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Pseudospin transformation of physical operators

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Abstract. A procedure for applications of the pseudospin transformation within the framework of nuclear oscillator shell model is developed. It is valid for operators expressed in terms of single-particle variables and is based on permutation rules for special rotational invariants. The procedure is applied to a number of physical operators including several rotational scalars, the spin and orbital momenta, and the quadrupole moment. An algorithm for generating an approximation to the pseudospin transformation, which gives a simple and accurate expression for dominant parts of required transforms, is also given. The algebras associated with pseudospin transformations are discussed.

1. Introduction

A promising advance relating to the development of a shell-model theory for heavy nuclei is the pseudospin (more precisely, pseudo space-spin) concept [1, 2]. It simplifies nuclear structure calculations considerably by re-assigning the orbital and spin momenta in such a way as to effectively reduce the strength of the spin–orbit coupling in the single-particle Hamiltonian. In combination with Elliott’s many-particle $SU(3)$ approach [3], and especially its $Sp(6, R)$ extension (see reviews [4, 5] and references therein) which looks after the monopole and quadrupole modes, it has developed into a powerful tool for microscopic studies of collective phenomena in strongly deformed nuclei [6–8].

The transformation from the normal representation to the pseudo space-spin representation, usually abbreviated as the *normal* \rightarrow *pseudo* transformation, is conventionally defined within the framework of the harmonic oscillator shell model. It can be viewed simply as being a scheme for relabelling the single-nucleon components of the oscillator shell-model states associated with the normal parity subspace [9]. Although this interpretation is too restrictive to be directly applicable in realistic mean-field and many-particle descriptions of nuclei, which require instead the helicity transformation [10], it is of primary importance because of the key role played by the oscillator shell model in microscopic nuclear calculations.

An alternative interpretation for the normal \rightarrow pseudo transformation in terms of the single-particle coordinates, momenta and spins variables has been suggested [11]. From an algebraic perspective, this new realization is a supersymmetric operation as it is constructed out of the rotational scalars which form the symplectic superalgebra $osp(1|2)$ [12].

The relabelling of single-particle states, which up until recently was the exclusive tool for effecting the normal \rightarrow pseudo transformation, is a working procedure that is well suited to

numerical calculation with a given model space. From the standpoint of operators, however, it only yields simple results for actions defined on single-particle basis states. For example, the relabelling procedure is very simple when applied to the pairing interaction which creates and annihilates pairs in time-reversed nucleon states [13]. However, the majority of physical operators, including the kinetic energy, internucleon potentials, electromagnetic transitions, and so on, are most easily expressed in terms of the variables \mathbf{r} , \mathbf{p} and \mathbf{s} . For these forms the relabelling can only be effected in terms of a second quantized representation which must be done numerically for every major shell by means of the symmetry-adapted tensorial expansion and this, in turn, complicates the interpretation of the result [6].

In this paper the analytical form of the normal \rightarrow pseudo transformation is used in constructing a procedure for finding images of operators that have an explicit dependence on single-particle variables. This procedure constitutes a basis for developing an analytical formalism and carrying out calculations within any microscopic theory using the pseudo space-spin concept, especially the pseudo- $SU(3)$ and pseudo- $Sp(6, R)$ theories. The analytical results are valid for any oscillator shell. The transformation of several important operators, including the spin and quadrupole moment, is discussed in detail. The images that are obtained are compared with tensorial expansions derived using the relabelling algorithm. A heuristic technique is developed to deduce simple approximations to the normal \rightarrow pseudo images which extract the dominant parts in a simple and accurate manner.

2. Normal \rightarrow pseudo transformation

For the system of A nucleons the normal \rightarrow pseudo transformation can be written in a multiplicative form [11]

$$U_{\text{total}} = \prod_{i=1}^A U(\mathbf{r}_i, \mathbf{p}_i, \boldsymbol{\sigma}_i) \quad (1)$$

where the \mathbf{r}_i stand for the position vectors, \mathbf{p}_i for the momentum, and $\boldsymbol{\sigma}_i = 2\mathbf{s}_i$ for the Pauli spin operators of the individual particles. The corresponding single-particle operators $U(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma})$ can be represented as follows [11, 12]:

$$U(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}) = d(d^+d)^{-1/2} \quad (2)$$

$$d = \mathbf{b} \cdot \boldsymbol{\sigma} \quad d^+ = \mathbf{b}^+ \cdot \boldsymbol{\sigma} \quad (3)$$

where $\mathbf{b} = (\mathbf{r}/r_0 + i r_0 \mathbf{p})/\sqrt{2}$, $\mathbf{b}^+ = (\mathbf{r}/r_0 - i r_0 \mathbf{p})/\sqrt{2}$ are the annihilation and creation operators, respectively, and $r_0 = \sqrt{\hbar/m\omega}$ is the characteristic oscillator length. There exists another representation [14] for the single-particle transformation operator

$$U(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}) = (d d^+)^{-1/2} d \quad (4)$$

which can be obtained from (2) by applying the identity

$$d f(d^+d) = f(d d^+) d.$$

The latter identity requires associative property for the operators d and d^+ for its proof, and holds for any analytic function $f(x)$ which is expandable in a power series.

