of η^2 that appears we get the desired result in creation operators, namely

$$|\nu lm> = \frac{(-)^{\frac{\nu-l}{2}}}{2^l l!} \sqrt{\frac{2^m(2l+1)(l-m)!}{(\nu+l+1)!!(\nu-l)!!}}$$

$$\times \sum_{S=0}^{l} \sum_{r=0}^{\frac{\nu-l}{2}+S} \frac{(-)^{r+S}\left(\frac{\nu-l}{2}+S\right)!\,2^{r}\,l!\,(2l-2S)!}{r!\left(\frac{\nu-l}{2}+S-r\right)!\,S!\,(l-S)!\,(l-2S-m)!}\;\eta_{+}^{\,r+m}\,\eta_{0}^{\,\nu-2r-m}\,\eta_{-}^{\,r}\,|0\rangle \qquad (m \geqslant 0) \qquad (2.11)$$

Taking the scalar product of (2.3) with this expression one obtains the closed formula

$$\langle n_{+}n_{0}n_{-} \mid \nu l m\rangle = (-)^{\frac{\nu-l}{2}}\, 2^{n_{-}-l} \sqrt{\frac{2^{m}(2l+1)(l-m)!\,(n_{+})!\,(n_{0})!}{(\nu+l+1)!!\,(\nu-l)!!\,(l+m)!\,(n_{-})!}}$$

$$\times\ \delta n_{0},\nu-2n_{-}-m\ \ \delta n_{+},n_{-}+m \sum_{S=0}^{l} \frac{(-)^{S}\left(\frac{\nu-l}{2}+S\right)!\,(2l-2S)!}{\left(\frac{\nu-l}{2}+S-n_{-}\right)!\,S!\,(l-S)!\,(l-2S-m)!} \qquad (m>0) \qquad (2.12)$$

For the case $m < 0$ one uses the property of the spherical harmonics $\mathcal{Y}_{l,-m} = (-)^{m}\,\mathcal{Y}_{lm}^{*}$ and the fact that $\eta_{\pm}^{*} = -\,\eta_{\mp}$, $\eta_{0}^{*} = \eta_{0}$ to obtain directly from (2.11) that

$$\langle n_{+}n_{0}n_{-} \mid \nu l,-m\rangle = \langle n_{-}n_{0}n_{+} \mid \nu l m\rangle \quad (m \geqslant 0) \qquad (2.13)$$

and so formula (2.12) can be used for negative values of m if one interchanges n_{+} with ν_{-} and n_{-} with n_{+}. Similarly, the scalar product of (2.4) with (2.11) yields the second working formula

$$\langle n_{x}n_{y}n_{z} \mid \nu l m\rangle = i^{n_y}\,[1+(-)^{n_x+n_y-m}]\,(-)^{1/2(\nu-l-m+n_x-n_y)}$$

$$\times \frac{\left(\frac{n_x+n_y+m}{2}\right)!}{2^{l+1}} \sqrt{\frac{(2l+1)\,(l-m)!\,n_x!\,n_y!\,n_z!}{(\nu+l+1)!!\,(\nu-l)!!\,(l+m)!}}\;\delta_{n_z,\,\nu-n_x-n_y}$$

$$\times \sum_{S=0}^{l} \sum_{\mu=0}^{n_x} \frac{(-)^{\mu+S} \left(\frac{\nu-l}{2}+S\right)! \, (2l-2S)!}{(n_x-\mu)! \left(\frac{n_y-n_x-m}{2}+\mu\right)! \, \mu! \left(\frac{n_x+n_y+m}{2}-\mu\right)! \left(\frac{\nu-l+m-n_x-n_y}{2}+S\right)! \, S! \, (l-S)! \, (l-2S-m)!}$$

$$\text{(for } m \geqslant 0) \qquad (2.14)$$

For negative values of m in $|\nu lm>$ one can use the above expression with an added phase of $(-)^{n_x}$ since

$$<n_x n_y n_z | \nu l -m> = (-)^{n_x} < n_x n_y n_z | \nu lm> \quad (m \geqslant 0) \qquad (2.15)$$

