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Shell-model matrix elements in a neutron–proton quasi-spin formalism for several shells

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Abstract. Previous work in the neutron–proton quasi-spin formalism to express shell-model Hamiltonian matrix elements in terms of a set of reduced matrix elements is extended to several interacting shells.

1. Introduction

In a previous paper [1], we used vector coherent-state methods [2] to derive formulae and tables for calculating shell-model matrix elements in a basis defined by the neutron–proton quasi-spin group $O(5)$. For simplicity, that paper was restricted to a single shell with angular momentum j. However, the general derivation is equally valid for a (multi-j) system of several shells so long as the pair state of $O(5)$ is defined as

$$A^{\dagger} = \sum_{i} \sqrt{\Omega_i/2}(a_i^{\dagger} \times a_i^{\dagger})^{J=0,T=1} \quad (1)$$

where $\Omega_i = j_i + \frac{1}{2}$. The irreducible representations of $O(5)$ are still labelled by (ω, t) with $\omega = \Omega - v/2$, where v is the seniority and t the reduced isospin, but now $\Omega = \sum_i \Omega_i$. Physically, v is the number of unpaired nucleons in the sense of the pairs (1) and t is the isospin of these unpaired nucleons. (Note that v is not given by the sum of seniorities in the separate shells which is used by some authors [3] as a loose definition of seniority in a multi-j system.) The purpose of this paper is to generalize to the multi-j system those sections of [1] which were written specifically for a single j-shell. In realistic calculations, there is almost always mixing of several shells.

The shell-model interaction V is analysed into components $V^{(00)}$, $V^{(11)}$, $V^{(20)}$ and $V^{(22)}$ which transform irreducibly under $O(5)$ and the coherent state arguments in [1] gave a crucial closed formula, (36) of [1], which, taken together with an appropriate K-matrix, provides shell-model matrix elements in the seniority basis for each $O(5)$ component of V. Since the derivation of this crucial equation relied entirely on the $O(5)$ structure it remains valid in the multi-j system. The formula is trivial for the invariant component $V^{(00)}$ and in a single j-shell it is not needed for $V^{(11)}$ since this component is then simply expressed in terms of the number operator. This simplification does not occur in a multi-j system and the formula ((36) of [1]) must be used for $V^{(11)}$ as well as for $V^{(20)}$ and $V^{(22)}$. In particular, the single-particle energy contributes to $V^{(11)}$. The evaluation of formula (36) for the case of $V^{(11)}$ is described in section 2 of the present paper, leading to table 2 which is an extension of table C in [1]. The calculation of reduced matrix elements of the two-body interaction in section 4 of [1] was written specifically for a single j and so requires significant modification, given here in section 3.

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2. The $V^{(11)}$ component of the interaction

The $V^{(11)}$ component of the two-body interaction is odd under particle–hole conjugation and so reduces to a one-body operator. In a single j-shell, the only scalar one-body operator is the number operator and so this component reduces to a multiple, given in equation (20) of [1], of the $O(5)$ group operator

$$H_1 = (n - 2\Omega)/2 \tag{2}$$

and is immediately evaluated. In the multi-j system there are several one-body scalars so their evaluation is non-trivial and equation (36) of [1] must be used. Although equation (36) of [1] refers to $V^{(2s)}$, it may be used for $V^{(11)}$ if the appropriate coefficients a, b and d are used. The values are $a_{00} = 1$, $a_{11} = -1$, and $d_{qT_q} = 1$ with b given in table 1, which corresponds to table 2 of [1]. Equation (36) of [1] then gives the general z-space matrix elements of $V^{(11)}$ in terms of the reduced matrix elements $\langle\omega' t'||V^{(11)}_{\omega-\omega' u}||\omega t\rangle$. In [1] we evaluated equation (36) for even n and $t = 0, 1$ and 2 by giving the coefficient of each reduced matrix element for the components $V^{(20)}$ and $V^{(22)}$. This process is completed in table 2 of the present paper where we give the coefficients for the component $V^{(11)}$. We use the same notation as in [1] and a full description is given in appendix C of that paper, including the use of the 'negative angular-momentum symmetry' for economy in printing.

3. The reduced matrix elements

The reduced matrix elements $\langle\omega' t'||V^{(ab)}_{\omega-\omega' u}||\omega t\rangle$ are defined as the matrix elements of the relevant component of the interaction between states of full seniority, reduced with respect to isospin t. The two subscripts on $V^{(ab)}_{\omega-\omega' u}$ define its isospin u and the value $\omega - \omega'$ of the $O(5)$ operator H_1 of equation (2). Since the interaction conserves both particle number and isospin, the strict 'components' of the interaction satisfy $\omega - \omega' = u = 0$ but the matrix elements of some other members of the $O(5)$ multiplet of operators containing each $V^{(ab)}_{00}$ are also required and can be constructed using $O(5)$ Wigner coefficients, as in [1]. The few additional coefficients needed for $V^{(11)}$ are given here in table 3 which is an extension of table 3 of [1].