The transformation operator, as given by (2) and (4), acts on the harmonic oscillator eigenstates

$$\psi_{nljm} = i^l R_{nl}(r)(\mathbf{Y}_l \otimes \chi)_{jm} \quad (5)$$

in the following manner [9, 11]:

$$U(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}) \psi_{nljm} = \psi_{\tilde{n}\tilde{l}jm} \quad (6)$$

where n is the number of quanta, j is the angular momentum, l and m are the orbital momentum and its projection, Y_l is a spherical harmonic, and χ is a Pauli spinor. The 'pseudo' values of n and l are determined by the rules

$$\tilde{n} = n - 1 \quad \tilde{l} = l \pm 1 \quad \text{if } j = l \pm \frac{1}{2}. \quad (7)$$

The normal \rightarrow pseudo transformation is rotationally invariant and unitary. Rotational invariance follows from the fact that the angular momentum $\mathbf{j} = \mathbf{l} + \mathbf{s}$ commutes with the d and d^+ operators. Unitarity holds within the subspace of normal parity orbitals only, that is, within the space spanned by the set of states of a major shell less the one with $(j = n + \frac{1}{2})$. The unique parity orbitals, which either defect out of the model space ($j = n + \frac{1}{2}$) or intrude into it from the shell above ($j = n + \frac{3}{2}$) due to the spin-orbit interaction, have no pseudo counterparts because they are annihilated by the d operator (cf the RHS of (4)). For instance, the $s_{1/2}$, $d_{3/2}$, $d_{5/2}$ and $g_{7/2}$ orbitals of the $n = 4$ shell map onto the $\tilde{p}_{1/2}$, $\tilde{p}_{3/2}$, $\tilde{f}_{5/2}$ and $\tilde{f}_{7/2}$ orbitals of the $\tilde{n} = 3$ shell, respectively, while the $g_{9/2}$ orbital has no pseudo image. The unitarity can be checked by comparing (2) and (4) with the condition

$$U U^+ = U^+ U = 1. \quad (8)$$

For the sake of notational simplicity the arguments of the transformation operator are omitted in what follows.

3. Permutation relations

The definitions (2) and (4) clearly indicate that the rotational invariants (3) are the simplest building blocks of the normal \rightarrow pseudo transformation operator. As shown in [12], these two operators are also the odd generators of the $osp(1|2)$ superalgebra. When combined with the bilinear forms of d and d^+ , namely

$$\begin{aligned} d^2 &= \mathbf{b} \cdot \mathbf{b} \\ h_0 &= \frac{1}{2}(d d^+ + d^+ d) = \hat{n} + \frac{3}{2} \\ (d^+)^2 &= \mathbf{b}^+ \cdot \mathbf{b}^+ \end{aligned} \quad (9)$$

they form an algebra closed with respect to commutation and anticommutation operations (see [12, equations (3.1) and (4.3)] for the relations connecting the $osp(1|2)$ generators). The symbol \hat{n} is used henceforth for denoting the number of quanta operator.

Since the operators (3) and (9) are related through both commutations and anticommutation, they should also be involved in general permutation relations. Indeed, by using the well known rule

$$(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})(\boldsymbol{\beta} \cdot \boldsymbol{\sigma}) = (\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}) + i \boldsymbol{\sigma} \cdot (\boldsymbol{\alpha} \times \boldsymbol{\beta}) \quad (10)$$

and the standard commutation relations for \mathbf{b} and \mathbf{b}^+ , it is easy to see that

$$\begin{aligned} (\mathbf{b} \cdot \boldsymbol{\sigma})(\mathbf{l} \cdot \boldsymbol{\sigma}) &= -(\mathbf{l} \cdot \boldsymbol{\sigma} + 2)(\mathbf{b} \cdot \boldsymbol{\sigma}) \\ (\mathbf{b} \cdot \boldsymbol{\sigma}) \hat{n} &= (\hat{n} + 1)(\mathbf{b} \cdot \boldsymbol{\sigma}). \end{aligned} \quad (11)$$

Here $\mathbf{l} = i \mathbf{b} \times \mathbf{b}^+$ is the orbital angular momentum. An iterative use of (11) leads to the permutation rule

$$(\mathbf{b} \cdot \boldsymbol{\sigma}) g(\hat{n}, \mathbf{l} \cdot \boldsymbol{\sigma}) = g(\hat{n} + 1, -\mathbf{l} \cdot \boldsymbol{\sigma} - 2) (\mathbf{b} \cdot \boldsymbol{\sigma}) \quad (12)$$

which is valid for operator-valued functions of the two variables. The operators n and $\mathbf{l} \cdot \boldsymbol{\sigma}$ naturally appear in this expression because they are simple linear combinations of $d d^+$ and

d^+d (see equations (2), (4), (16) and (17)). A similar formula can be given for the d^+ operator:

$$(\mathbf{b}^+ \cdot \boldsymbol{\sigma}) g(\hat{n}, \mathbf{l} \cdot \boldsymbol{\sigma}) = g(\hat{n} - 1, -\mathbf{l} \cdot \boldsymbol{\sigma} - 2) (\mathbf{b}^+ \cdot \boldsymbol{\sigma}). \quad (13)$$

Note that equations (12) and (13) can be folded into the same relation

$$(\mathbf{b}^\pm \cdot \boldsymbol{\sigma}) g(\hat{n}, \mathbf{l} \cdot \boldsymbol{\sigma}) = g(\hat{n} \mp 1, -\mathbf{l} \cdot \boldsymbol{\sigma} - 2) (\mathbf{b}^\pm \cdot \boldsymbol{\sigma}) \quad (14)$$

provided \mathbf{b}^- stands for \mathbf{b} .

The permutation rule (14) is a cornerstone of the procedure for developing analytical results for pseudo transforms. It is of primary use for transforming monopole operators, that is, operators that are rotational scalars. In the case of higher multipolarity operators there are more complex rules which are not reducible to permutations alone. The rules are different for different operators, but generally, the degree of complexity increases rapidly with the multipolarity of the operator. For instance, the rule for transposing the spin operator with an analytic function of the $\mathbf{l} \cdot \boldsymbol{\sigma}$ operator goes as follows:

$$\boldsymbol{\sigma} f(\mathbf{l} \cdot \boldsymbol{\sigma}) = f(-\mathbf{l} \cdot \boldsymbol{\sigma} - 1) \boldsymbol{\sigma} + \frac{f(\mathbf{l} \cdot \boldsymbol{\sigma}) - f(-\mathbf{l} \cdot \boldsymbol{\sigma} - 1)}{\mathbf{l} \cdot \boldsymbol{\sigma} + \frac{1}{2}} \mathbf{j} \quad (15)$$

where the symbolic operator-valued fraction is used because the numerator and denominator do commute. This formula is derived in the appendix and will be used in section 6 where the image of the spin operator is given.

