CLASSIFICATION OF INTERACTION OPERATORS WITH RESPECT TO MANY-PARTICLE PERMUTATION SYMMETRY

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Two procedures are developed for the classification of interaction operators with respect to the permutation symmetry of a many (N) particle system, which is a necessary first step for deriving selection rules for matrix elements of spin dependent operators over many-particle wavefunctions. The first method, based on character relations in the symmetric group $S_N$, is applied to one- and two-particle operators. The second, using Young diagrams is easily applied to the general case of $n$-particle interaction operators.

1. Introduction

Recently, Musher [1] has derived selection rules for matrix elements of spin-dependent operators over many-electron wavefunctions, only using the property that such operators should be symmetric under permutations of the electrons, whereas the wavefunctions must be antisymmetric. The formalism works for symmetric wavefunctions as well and, therefore, can be applied to all systems containing $N$ identical particles. It is based on the decomposition of the configuration space and the spin space separately into sub-spaces which span the irreducible representations of the symmetric group $S_N$. A symmetric/antisymmetric wavefunction can be written as a sum of space functions which transform according to the irreducible representations of $S_N$, each term multiplied by a spin function which is a basis vector of the same/associ­­ate representation [2, 3]. If the wavefunction is an eigenfunction of the total spin operator $S^2$ it corresponds to one specific irreducible representation. An analogous expansion can be made for the symmetric space—spin operators. After this decomposition of the wavefunctions and the operator, matrix elements can be calculated by integrating over space and spin coordinates separately and applying the Wigner—Eckart theorem for the permutation group. The reduced matrix elements describe the dynamics of the problem; the 3-\( j \) symbols contain all information regarding the symmetry. Matrix elements are zero, by vanishing of all 3-\( j \) symbols, if the threefold (inner) product of the irreducible representations spanned by the components of the bra-vector, the operator and the ket-vector does not include the symmetric representation. Since the operator only contains some specific irreducible representations of $S_N$, this results in certain spin selection rules between the bra-vector and the ket-vector [1].

Methods for calculating non-vanishing 3-\( j \) symbols of the permutation group are given by Gallup [4], Sullivan [5], Cooper and Musher [6]. In order to apply this procedure for the simplification of matrix elements explicitly one must find out which irreducible representations of $S_N$ are carried by the separate space and spin operators that constitute the $N$-particle interaction operator.

(i) One-particle operators

\[ \{ f(i) | i = 1, \ldots, N \} \]

are contained in the general interaction operator

\[ O_1 = \sum_{i=1}^{N} a(r_i) b(s_i) , \]

which describes, e.g., spin—orbit coupling or the Fermi hyperfine interaction.
(ii) Two-particle operators
\{h(i,j)|i=1,...,N;j=1,...,i-1\}

occur in interactions of the type

\[ O_2 = \sum_{i=1}^{N} \sum_{j=1}^{i-1} g(r_i,r_j) h(\sigma_i,\sigma_j) . \]

They can be symmetric, \( f(i,j) = f(j,i) \), such as electron-electron, spin-spin coupling, or antisymmetric, \( f(i,j) = -f(j,i) \), in case of vector forces [7]. Non-symmetric two-particle operators, appearing in the spin-other-orbit coupling [8], can be written as sums of a symmetric and an antisymmetric part. An important class of two-particle spin operators is given by various effective hamiltonians, symmetric if they are of the Heisenberg type [9], antisymmetric in some more extended models [10].

(iii) Many-particle operators
\{f(i,j,k,...)|N \geq i > j > k > ... \geq 1\}

involving interactions between more than two particles simultaneously, are not found in any "physical" hamiltonian. Still they do arise in effective interaction operators [11, 12].

In this letter we first use the character relations in order to prove the decomposition of the spaces spanned by the one-particle and two-particle operators, given by Musher [1] and Gallup [4]. We then treat the general case of \( n \)-particle operators in the \( N \)-particle Hilbert space.

2. One- and two-particle operators

(a) The one-particle operators:
\{f(i)|i=1,...,N\}

carry an \( N \)-dimensional (reducible) representation \( \Gamma_1 \) of the symmetric group \( S_N \), which should be decomposed as a direct sum of irreducible representations. The character of this "permutation representation" \( \Gamma_1 \) for a certain class of \( S_N \) is derived by acting with a permutation from this class on the basis of 1-particle operators. The character equals the number of basis vectors mapped on itself. The class structure of \( S_N \) is completely determined by the cycle structure of the permutations, so that we can denote an arbitrary class of permutations consisting of \( k \) 1-cycles, \( l \) 2-cycles, \( m \) 3-cycles, etc. as:

\[ (k,l,m,...) = (1^k,2^l,3^m,...) , \]

with
\[ k + 2l + 3m + ... = N . \]

If an operator from this class acts on the basis (1) all 2-cycles and larger cycles interchange operators. Each 1-cycle leaves one operator invariant. So the character of this permutation representation is:

\[ \chi_{(k,l,m,...)}^{[N]} = k . \]