Table 1. The coefficients $b(mc_qT'_qu)$ in equation (36) of [1] for the component $V^{(11)}$.

ω'	m	c	q	T'_q	$u=0$	$u=1$
$\omega+1$	1	1	0	0	—	1
ω	1	1	1	1	$-\sqrt{3}$	$-\sqrt{2}$
	0	0	0	0	1	—

In [1] we referred to these other components as 'extensions' of the interaction. However, the discussion in section 4 of that paper was limited to a single shell and must now be generalized. The strict components of the interaction, including the single-particle energies, are given by

$$V^{(11)}_{00} = \tfrac{1}{2}\sum_{1,3}(N_{13} - 2\Omega_3\delta_{13})(f^0_{13} - 3f^1_{13} + 2p_{13}) \tag{3}$$

Table 2. Coefficients of reduced matrix elements $\langle\omega' t'\|V^{(11)}_{\omega-\omega' u}\|\omega t\rangle$ in equation (36) of [1].

t'	t	T'_p	T_p	u	$((\omega' t')p' T'_p T\|\Gamma(V^{(11)})\|(\omega t)pT_pT)$
		$\omega' = \omega + 1$			
1	0	$T\pm1$	T	1	$\sqrt{(T+1)(p+T+3)/(2T+1)}$
0	1	T	$T\pm1$	1	$-\sqrt{(T+1)(p-T+1)/3(2T+1)}$
1	1	$T\pm1$	T	1	$-\sqrt{T(p+T+3)/2(2T+1)}$
		T	$T\pm1$	1	$-\sqrt{T(p-T+1)/2(2T+1)}$
2	1	$T\pm2$	$T\pm1$	1	$\sqrt{(T+2)(p+T+4)/(2T+3)}$
		T	$T\pm1$	1	$-\sqrt{T(2T-1)(p-T+1)/6(2T+1)(2T+3)}$
		$T\pm1$	T	1	$\sqrt{(p+T+3)(T+2)/2(2T+1)}$
1	2	$T\pm1$	$T\pm2$	1	$-\sqrt{3(T+2)(p-T)/5(2T+3)}$
		$T\pm1$	T	1	$\sqrt{T(2T-1)(p+T+3)/10(2T+1)(2T+3)}$
		T	$T\pm1$	1	$-\sqrt{3(T+2)(p-T+1)/10(2T+1)}$
2	2	$T\pm2$	$T\pm1$	1	$-\sqrt{T(p+T+4)/3(2T+3)}$
		T	$T\pm1$	1	$-\sqrt{(T+2)(2T-1)(p-T+1)/2(2T+1)(2T+3)}$
		$T\pm1$	$T\pm2$	1	$-\sqrt{T(p-T)/3(2T+3)}$
		$T\pm1$	T	1	$-\sqrt{(T+2)(2T-1)(p+T+3)/2(2T+1)(2T+3)}$
		$(\omega' = \omega)$			
0	0	T	T	0	$(\omega-p)/\omega$
0	1	T	T	1	$\sqrt{T(T+1)/3}/(\omega+1)$
1	1	$T\pm1$	$T\pm1$	0	$\sqrt{2}\{2T(T+1)(3+2\omega)-(p-\omega)[1+(2T+1)(1+2\omega^2+4\omega)]\}/D$
				1	$[-2T(T+1)\omega(3+2\omega)+\omega(p-\omega)+(2T+1)(p-\omega)(4+3\omega)]/D$ $D=2\sqrt{2}(\omega+2)(\omega+1)(\omega-1)(2T+1)$
		$T+1$	$T-1$	0	$\sqrt{T(T+1)(p+T+2)(p-T+1)}/(\omega+2)(\omega+1)(\omega-1)(2T+1)$
				1	$-\omega\sqrt{T(T+1)(p+T+2)(p-T+1)}/\sqrt{2}(\omega+2)(\omega+1)(\omega-1)(2T+1)$
		T	T	0	$-\omega(p-\omega)/(\omega+1)(\omega-1)$
				1	$(p-\omega)/\sqrt{2}(\omega+1)(\omega-1)$
1	2	$T\pm1$	$T\pm1$	1	$\sqrt{3T(T+2)}[T(2\omega+5)+\omega-p+1]/\sqrt{10}(\omega+3)(\omega+1)(2T+1)$
		$T\pm1$	$T\mp1$	1	$\sqrt{3T(T-1)(p+T+2)(p-T+1)}/\sqrt{10}(\omega+3)(\omega+1)(2T+1)$
		T	$T\pm2$	1	$-\sqrt{3T(T+2)(p+T+3)(p-T)/5(2T+1)(2T+3)}/(\omega+3)(\omega+1)$
		T	T	1	$[-3(p-\omega)+2(2\omega+5)T(T+1)-6(\omega+2)]/[(\omega+3)(\omega+1)$ $\times\sqrt{10(2T-1)(2T+3)}]$
2	2	$T\pm2$	$T\pm2$	0	$\{2T(T+2)(3+2\omega)-(p-\omega)[(3+4\omega+2\omega^2)+\omega(\omega+2)(2T+1)]\}/[(\omega+3)$ $\times(\omega+1)(\omega-2)(2T+3)]$
				1	$\{-2T(T+2)\omega(3+2\omega)+(p-\omega)[(12+13\omega)+(5\omega+6)(2T+1)]\}/[\sqrt{6}(\omega+3)$ $\times(\omega+1)(\omega-2)(2T+3)]$
		$T\pm2$	T	0	$\sqrt{6T(T+2)(2T-1)(p+T+3)(p-T)/(2T+1)}/[(\omega+3)(\omega+1)$ $\times(\omega-2)(2T+3)]$
				1	$-\omega\sqrt{T(T+2)(2T-1)(p+T+3)(p-T)/(2T+1)}/[(\omega+3)(\omega+1)$ $\times(\omega-2)(2T+3)]$
		T	T	0	$\{-6(3+2\omega)+(p-\omega)[3(\omega^2+2\omega-6)-4(\omega^2+2\omega-2)T(T+1)]\}/[(\omega+3)$ $\times(\omega+1)(\omega-2)(2T+3)(2T-1)]$
				1	$\sqrt{6}\{2\omega(3+2\omega)+(p-\omega)[(\omega-6)+4(\omega+2)T(T+1)]\}/[2(\omega+3)(\omega+1)$ $\times(\omega-2)(2T+3)(2T-1)]$
		$T\pm1$	$T\pm1$	0	$\{2(T+2)(T-1)(3+2\omega)-(p-\omega)[9+(2\omega^2+4\omega-3)(2T+1)]\}/[2(\omega+3)$ $\times(\omega+1)(\omega-2)(2T+1)]$
				1	$\{-2(T+2)(T-1)\omega(3+2\omega)+(p-\omega)[9\omega+(7\omega+12)(2T+1)]\}/[2\sqrt{6}(\omega+3)$ $\times(\omega+1)(\omega-2)(2T+1)]$
		$T+1$	$T-1$	0	$3\sqrt{(T+2)(T-1)(p+T+2)(p-T+1)}/(\omega+3)(\omega+1)(\omega-2)(2T+1)$
				1	$-\omega\sqrt{6(T+2)(T-1)(p+T+2)(p-T+1)}/2(\omega+3)(\omega+1)(\omega-2)(2T+1)$