4. Double transformation

A simple, although rather interesting, application of equation (12) is a derivation of an analytic expression for the twofold normal \rightarrow pseudo transformation. An important property of the double transformation is that it actually depends only on the orbital degrees of freedom. This property will prove useful for finding the transform of the spin operator (see section 6).

To obtain the double transformation result, note that

$$d^+d = \hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma} \quad (16)$$

$$d d^+ = \hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3 \quad (17)$$

and rewrite the single transformation (see equations (2) and (4)) in the form [11]

$$U = (\mathbf{b} \cdot \boldsymbol{\sigma}) (\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})^{-1/2} \quad (18)$$

or, equivalently [14],

$$U = (\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3)^{-1/2} (\mathbf{b} \cdot \boldsymbol{\sigma}). \quad (19)$$

Note that equation (12) provides an additional and direct proof of the identity between the operators (18) and (19) acting in the normal parity subspace.

The double transformation can now formally be defined as a product of two single transformations. For instance, equation (19) yields

$$U^2 = (\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3)^{-1/2} (\mathbf{b} \cdot \boldsymbol{\sigma}) (\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3)^{-1/2} (\mathbf{b} \cdot \boldsymbol{\sigma}).$$

By applying (12), the $\mathbf{b} \cdot \boldsymbol{\sigma}$ operator can be moved to the right resulting in

$$U^2 = ((\hat{n} + 2)(\hat{n} + 3) - \mathbf{l}^2)^{-1/2} \mathbf{b}^2. \quad (20)$$

To arrive at (20), the identities

$$(\mathbf{l} \cdot \boldsymbol{\sigma})^2 = l^2 - \mathbf{l} \cdot \boldsymbol{\sigma} \quad (21)$$

$$(\mathbf{b} \cdot \boldsymbol{\sigma})^2 = \mathbf{b}^2 \quad (22)$$

were used along with the fact that the n and $\mathbf{l} \cdot \boldsymbol{\sigma}$ operators commute. Since

$$(\hat{n} + 2)(\hat{n} + 3) - l^2 = \mathbf{b}^2(\mathbf{b}^+)^2$$

Equation (20) can be rewritten as

$$U^2 = (\mathbf{b}^2(\mathbf{b}^+)^2)^{-1/2} \mathbf{b}^2. \quad (23)$$

Thus, the double normal \rightarrow pseudo transformation is reduced to an action of the \mathbf{b}^2 operator with a subsequent normalization (cf equation (6)):

$$U^2 \psi_{nljm} = \psi_{n-2,ljm}. \quad (24)$$

From an algebraic viewpoint, this transformation can be expressed in terms of the enveloping algebra of the non-compact symplectic algebra $sp(2, R)$ which is a subalgebra of $osp(1|2)$. The three generators of $sp(2, R)$ are defined in (9). It is important to note, however, that while the $sp(2, R)$ algebra that emerges is related to the $sp(2, R)$ subalgebra of the nuclear collective motion algebra of $sp(6, R)$ [4, 5], in general these two algebras only coincide at the single-particle level. In the many-particle case the generators of the collective $sp(2, R)$ algebra include a summation over single-particle operators (9). In the pseudospin-related problems only single-particle operators are considered; for instance, the many-particle double transformation is just a product of single-particle transformations (23). This product structure of U_{total}^2 is an indication of the *non-collective* nature of the pseudospin transformation.

Note that in contrast to the single transformation, the double form changes neither the orbital momentum nor parity—it is an $O(3)$ scalar operator. As a result, the spin is also invariant with respect to the double transformation. In short, the double transformation carries the n of the oscillator into $n - 2$ while leaving both l and s unchanged.

The technique used for deriving (20) and (23) can be used to produce another form of the double transformation operator

$$\begin{aligned} U^2 &= \mathbf{b}^2 (\hat{n}(\hat{n} + 1) - l^2)^{-1/2} \\ &= \mathbf{b}^2 ((\mathbf{b}^+)^2 \mathbf{b}^2)^{-1/2}. \end{aligned} \quad (25)$$

Which form is used in an application is simply a matter of convenience so long as consideration is confined to normal parity subspace.

5. One-body rotational invariants

One-body rotationally invariant operators naturally emerge in microscopic, shell-model based approaches to nuclear structure. For pseudospin-related problems the d , d^+ operators and the single-nucleon Hamiltonian are the characteristic rotational scalars. The normal \rightarrow pseudo transforms of these operators are derived in this section.