Both brackets are very simple to evaluate for particular shells and the orbital state transformation brackets $< n_+ n_0 n_- | \nu lm>$ and $< n_x n_y n_z | \nu lm>$ for the $2s$-$1d$ nuclear shell are given in Tables I and II. They constitute unitary transformation matrices in both cases, so that orthonormality properties are given by

$$\sum_{\nu lm} <n_1' n_2' n_3' | \nu lm>^* <\nu lm | n_1 n_2 n_3> = \delta n_1' n_1 \; \delta n_2' n_2 \; \delta n_3' n_3$$

$$\sum_{n_1 n_2 n_3} <n_1 n_2 n_3 | \nu' l' m'>^* <\nu lm | n_1 n_2 n_3> = \delta \nu' \nu \; \delta l' l \; \delta m' m. \qquad (2.16)$$

The cœfficients in Table II were calculated by Smirnov using a tecnique [3] different from the creation-operator method used here.

The spin-orbit coupled states $|\nu lj\mu>$ are constructed in the following way:

$$|\nu lj\mu> = \sum_{m\sigma} <l \tfrac{1}{2} \; m\sigma | j\mu> | \nu lm, \sigma> \qquad (2.17)$$

Using the orthonormality of Clebsch-Gordan coefficients this equation can be inverted to

$$|\nu lm,\sigma> = \sum_{j\mu} < l \frac{1}{2} m\sigma | j\mu> | \nu lj\mu> \qquad (2.18)$$

Hence,

$$|n_1 n_2 n_3, \sigma> = \sum_{\nu\, lm} < \nu lm | n_1 n_2 n_3 > | \nu lm, \sigma >$$

$$= \sum_{\nu lj\,\mu} \{ \sum_{m} < \nu lm | n_1 n_2 n_3 > < l \frac{1}{2} m\sigma | j\mu> \} | \nu lj\mu> \qquad (2.19)$$

Thus our transformation coefficients for spin-orbital states in the 2s-1d shell can be constructed from Tables I and II with the help of Clebsch-Gordan coefficients since by definition

$$\sum_{m} < \nu lm | n_1 n_2 n_3 > < l \frac{1}{2} m\sigma | j\mu> \equiv < \nu lj\mu | n_1 n_2 n_3, \sigma > . \qquad (2.20)$$

These are tabulated in Tables III and IV and their orthonormality relations are given by

$$\sum_{n_1 n_2 n_3 \sigma} < \nu' l' j' \mu' | n_1 n_2 n_3, \sigma>^{*} < n_1 n_2 n_3 \sigma | \nu lj\mu > = \delta\nu' \nu \; \delta l' l \; \delta j' j \; \delta\mu' \mu,$$

$$(2.21)$$

$$\sum_{\nu lj\mu} < \nu lj\mu | n_1' n_2' n_3' , \sigma>^{*} < n_1 n_2 n_3 \sigma | \nu lj\mu> = \delta n_1' n_1 \; \delta n_2' n_2 \; \delta n_3' n_3 \; \delta\sigma' \sigma.$$

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$\lvert \nu l m\rangle$ / $\lvert n_+ n_o n_-\rangle$	$\lvert 222\rangle$	$\lvert 221\rangle$	$\lvert 220\rangle$	$\lvert 200\rangle$	$\lvert 221\rangle$	$\lvert 222\rangle$
$\lvert 200\rangle$	1 1	0	0	0	0	0
$\lvert 110\rangle$	0	1	0	0	0	0
$\lvert 101\rangle$	0	0	$\frac{1}{\sqrt{3}}$	$\frac{\sqrt{2}}{\sqrt{3}}$	0	0
$\lvert 020\rangle$	0	0	$\frac{\sqrt{2}}{\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$	0	0
$\lvert 011\rangle$	0	0	0	0	1	0
$\lvert 002\rangle$	0	0	0	0	0	1