Table 3. Wigner coefficients for $V^{(11)}$.

		(10)×(10)					(11)×(11)						
	h	0			−1		0			−1			
	h_1t_1	−10	01	10	−10	01	−11	01	11	−11	−11	00	01
	h_2t_2	10	01	−10	01	−10	11	01	−11	00	01	−11	−11
(11)	$u=0$	$\sqrt{\frac{1}{2}}$		$-\sqrt{\frac{1}{2}}$			$\sqrt{\frac{1}{2}}$		$-\sqrt{\frac{1}{2}}$				
	$u=1$		−1		$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{3}}$	$-\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{3}}$

$$V_{00}^{(20)} = \tfrac{1}{5}\sum_{1,3}(N_{13} - \Omega_3\delta_{13})(f_{13}^1 - 3f_{13}^0 - e_{13}) + \bar{V}^{(20)} \tag{4}$$

$$V_{00}^{(22)} = \tfrac{1}{2}\sum_{1,3}(N_{13} - \Omega_3\delta_{13})(2f_{13}^1 + e_{13}) + \bar{V}^{(22)} \tag{5}$$

where $\bar{V}$ denotes two-body interactions with matrix elements

$$\langle 12J, T=0|\bar{V}_{00}^{(20)}|34J, T=0\rangle = \tfrac{3}{5}[E_{J0}(1234) + F_{J0}^0(1234) + F_{J0}^1(1234)] \tag{6}$$