Analytic results for the transformed d and d^+ operators, which are an integral part of the normal \rightarrow pseudo transformation itself, follow from the definition of a transformed operator,

$$F' = U F U^+ \quad (26)$$

where F' is the transform of F . For the $F = d = \mathbf{b} \cdot \boldsymbol{\sigma}$ case it is convenient to utilize (19) for U and the Hermitian conjugate of (18) for U^+ . Applying equation (17) to this result yields

$$U \mathbf{b} \cdot \boldsymbol{\sigma} U^+ = \left(\frac{\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma} + 2}{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3} \right)^{1/2} \mathbf{b} \cdot \boldsymbol{\sigma}. \quad (27)$$

The transform of $d^+ = \mathbf{b}^+ \cdot \boldsymbol{\sigma}$ is given by the Hermitian conjugate of (27). For convenience of having the normalization factor on the left, the rule (13) can be applied to obtain the result

$$U \mathbf{b}^+ \cdot \boldsymbol{\sigma} U^+ = \left(\frac{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3}{\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma}} \right)^{1/2} \mathbf{b}^+ \cdot \boldsymbol{\sigma}. \quad (28)$$

Given the transformation properties of d and d^+ , it becomes easy to transform the single-nucleon Hamiltonian for the oscillator shell model (in units of $\hbar\omega$)

$$H = h_0 - k (\mathbf{l} \cdot \boldsymbol{\sigma} + \mu (\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n)) \quad (29)$$

where h_0 is the oscillator energy operator (see equation (9)) and $\langle \mathbf{l}^2 \rangle_n = \frac{1}{2}n(n+3)$ is the mean value of \mathbf{l}^2 within the n th shell. The $\langle \mathbf{l}^2 \rangle_n$ term is subtracted from \mathbf{l}^2 to ensure that the average value of the single-nucleon Hamiltonian remains fixed by h_0 [15].

The transformation of the oscillator energy is obvious:

$$U h_0 U^+ = h_0 + 1 \quad (30)$$

because U reduces the number of oscillator quanta by 1. To understand how the spin-orbit term transforms, recall relations (16) and (17). Since the transforms for d , d^+ and h_0 are known, it is easy to show that

$$U \mathbf{l} \cdot \boldsymbol{\sigma} U^+ = -\mathbf{l} \cdot \boldsymbol{\sigma} - 2. \quad (31)$$

And finally, by making use of (21), the transform of \mathbf{l}^2 can be determined:

$$U \mathbf{l}^2 U^+ = \mathbf{l}^2 + 2\mathbf{l} \cdot \boldsymbol{\sigma} + 2. \quad (32)$$

Since $\boldsymbol{\sigma}^2$ has a unique eigenvalue it is invariant under the normal \rightarrow pseudo transformation, and furthermore, equations (31) and (32) provide proof for the invariance of $\mathbf{j}^2 = \mathbf{l}^2 + \mathbf{l} \cdot \boldsymbol{\sigma} + \frac{1}{4}\boldsymbol{\sigma}^2$. The latter result is simply a consequence of the rotational invariance of the normal \rightarrow pseudo transformation itself.

By combining the results of equations (30)–(32), the transformation of the Hamiltonian (29) can be given as

$$U H U^+ = h_0 + 1 - k ((2\mu - 1)\mathbf{l} \cdot \boldsymbol{\sigma} + \mu (\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n)) + k (\mu (h_0 - \frac{3}{2}) + 2). \quad (33)$$

This expression for the transformed Hamiltonian coincides with the corresponding formula in [11], with the exception of the $\langle \mathbf{l}^2 \rangle_n$ term and its transform which were not considered in the earlier pseudospin studies. (Note that the inclusion of the $\langle \mathbf{l}^2 \rangle_n$ term in the original Hamiltonian induces a slight change in the oscillator frequency of the transformed Hamiltonian because the value of $k\mu$ is about 0.02–0.04 for heavy nuclei.) Also, there is no easy way to apply the commutator technique employed in [11] to operators whose transforms have a more complicated form, for example equations (27) and (28), as well as many other operators of physical significance. The techniques based on the rule (14) and its generalizations are applicable in all cases.

The expressions derived so far are sufficient for calculating the transforms for any polynomial (or more complex) functions of the d and d^+ operators. Important examples of this kind are the bilinear combinations $d^2 = \mathbf{b}^2$ and $(d^+)^2 = (\mathbf{b}^+)^2$ which together with the

n operator generate the $sp(2, R)$ algebra (see the comment following (9)). Their transforms can be found by squaring both sides of (27) and (28) and applying rule (14):

$$U\mathbf{b}^2U^+ = \left(\frac{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 5}{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3} \right)^{1/2} \mathbf{b}^2 \quad (34)$$

$$U(\mathbf{b}^+)^2U^+ = \left(\frac{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3}{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 1} \right)^{1/2} (\mathbf{b}^+)^2. \quad (35)$$

An obvious application of the above results is a calculation of the transform of the monopole transition operator r^2 which is a linear combination of the three symplectic generators (9).

6. Spin and quadrupole moment operators

While rotational scalars transform in a rather simple manner, the transformation of the higher multipolarity operators requires a more advanced prescription. Below, such a transformation is developed for the spin and Elliott quadrupole operator (the latter is that part of the quadrupole moment operator which conserves the number of oscillator quanta). These operators are important for applications because their matrix elements enter into expressions for moments and transition rates. The transformation for the orbital momentum is also found since the total angular momentum \mathbf{j} is known to be invariant under the normal \rightarrow pseudo transformation.

By using the definition (18), the image of the spin operator can be written in the form

$$U\boldsymbol{\sigma}U^+ = (\mathbf{b} \cdot \boldsymbol{\sigma})(\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})^{-1/2} \boldsymbol{\sigma} (\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})^{-1/2} (\mathbf{b}^+ \cdot \boldsymbol{\sigma}). \quad (36)$$

Now recall (15) to discover that

$$\begin{aligned} (\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})^{-1/2} \boldsymbol{\sigma} (\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})^{-1/2} &= [(\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 1)(\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})]^{-1/2} \boldsymbol{\sigma} \\ &+ \frac{(\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})^{-1} - [(\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 1)(\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})]^{-1/2}}{\mathbf{l} \cdot \boldsymbol{\sigma} + \frac{1}{2}} \mathbf{j}. \end{aligned} \quad (37)$$