TABLE I $\langle n_+ n_o n_- \lvert \nu l m\rangle$ $\nu = 2$

$\|\nu l m\rangle$ / $\|n_x n_y n_z\rangle$	$\|222\rangle$	$\|221\rangle$	$\|220\rangle$	$\|200\rangle$	$\|221\rangle$	$\|222\rangle$
$\|200\rangle$	$\frac{1}{2}$	0	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{3}}$	0	$\frac{1}{2}$
$\|110\rangle$	$\frac{i}{\sqrt{2}}$	0	0	0	0	$\frac{i}{\sqrt{2}}$
$\|101\rangle$	0	$-\frac{1}{\sqrt{2}}$	0	0	$\frac{1}{\sqrt{2}}$	0
$\|020\rangle$	$-\frac{1}{2}$	0	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{3}}$	0	$-\frac{1}{2}$
$\|011\rangle$	0	$-\frac{i}{\sqrt{2}}$	0	0	$-\frac{i}{\sqrt{2}}$	0
$\|002\rangle$	0	0	$\frac{2}{\sqrt{6}}$	$-\frac{1}{\sqrt{3}}$	0	0

TABLE II $\langle n_x n_y n_z | \nu l m \rangle$ $\nu = 2$

$\vert n_+ n_o n_- \sigma\rangle$ / $\vert 2 l j \mu\rangle$	$\sigma = 1/2$						$\sigma = -1/2$					
	$\vert 002\rangle$	$\vert 101\rangle$	$\vert 011\rangle$	$\vert 200\rangle$	$\vert 110\rangle$	$\vert 020\rangle$	$\vert 002\rangle$	$\vert 101\rangle$	$011\rangle$	$\vert 200\rangle$	$\vert 110\rangle$	$\vert 020\rangle$
$0\ \frac{1}{2}\ -\frac{1}{2}$	0	$+\sqrt{\frac{2}{3}}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0	0
$2\ \frac{3}{2}\ \frac{3}{2}$	0	0	0	0	0	0	0	$+\sqrt{\frac{2}{3}}$	0	0	0	$-\frac{1}{\sqrt{3}}$
$2\ \frac{3}{2}\ \frac{1}{2}$	0	0	0	0	$-\frac{1}{\sqrt{6}}$	0	0	0	0	$\frac{2}{\sqrt{5}}$	0	0
$2\ \frac{3}{2}\ -\frac{1}{2}$	0	$-\sqrt{\frac{2}{15}}$	0	0	0	$\frac{-2}{\sqrt{15}}$	0	0	0	0	$+\sqrt{\frac{3}{5}}$	0
$2\ \frac{3}{2}\ \frac{1}{2}$	0	0	$-\sqrt{\frac{3}{5}}$	0	0	0	0	$+\sqrt{\frac{2}{15}}$	0	0	0	$\frac{2}{\sqrt{15}}$
$2\ \frac{3}{2}\ -\frac{3}{2}$	$-\frac{2}{\sqrt{5}}$	0	0	0	0	0	0	0	$\frac{1}{\sqrt{5}}$	0	0	0
$2\ \frac{5}{2}\ \frac{5}{2}$	0	0	0	1	0	0	0	0	0	0	0	0
$2\ \frac{5}{2}\ \frac{3}{2}$	0	0	0	0	$+\frac{2}{\sqrt{5}}$	0	0	0	0	$\frac{1}{\sqrt{5}}$	0	0
$2\ \frac{5}{2}\ \frac{1}{2}$	0	$+\frac{1}{\sqrt{5}}$	0	0	0	$\sqrt{\frac{2}{5}}$	0	0	0	0	$+\sqrt{\frac{2}{5}}$	0
$2\ \frac{5}{2}\ -\frac{1}{2}$	0	0	$\sqrt{\frac{2}{5}}$	0	0	0	0	$+\frac{1}{\sqrt{5}}$	0	0	0	$\sqrt{\frac{2}{5}}$
$2\ \frac{5}{2}\ -\frac{3}{2}$	$\frac{1}{\sqrt{5}}$	0	0	0	0	0	0	0	$\frac{2}{\sqrt{5}}$	0	0	0
$2\ \frac{5}{2}\ -\frac{5}{2}$	0	0	0	0	0	0	1	0	0	0	0	0