$$\langle 12J, T=1|\bar{V}_{00}^{(20)}|34J, T=1\rangle = \tfrac{1}{15}[E_{J1}(1234) + 3F_{J1}^0(1234) - F_{J1}^1(1234)] \tag{7}$$

$$\langle 12J, T=1|\bar{V}_{00}^{(22)}|34J, T=1\rangle = \tfrac{1}{3}[E_{J1}(1234) + 2F_{J1}^1(1234)] \tag{8}$$

and

$$e_{13} = \Delta_{13}\sum_2\sqrt{\Omega_2/\Omega_1}\,E_{01}(1322) \tag{9}$$

$$f_{13}^T = \Delta_{13}\sum_2\sqrt{\Omega_2/\Omega_1}\,F_{01}^T(1322) \tag{10}$$

$$N_{13} = 2\sqrt{\Omega_1}(a_1^\dagger \times a_3)^{00} \tag{11}$$

with p_{13} defining the single-particle energy term in the form

$$h = \sum_{1,3} p_{13}N_{13}. \tag{12}$$

In equation (11), the superscripts after the brackets denote the vector-coupling resultants in angular momentum and isospin, respectively. For brevity we use 1, 2, 3 and 4 for the single-particle state labels and write $\Delta_{13} = [(1+\delta_{13})/2]^{1/2}$ with $E_{JT}(1234) = \langle 12JT|V|34JT\rangle$, where $|34JT\rangle$ is a two-particle antisymmetrized state and

$$F_{JT}^{T'}(1234) = \frac{(-1)^{j_2+j_3+T'}}{2\Delta_{12}\Delta_{34}}\sum_{J'}(-1)^{J'}(2J'+1)\left[\Delta_{23}\Delta_{14}\begin{Bmatrix} j_2 & j_3 & J' \\ j_4 & j_1 & J\end{Bmatrix}E_{J'T'}(2314) + (-1)^{J+T+1}\Delta_{13}\Delta_{24}\begin{Bmatrix} j_1 & j_3 & J' \\ j_4 & j_2 & J\end{Bmatrix}E_{J'T'}(1324)\right]. \tag{13}$$

Note that, whereas the components $(a^\dagger)_{mm_t}$ of the tensor operator $a^\dagger$ are precisely the creation operators $a^\dagger_{mm_t}$, the components of a are given in terms of the destruction operators by $(a)_{mm_t} = (-1)^{j+1/2-m-m_t} a_{-m\,-m_t}$. In most calculations the expressions (9)–(12) will contain a factor δ_{13} because $j_1 = j_3$ and it is rare to involve states with the same j but different nl.

The remaining component $V^{(00)}_{00}$ is obtained by subtraction from the original interaction V

$$V^{(00)}_{00} = V - V^{(11)}_{00} - V^{(20)}_{00} - V^{(22)}_{00}. \tag{14}$$

The extensions of V which conserve the particle number are given by two-body interactions with reduced matrix elements

$$\langle 12J, T = 1 || V^{(20)}_{02} || 34J, T = 1\rangle = \frac{\sqrt{2}}{3}[E_{J1}(1234) + 3F^0_{J1}(1234) - F^1_{J1}(1234)] \tag{15}$$

$$\langle 12J, T = 1 || V^{(22)}_{02} || 34J, T = 1\rangle = \frac{\sqrt{5}}{3}[E_{J1}(1234) + 2F^1_{J1}(1234)] \tag{16}$$

$$\langle 12J, T = 1 || V^{(22)}_{01} || 34J, T = 1\rangle = -\frac{1}{\sqrt{3}}[E_{J1}(1234) + 2F^1_{J1}(1234)] \tag{17}$$

together with the one-body terms

$$V^{(11)}_{01}(\text{one-body}) = -\sum_{1,3} T_{13}(f^0_{13} - 3f^1_{13} + 2p_{13}) \tag{18}$$

$$V^{(22)}_{01}(\text{one-body}) = -\sqrt{\frac{2}{3}} \sum_{1,3} T_{13}(2f^1_{13} + e_{13}) \tag{19}$$

where

$$T_{13} = \sqrt{\Omega_1}(a^\dagger_1 \times a_3)^{01}. \tag{20}$$

Reduced matrix elements which are diagonal in the seniority $\omega = \omega'$ may be calculated directly from these expressions in the states of full seniority $n = v$. This is simple for small $v \leqslant 2$ but for greater v one must first define the basis and then use fractional parentage coefficients, as in [1], or some other numerical technique.