By inserting the RHS of the latter expression in the RHS of (36) and applying the permutation rule, the following expression for the transformed spin operator is obtained:

$$U\boldsymbol{\sigma}U^+ = \frac{(\mathbf{b} \cdot \boldsymbol{\sigma})\boldsymbol{\sigma}(\mathbf{b}^+ \cdot \boldsymbol{\sigma}) + 2 \left[1 + \left(\frac{\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma}}{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3} \right)^{1/2} \right]^{-1} \mathbf{j}}{[(\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3)(\hat{n} - \mathbf{l} \cdot \boldsymbol{\sigma})]^{1/2}}. \quad (38)$$

The use of symbolic division in this formula is justified because the operators that enter into both the numerator and denominator factors commute with one another. The fact that the $(\mathbf{b} \cdot \boldsymbol{\sigma})\boldsymbol{\sigma}(\mathbf{b}^+ \cdot \boldsymbol{\sigma})$ operator commutes with the denominator follows as a particular case from a generic identity:

$$[(\mathbf{b} \cdot \boldsymbol{\sigma})\boldsymbol{\sigma}(\mathbf{b}^+ \cdot \boldsymbol{\sigma}), G(\hat{n}, \mathbf{l}^2 + \mathbf{l} \cdot \boldsymbol{\sigma} + 2)] = 0 \quad (39)$$

which is valid for an operator-valued analytical function $G(x, y)$ of the two variables. This result follows from the fact that

$$[\boldsymbol{\sigma}, G(\hat{n}, \mathbf{l}^2)] = 0 \quad (40)$$

by applying the operators $\mathbf{b} \cdot \boldsymbol{\sigma}$ and $\mathbf{b}^+ \cdot \boldsymbol{\sigma}$ on the left and right, respectively.

Equation (38) is one of several equivalent forms for the transformed spin operator. The equality

$$U^+ \sigma U = \frac{(\mathbf{b}^+ \cdot \sigma) \sigma (\mathbf{b} \cdot \sigma) - 2 \left[1 + \left(\frac{\hat{n} + \mathbf{l} \cdot \sigma + 3}{\hat{n} - \mathbf{l} \cdot \sigma} \right)^{1/2} \right]^{-1} \mathbf{j}}{[(\hat{n} + \mathbf{l} \cdot \sigma + 3)(\hat{n} - \mathbf{l} \cdot \sigma)]^{1/2}} \quad (41)$$

which can be derived in a similar manner, is another form for the same expression because of the invariance of the spin under the double normal \rightarrow pseudo transformation. By taking an average of the RHS of (38) and (41) and using the identity

$$(\mathbf{b} \cdot \sigma) \sigma_i (\mathbf{b}^+ \cdot \sigma) + (\mathbf{b}^+ \cdot \sigma) \sigma_i (\mathbf{b} \cdot \sigma) = 4q_{ij} \sigma^j - \frac{2}{3} (\hat{n} + \frac{3}{2}) \sigma_i \quad (42)$$

where a summation over repeated indices is implied and

$$q_{ij} = \frac{1}{2} (b_i b_j^+ + b_j b_i^+) - \frac{1}{3} (\hat{n} + 3) \delta_{ij} \quad (43)$$

are the Cartesian components of the Elliott quadrupole tensor, the transform of the spin operator can be re-expressed in terms of the spin, orbital momentum and quadrupole single-particle operators alone:

$$U \sigma U^+ = [(\hat{n} + \mathbf{l} \cdot \sigma + 3)(\hat{n} - \mathbf{l} \cdot \sigma)]^{-1/2} \times \left(2(\mathbf{q} \otimes \sigma)^{(1)} - \frac{1}{3} (\hat{n} + \frac{3}{2}) \sigma + \frac{3\mathbf{j}}{[(\hat{n} + \mathbf{l} \cdot \sigma + 3)^{1/2} + (\hat{n} - \mathbf{l} \cdot \sigma)^{1/2}]^2} \right). \quad (44)$$

In this expression $(\mathbf{q} \otimes \sigma)_i \equiv q_{ij} \sigma^j$. Although the resulting expression looks more complicated than any of the monopole operator transforms discussed in the previous section, evaluation of the corresponding matrix elements poses no problem in the spherical oscillator single-particle basis.

Proceeding to a derivation of the transform of the Elliott quadrupole tensor, it is convenient to start from the definition

$$U \mathbf{q} U^+ = (\hat{n} + \mathbf{l} \cdot \sigma + 3)^{-1/2} (\mathbf{b} \cdot \sigma) \mathbf{q} (\mathbf{b}^+ \cdot \sigma) (\hat{n} + \mathbf{l} \cdot \sigma + 3)^{-1/2}. \quad (45)$$

By utilizing equations (43) and (17), the boson commutation relations, and the definition of the orbital momentum, it is possible to prove the identity

$$(\mathbf{b} \cdot \sigma) q_{ij} (\mathbf{b}^+ \cdot \sigma) = \frac{1}{2} \{ q_{ij} (\hat{n} + \mathbf{l} \cdot \sigma + 4) + (\hat{n} + \mathbf{l} \cdot \sigma + 4) q_{ij} + \frac{1}{3} \mathbf{l} \cdot \sigma \delta_{ij} - \frac{1}{2} (l_i \sigma_j + l_j \sigma_i) \} \quad (46)$$

and rewrite the previous equation as follows:

$$U \mathbf{q} U^+ = \frac{1}{2} (\hat{n} + \mathbf{l} \cdot \sigma + 3)^{-1/2} \{ \mathbf{q} (\hat{n} + \mathbf{l} \cdot \sigma + 4) + (\hat{n} + \mathbf{l} \cdot \sigma + 4) \mathbf{q} - (\mathbf{l} \otimes \sigma)^{(2)} \} \times (\hat{n} + \mathbf{l} \cdot \sigma + 3)^{-1/2} \quad (47)$$

where $(\mathbf{l} \otimes \sigma)_{ij}^{(2)} = \frac{1}{3} (l_i \sigma_j + l_j \sigma_i - (\mathbf{l} \cdot \sigma) \delta_{ij})$ stands for the spherical tensor of rank 2 formed out of the orbital and spin momenta. Rewriting equation (47) as a fraction of commuting operators as was done for (38) and (41) does not result in any obvious advantage, as the resulting expression is neither transparent nor particularly convenient for applications. Moreover, as will be discussed in section 7, the present form is well suitable for an analysis which reveals the principal components of the tensorial structure of its image and which can easily be generalized in the many-particle case.