TABLE III $\langle \nu l j \mu \vert n_+ n_o n_- \sigma \rangle$ $\nu = 2$

$\|n_x n_y n_z \sigma\rangle$ / $\|2 l j \mu\rangle$	$\sigma = 1/2$						$\sigma = -1/2$					
	$\|002\rangle$	$\|101\rangle$	$\|011\rangle$	$\|200\rangle$	$\|110\rangle$	$\|020\rangle$	$\|002\rangle$	$\|101\rangle$	$\|011\rangle$	$\|200\rangle$	$\|110\rangle$	$\|020\rangle$
$0\ \frac{1}{2}\ \frac{1}{2}$	$\frac{-1}{\sqrt{3}}$	0	0	$\frac{-1}{\sqrt{3}}$	0	$\frac{-1}{\sqrt{3}}$	0	0	0	0	0	0
$0\ \frac{1}{2}\ \frac{1}{2}$	0	0	0	0	0	0	$\frac{-1}{\sqrt{3}}$	0	0	$\frac{-1}{\sqrt{3}}$	0	$\frac{-1}{\sqrt{3}}$
$2\ \frac{3}{2}\ \frac{3}{2}$	0	$\frac{1}{\sqrt{10}}$	$\frac{-i}{\sqrt{10}}$	0	0	0	0	0	0	$\frac{1}{\sqrt{5}}$	$-i\sqrt{\frac{2}{5}}$	$\frac{-1}{\sqrt{5}}$
$2\ \frac{3}{2}\ \frac{1}{2}$	$\frac{-2}{\sqrt{15}}$	0	0	$\frac{1}{\sqrt{15}}$	0	$\frac{1}{\sqrt{15}}$	0	$-\sqrt{\frac{3}{10}}$	$i\sqrt{\frac{3}{10}}$	0	0	0
$2\ \frac{3}{2} - \frac{1}{2}$	0	$-\sqrt{\frac{3}{10}}$	$-i\sqrt{\frac{3}{10}}$	0	0	0	$\frac{2}{\sqrt{15}}$	0	0	$\frac{-1}{\sqrt{15}}$	0	$\frac{-1}{\sqrt{15}}$
$2\ \frac{3}{2} - \frac{3}{2}$	0	0	0	$\frac{-1}{\sqrt{5}}$	$-i\sqrt{\frac{2}{5}}$	$\frac{1}{\sqrt{5}}$	0	$\frac{1}{\sqrt{10}}$	$\frac{i}{\sqrt{10}}$	0	0	0
$2\ \frac{5}{2}\ \frac{5}{2}$	0	0	0	$\frac{1}{2}$	$\frac{-i}{\sqrt{2}}$	$\frac{-1}{2}$	0	0	0	0	0	0
$2\ \frac{5}{2}\ \frac{3}{2}$	0	$-\sqrt{\frac{2}{5}}$	$i\sqrt{\frac{2}{5}}$	0	0	0	0	0	0	$\frac{1}{2\sqrt{5}}$	$\frac{-i}{\sqrt{10}}$	$\frac{-1}{2\sqrt{5}}$
$2\ \frac{5}{2}\ \frac{1}{2}$	$\sqrt{\frac{2}{5}}$	0	0	$\frac{-1}{\sqrt{10}}$	0	$\frac{-1}{\sqrt{10}}$	0	$\frac{-1}{\sqrt{5}}$	$\frac{i}{\sqrt{5}}$	0	0	0
$2\ \frac{5}{2} - \frac{1}{2}$	0	$\frac{1}{\sqrt{5}}$	$\frac{i}{\sqrt{5}}$	0	0	0	$\sqrt{\frac{2}{5}}$	0	0	$\frac{-1}{\sqrt{10}}$	0	$\frac{-1}{\sqrt{10}}$
$2\ \frac{5}{2} - \frac{3}{2}$	0	0	0	$\frac{1}{2\sqrt{5}}$	$\frac{i}{\sqrt{10}}$	$\frac{-1}{2\sqrt{5}}$	0	$\sqrt{\frac{2}{5}}$	$i\sqrt{\frac{2}{5}}$	0	0	0
$2\ \frac{5}{2} - \frac{5}{2}$	0	0	0	0	0	0	0	0	0	$\frac{1}{2}$	$\frac{i}{\sqrt{2}}$	$\frac{-1}{2}$

TABLE IV $\langle \nu l j \mu \| n_x n_y n_z \sigma \rangle$ $\nu = 2$