Since the implementation of equation (36) of [1] requires reduced matrix elements only between states of full seniority, the calculation of reduced matrix elements between different seniorities requires extensions of V which change the particle number. Using the $O(5)$ commutation relations, we find them to be

$$V^{(11)}_{-11} = -\tfrac{1}{2} \sum_{1,3} \hat{j}_1 (f^0_{13} - 3f^1_{13} + 2p_{13})(a_1 \times a_3)^{01} \tag{21}$$

$$V^{(20)}_{-11} = \frac{1}{2\sqrt{30}} \sum_{1,2,3,4,J} \Delta_{12}\Delta_{34}\hat{J}\Big[3E_{J0}(3412)[(a^\dagger_3 \times a_4)^{J1} \times (a_1 \times a_2)^{J0}]^{01}$$
$$- E_{J1}(3412)\{\sqrt{2}[(a^\dagger_3 \times a_4)^{J1} \times (a_1 \times a_2)^{J1}]^{01} - [(a^\dagger_3 \times a_4)^{J0} \times (a_1 \times a_2)^{J1}]^{01}\}\Big]$$

$$+\frac{1}{2\sqrt{15}}\sum_{1,3}\hat{j}_1(f^1_{13}-3f^0_{13}-e_{13})(a_1\times a_3)^{01} \tag{22}$$

$$V^{(22)}_{-11}=\frac{1}{2\sqrt{6}}\sum_{1,2,3,4,J}\Delta_{12}\Delta_{34}\hat{J}E_{J1}(3412)\{[(a^\dagger_3\times a_4)^{J1}\times(a_1\times a_2)^{J1}]^{01}$$
$$+\sqrt{2}[(a^\dagger_3\times a_4)^{J0}\times(a_1\times a_2)^{J1}]^{01}\}-\frac{1}{\sqrt{6}}\sum_{1,3}\hat{j}_1(2f^1_{13}+e_{13})(a_1\times a_3)^{01} \tag{23}$$

$$V^{(22)}_{-12}=-\frac{1}{2\sqrt{2}}\sum_{1,2,3,4,J}\Delta_{12}\Delta_{34}\hat{J}E_{J1}(3412)[(a^\dagger_3\times a_4)^{J1}\times(a_1\times a_2)^{J1}]^{02} \tag{24}$$

$$V^{(20)}_{-20}=\frac{1}{4\sqrt{10}}\sum_{1,2,3,4,J}\Delta_{12}\Delta_{34}\hat{J}\{\sqrt{3}E_{J0}(3412)[(a_3\times a_4)^{J0}\times(a_1\times a_2)^{J0}]^{00}$$
$$-E_{J1}(3412)[(a_3\times a_4)^{J1}\times(a_1\times a_2)^{J1}]^{00}\} \tag{25}$$

$$V^{(22)}_{-22}=-\frac{1}{4\sqrt{2}}\sum_{1,2,3,4,J}\Delta_{12}\Delta_{34}\hat{J}E_{J1}(3412)[(a_3\times a_4)^{J1}\times(a_1\times a_2)^{J1}]^{02} \tag{26}$$

where $\hat{J}=(2J+1)^{1/2}$. In all cases, the sums run independently over the single-particle labels and J. To calculate reduced matrix elements for the operators (21) to (24), one must use full seniority states with $n=v$ on the right and $n'=v'=n-2$ on the left while for (25) and (26) $n'=v'=n-4$ on the left.

There is an alternative method for calculating reduced matrix elements which is less direct and makes use only of the strict components $V^{(ab)}_{00}$ of the interaction. The method would involve making a shell-model calculation for states of less than full seniority, that is for states with $n>v$. These results could be equated to the results from equation (36) of [1] and then solved to find the reduced matrix elements. Although this procedure may be advantageous in some simple cases it is not generally preferable.

4. Discussion

The formulae and tables in this paper provide a generalization of a previous paper [1] away from a single shell to the more realistic situation of several interacting shells. It enables the shell-model energy matrix to be calculated for arbitrary particle number in a neutron–proton quasi-spin basis in terms of a set of reduced matrix elements. Although it may be possible to develop a technique which treats the reduced matrix elements as parameters, we give formulae by which they can be calculated from a given two-body Hamiltonian and single-particle energies. The formulae for a single shell in the earlier paper [1] have been used in [4] to derive the dependence of the interacting-boson Hamiltonian on number and isospin in the isospin-invariant version IBM-3, see [5] and [6]. The more general formulation of the present paper can now be used to extend that work [4] to the more realistic case of several valence shells.

Errata in reference [1].

(i) The symbol $g_{m'_t m_t}$ was omitted after the summation sign in equation (26).

(ii) The two symbols (11) in the sum over odd J in equation (42) should read (10).

(iii) The entry $\sqrt{1/2}$ in the seventh row and thirteenth column of table 3 should be deleted.

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