7. Approximate pseudospin transforms

A comparison of the results of sections 5 and 6 confirms that the normal \rightarrow pseudo transforms of higher multipolarity operator forms are more complicated than those for monopole operators. This is especially true for Hermitian forms that conserve the total number of oscillator quanta.

It is interesting to juxtapose the analytical results from the above for the single-particle case with many-particle $SU(3)$ -tensorial expansions for multipole operators determined numerically using the relabelling procedure referred to above together with standard group-theoretical coupling techniques [6]. The results show that the dominant parts of these seemingly complex operators have a relatively simple structure that in each case is very close to the structure of the original operator. For example, the transformed spin operator has the analytical form

$$U_{\text{total}} S U_{\text{total}}^+ = -\frac{1}{3} S + \left(\sum_{i=1}^A \lambda_i^{(l=2)} \otimes s_i \right)^{(J=1)} \quad (48)$$

where $\lambda^{(l=2)}$ is an orbital operator of the quadrupole type. The $SU(3)$ tensorial expansion of the λ operator, obtained in [6], consists of a leading term proportional to the Elliott quadrupole operator with the rest of the series not reducible to $SU(3)$ generators but adding up to a very small part of the total value of the calculated matrix elements. The coefficients in this expansion are oscillator-shell dependent. (A further transformation of (44) also yields (48), although in a tedious and non-transparent way.)

For the Elliott quadrupole tensor as well as for the spherical rank-0 and rank-2 tensors which are $Sp(6, R)$ generators that increase/decrease the number of oscillator quanta by two, the transformation rule is even simpler:

$$U_{\text{total}} F U_{\text{total}}^+ = \kappa_F F + \dots \quad (49)$$

where the dots represent other $SU(3)$ tensors that have expansion coefficients which are less than ten percent of the leading term and tend effectively to cancel on average so as to yield less than one percent change in calculated transition rates [16, 17]. The coefficients κ are usually operator and shell dependent with the latter dependence decreasing monotonically towards unity with increasing shell number.

Given the simple form for the leading term in these expansions, it seems reasonable to expect that the analytical techniques developed for the single-particle case should lead to an easy way of predicting the structure of the dominant parts of a transformed operator as well as a prescription for evaluating the corresponding expansion coefficients. An approximate method for doing this is proposed below; however, caution is advised as there is no simple method short of a full calculation for giving an estimate for errors that might be associated with the use of such approximations.

The procedure is based on the following observation. In general, for a given single-particle operator F there exists several different pairs of operators \check{F} and G satisfying the identity

$$d F d^+ = \frac{1}{2} (d d^+ \check{F} + \check{F} d d^+) + G \quad (50)$$

with d and d^+ defined in (3). Different choices for \check{F} and G are possible because the operator F may be encountered not only in commutation relations with d and d^+ but also in the anticommutation and generic permutation relations (see section 3). While \check{F} usually has a tensorial structure similar to F , the structure of the residual term G is dependent upon the choice of the permutation relation that is used in the derivation. In what follows, the

choice that renders the structure of G as simple as possible is made, namely, that choice which involves a minimum number of $SU(3)$ tensor operators.

The transformed operator can be written in the form

$$UFU^+ = \frac{1}{2} \left((dd^+)^{1/2} \check{F} (dd^+)^{-1/2} + (dd^+)^{-1/2} \check{F} (dd^+)^{1/2} \right) + (dd^+)^{-1/2} G (dd^+)^{-1/2}. \quad (51)$$

Note that within a given oscillator shell the $(dd^+)^{-1/2} = (\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3)^{-1/2}$ factor, as well as its inverse, is a positive definite, monotonic, and slowly changing function of the $\mathbf{l} \cdot \boldsymbol{\sigma}$ operator, especially for higher shells. Since the pseudospin symmetry is relevant for heavy nuclei and high single-particle orbitals, it is not unreasonable to approximate the RHS of (51) by taking average values within the shell for both factors, and these in turn can be estimated by setting $\mathbf{l} \cdot \boldsymbol{\sigma} \rightarrow 0$ (or in a better way if possible).

It is important to recall, however, that average values of the single-particle angular momenta and quadrupole moments within a given major shell correlate with the shell number. So while a formal expansion in powers of $\mathbf{l} \cdot \boldsymbol{\sigma}$, which is the basis of the subsequent consideration, apparently is asymptotic, the result remains approximate and should be used with appropriate caution.

The $\frac{1}{2}((dd^+)^{1/2} \check{F} (dd^+)^{-1/2} + (dd^+)^{-1/2} \check{F} (dd^+)^{1/2})$ operator of (51) can be approximated by \check{F} . This is appropriate because the two operators behave similarly under Hermitian conjugation, have the same traces in any subspace of single-particle states, and their difference can only be of the order of $O(n^{-2})$. The latter estimate is valid because of the absence of a linear $\mathbf{l} \cdot \boldsymbol{\sigma}$ term in the MacLaurin series for $\frac{1}{2}((dd^+)^{1/2} \check{F} (dd^+)^{-1/2} + (dd^+)^{-1/2} \check{F} (dd^+)^{1/2})$. For the residual $(dd^+)^{-1/2} G (dd^+)^{-1/2}$ term the estimate $\beta_F (\hat{n} + 3)^{-1} G$ is acceptable with β_F an adjustable parameter that is close to unity. This parameter accounts for higher-order corrections due to averaging and renormalization and can be evaluated directly or by comparison with known results.

These considerations lead to the following approximation:

$$UFU^+ = \check{F} + \frac{\beta_F}{\hat{n} + 3} G + O(n^{-2}) \quad (52)$$

for the transform of the operator F . The accuracy of this approximation is expected to increase with increasing shell number. Obviously, such an approximation is not unique, and there is always a chance to improve it by using a more sophisticated initial expression. For instance, as will be demonstrated below, equation (44) allows for immediate averaging without any preliminary transformation.

As examples, three cases from the previous sections, namely the transformation of the $\mathbf{l} \cdot \boldsymbol{\sigma}$, $\boldsymbol{\sigma}$ and \mathbf{q} operators, will now be considered. The result for $F = \mathbf{l} \cdot \boldsymbol{\sigma}$ is particularly simple because in this case $\check{F} = -(\mathbf{l} \cdot \boldsymbol{\sigma} + 2)$ and $G = 0$ by virtue of (11), (12) or (13). In this case the exact result, (31), is obtained as a consequence of the commutation of the dd^+ and \check{F} operators.

For $F = \boldsymbol{\sigma}$ there is no need to apply the generic scheme based on (50) because it is more convenient to average the values of the slowly changing coefficients in the RHS of (44). If accuracy is maintained to $O(n^{-2})$, the approximate transform for the spin operator $s = \boldsymbol{\sigma}/2$ has the form

$$UsU^+ = -\frac{1}{3} s + \frac{2\beta_s}{\hat{n} + \frac{3}{2}} (\mathbf{q} \otimes s)^{(1)} + \dots \quad (53)$$

which can be compared directly with its many-particle generalization (48). This shows that the coefficient of the spin operator is exact, and the $SO(3)$ tensorial structure is

represented correctly. Moreover, as mentioned above, the $SU(3)$ tensorial expansion for $\lambda^{(l=2)}$, found in [6], shows that the dominant term has the transformation properties of the Elliott quadrupole operator. Therefore, these two approaches are in a good agreement. An estimate for the coefficient β_s from (44) is simply unity. As an alternative, equation (53) can be raised to the second power and then if the expression were exact the RHS should be equal to $\frac{3}{4}$. In general, the result depends on both the $\mathbf{l} \cdot \boldsymbol{\sigma}$ and l^2 operators; however, the value of $\beta_s = \sqrt{8/5}$ guarantees the correct average value for s^2 within a shell. These two estimates are very close with the differences attributable to corrections that are of the order of n^{-2} and higher which are effectively taken into account in the latter estimate.

To determine the dominant part of the transform for the single-particle Elliott quadrupole operator q , compare equation (47) with the definition (51) and note that in this case $\tilde{F} = q$ and $G = q - (\mathbf{l} \otimes \mathbf{s})^{(2)}$. Then, by making use of prescription (52), this can be rewritten as

$$UqU^+ = q + \frac{\beta_q}{\hat{n} + 3} (q - (\mathbf{l} \otimes \mathbf{s})^{(2)}) + \dots \quad (54)$$

Although there is no rigorous way to evaluate β_q , the following heuristic estimate proves to be rather precise. By comparing the corresponding terms from (47) and (54), the ratio $\beta_q/(\hat{n} + 3)$ within the given shell can be shown to be close to the average value of the $(\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3)^{-1}$ operator within the same shell. Using the formal expansion

$$\frac{\hat{n} + 3}{\hat{n} + \mathbf{l} \cdot \boldsymbol{\sigma} + 3} = 1 - \frac{\mathbf{l} \cdot \boldsymbol{\sigma}}{\hat{n} + 3} + \frac{l^2 - \mathbf{l} \cdot \boldsymbol{\sigma}}{(\hat{n} + 3)^2} + O(n^{-3}) \quad (55)$$

and the familiar formulae $\langle \mathbf{l} \cdot \boldsymbol{\sigma} \rangle_n = 0$ and $\langle l^2 \rangle_n = \frac{1}{2}n(n + 3)$ for the average values within the n th oscillator shell, the following approximation is obtained:

$$\beta_q \approx 1 + \frac{\hat{n}}{2(\hat{n} + 3)}.$$

Note that the comparison of the ‘empirical’ relation (49) with (54) displays the simple connection

$$\kappa_q = 1 + \frac{\beta_q}{\hat{n} + 3}.$$

To illustrate the accuracy of the result, compare the estimates for κ_q , calculated according to this formula, with the exact numerical values from [16]. The relevant numbers are 1.208 versus 1.221 for $n = 3$, 1.184 versus 1.193 for $n = 4$, and 1.164 versus 1.171 for $n = 5$, respectively. The difference is about one per cent and decreasing, i.e. the accuracy is apparently higher than can be expected from the rough estimates given above.

The occurrence of the residual term proportional to $(\mathbf{l} \otimes \mathbf{s})^{(2)}$, that is predicted by (54), is also corroborated by the results given in [16]. Indeed, the $SU(3) \supset SO(3)$ tensorial expansion of the many-particle image of Q contains a term with the structure of $(\sum_{i=1}^A \mathbf{l}_i \otimes \mathbf{s}_i)^{(J=2)}$ although its influence on the E2 transition rates is weak compared to that of the leading term.

8. Conclusion

A general prescription for generating normal \rightarrow pseudo transforms of physical operators in the context of a spherical harmonic oscillator shell-model theory has been introduced. The procedure applies to operators that can be expressed in terms of single-particle oscillator boson operators \mathbf{b} , \mathbf{b}^+ (or coordinates \mathbf{r} and momenta \mathbf{p}) and spins \mathbf{s} , and is based on the existence of permutation relations among the rotational invariants constructed out of \mathbf{b} ,

\mathbf{b}^+ and \mathbf{s} . A simple and straightforward consequence of these permutation relations is the existence of an analytical result for the double transformation in terms of rotational scalars bilinear in \mathbf{b} and \mathbf{b}^+ that form the non-compact $sp(2, R)$ symplectic algebra.

Although the pseudospin representation has been widely used in the past, the option of applying it in an analytical form adds a new dimension to the many-particle studies of the structure of heavy deformed nuclei. In contrast to the general and powerful but formal algebraic technique, using the $SU(3) \supset SO(3)$ tensorial expansions plus relabelling of the single-particle states, the procedure of analytical transformation allows to derive the normal \rightarrow pseudo images for the operators expressed in customary physical variables.

The application of the transformation procedure to different operators yields results of different complexity. For instance, the transforms for the number of oscillator quanta, spin-orbit and orbit-orbit terms from the spherical Nilsson Hamiltonian are very simple and already well known [9, 11, 18]. The transforms of other rotational scalars are slightly more complicated. The operators of higher multipolarity tend to have images that are not reducible to any simple or transparent form, and arriving at the exact final expressions usually requires some creative thought.

Fortunately, for cases of real physical interest the exactness of the normal \rightarrow pseudo transformation can be easily compromised in favour of relative simplicity. Indeed, by using the appropriate permutation relation and averaging over slowly varying operator-valued factors within a given oscillator shell, it is feasible to extract the leading part of the transform which has a simple structure and accurately approximates the entire operator. These approximations can be used to streamline applications of the theory by rendering it no more complicated than the usual physical representation while reducing the spin-orbit interaction in the mean-field and the space of states to the normal parity subspace only. Representative operators for which an approximate form has proven to be advantageous include the electromagnetic transition operators and the multipole interactions which are highly significant for the studies of the collective phenomena in heavy nuclei.

A noteworthy aspect of the normal \rightarrow pseudo transformation is its underlying algebraical structure. The results of sections 4–7 underscore the significance of the connection between this transformation and the orthosymplectic supersymmetry and its subsymmetries.

Once the normal \rightarrow pseudo transformation is expressed in terms of the $osp(1|2)$ superalgebra [12] of the rotational invariants of \mathbf{b} , \mathbf{b}^+ and \mathbf{s} , it is natural to expect that the transforms of these rotational invariants are themselves expressible in terms of the same superalgebra, and this fact is demonstrated explicitly. The double transformation is shown to separate the orbital and spin variables and therefore can be expressed in terms of the $sp(2, R)$ Lie algebra which is the subalgebra of $osp(1|2)$. The double transforms of the bilinear rotational invariants (9) are, in turn, written in terms of $sp(2, R)$. The inclusion of the non-scalar bilinear combinations would extend the dynamical symmetry algebra to $sp(6, R)$.

The normal \rightarrow pseudo transforms of the spin and orbital momenta and the Elliott quadrupole operator are expressible in terms of these same three operators in the normal space. The \mathbf{l} and \mathbf{q} operators form the Lie algebra of the Elliott $SU(3)$ group [3], an important subgroup of the $Sp(6, R)$ group. Therefore, in the single-particle case the normal \rightarrow pseudo transformation produces an automorphism of the universal enveloping algebra of the $SU(3) \otimes SU(2)$ group. This algebraic property is no longer exact for the many-particle operators \mathbf{L} , \mathbf{Q} and \mathbf{S} , which comprise the collective $su(3) \oplus su(2)$ algebra. Nevertheless, the dominant parts of the pseudospin transforms of these operators are known to be proportional to the operators themselves. This is apparently the reason why the corresponding operators in the many-particle pseudospace are well defined, and this in turn

leads to the pseudo- $SU(3)$ and pseudo- $Sp(6, R)$ models being valid physical theories of the collective phenomena in heavy nuclei.

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Appendix. Permutation relation for spin

The purpose of this section is to derive the permutation relation (15) for the spin operator and an arbitrary analytic function of $l \cdot \sigma$.

Note that the anticommutation rule

$$\sigma(l \cdot \sigma) + (l \cdot \sigma)\sigma = 2l$$

can be rewritten in the form

$$\sigma(l \cdot \sigma) = -(l \cdot \sigma + 1)\sigma + 2j. \quad (\text{A1})$$

Since the $l \cdot \sigma$ operator commutes with j , this equation can be used recursively for permuting σ with a power function of $l \cdot \sigma$. Assume that a general solution for this recursion goes as follows:

$$\sigma(l \cdot \sigma)^k = (-l \cdot \sigma - 1)^k \sigma + 2\xi_k(l \cdot \sigma)j \quad (\text{A2})$$

where $\xi_k(x)$ is an unknown function and $\xi_1(x) = 1$. Multiply equation (A2) by $l \cdot \sigma$ from the right and use (A1) to arrive at the relation

$$\xi_{k+1}(x) = x\xi_k(x) + (-x - 1)^k$$

which has a solution

$$\xi_k(x) = \frac{x^k - (-x - 1)^k}{2x + 1}.$$

The latter formula provides the missing element in the permutation relation (A2) which in turn yields (15) as a consequence of the linearity of the original expression.

It is of some interest to note that the operator-valued function

$$\frac{f(l \cdot \sigma) - f(-l \cdot \sigma - 1)}{l \cdot \sigma + \frac{1}{2}}$$

which occurs as a coefficient of j in (15), is in fact spin independent. To determine this result, observe that the function is symmetric under the substitution $l \cdot \sigma \rightarrow -l \cdot \sigma - 1$. A simple analysis shows that it actually depends only on the $l \cdot \sigma(l \cdot \sigma + 1)$ combination which is just l^2 (cf equation (21)).

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