This character must be written as a sum of irreducible characters of \( S_N \), which can be derived by an algorithm described in Hamermesh [13]. Using the partition notation for the irreducible representations of \( S_N \) one finds that

\[ \chi_{(k,l,m,...)}^{[N]} = 1 , \]

\[ \chi_{(k,l,m,...)}^{[N-1,1]} = k - 1 , \]

so that the unique decomposition of the representation \( \Gamma_1 \) is given by:

\[ \Gamma_1 = [N] \oplus [N-1,1] . \]

(b) The two-particle operators:
\{f(i,j)|i=1,...,N;j=1,...,i-1\}

span a \( \frac{1}{2}N(N-1) \) dimensional representation. Let us again act with a permutation operator of the arbitrary class \((1^k,2^l,3^m,...)\) on all \( f(i,j) \). The \( k \) 1-element partitions leave a certain \( f(i,j) \) invariant if they include both \((i)\) and \((j)\). A sequence of \( k \) numbers contains \( \frac{1}{2}k(k-1) \) different pairs \((i,j)\) with \( i > j \), so that the 1-element partitions in the permutation operator leave \( \frac{1}{2}k(k-1) \) operators \( f(i,j) \) unaltered. Besides, if we assume that the operators \( f(i,j) \) are all symmetric or all antisymmetric under the transposition \((ij)\), an \( f(i,j) \) is left invariant or turned into \(-f(i,j)\), respectively, by this transposition. Therefore, every 2-cycle in the permutation operator maps one \( f(i,j) \) on itself in the symmetric case or on its negative for antisymmetric operators. Since all larger cycles necessarily interchange the \( f(i,j) \), the characters of the representations spanned by the symmetric and antisymmetric 2-particle operators are, respectively:

\[ \chi_{(k,l,m,...)}^{[N]} = \frac{1}{2}k(k-1) + l , \]
\[ \Gamma^2 \text{anti} = \frac{1}{2}k(k-1) - l. \]  
(9)

Inspecting the irreducible characters of \( S_N \) given by Hamermesh [13]:

\[ \chi^{[N-2,2]}_{k,l,m,...} = \frac{1}{2}(k-1)(k-2) + l - 1, \]  
(10)

\[ \chi^{[N-2,1^2]}_{k,l,m,...} = \frac{1}{2}(k-1)(k-2) - l, \]  
(11)

we find that:

\[ \Gamma^2 \text{sym} = \{ N \} \oplus \{ N - 1, 1 \} \oplus \{ N - 2, 2 \}, \]  
(12)

\[ \Gamma^2 \text{anti} = \{ N - 1, 1 \} \oplus \{ N - 2, 1^2 \}. \]  
(13)

Although possible in principle, the treatment of three- or more-particle operators in a similar manner would become very laborious. For this reason we shall consider the general case of \( n \)-particle operators by an alternative technique, which basically is derived from character relations as well [14].

3. General theory

The general problem is to find, which representations are carried by the set of all \( n \)-particle operators in \( N \)-particle space (\( 1 \leq n \leq N \)). Without loss of generality the \( n \)-particle operators are assumed to be symmetry adapted with respect to the permutation group \( S_n \); they are irreducible tensor operators which transform according to the representation \([\lambda]\) of \( S_n \) (i.e., the symmetric or the antisymmetric one in case of 2-particle operators). If this would not be the case for any practical set of operators we could always expand them as linear combinations of such symmetry adapted operators. We denote these operators by:

\[ \{ f_k^\lambda(I_n) \mid k=1, ..., f_\lambda \}, \]  
(14)

where \( I_n \) stands for a set of \( n \) different particle coordinates (taken from the total set \( I_N \) of \( N \) particle coordinates) and \( f^\lambda_k \) is the dimension of the irreducible representation \([\lambda]\). Special cases of this formula are given by the expressions (1) and (7). We factorize the \( N \)-particle Hilbert space as a twofold tensorial product, one factor being the space of functions on \( I_n \), the other one the space of functions on the set of coordinates which do not occur in \( I_n \). This difference set is denoted by \( I_N \setminus I_n \). This factorization of the \( N \)-particle Hilbert space corresponds to an equivalent factorizing of the operators on this space. So we write the operators \( f_k^\lambda(I_n) \) in \( N \)-particle space as:

\[ f_k^\lambda(I_n) \otimes 1(I_N \setminus I_n), \]  
(15)

where \( 1(I_N \setminus I_n) \) stands for the identity operator in the space of the particles in the difference set \( I_N \setminus I_n \).

Consider a particular one of these operators, for instance:

\[ f_k^\lambda(1, ..., n) \otimes 1(n+1, ..., N). \]  
(16)

It is apparent that \( 1(n+1, ..., N) \) transforms according to the symmetric representation of \( S_{N-n} \), corresponding to the partition \([N-n]\). Since \( f_k^\lambda(I_n) \) transforms according to the representation \([\lambda]\) of \( S_n \), the operator given by (16) must carry the (irreducible) representation \([\lambda] \otimes [N-n]\) of the product group \( S_n \otimes S_{N-n} \), which is a subgroup of \( S_N \). The total set of \( n \)-particle operators in \( N \)-particle space can be generated from this particular operator (16) by the coset generators of \( S_n \otimes S_{N-n} \) in \( S_N \). The representation spanned by these operators is thus obtained by inducing the representation \([\lambda] \otimes [N-n]\) to the permutation group \( S_N \). It is symbolically denoted by \([\lambda] \otimes [N-n] \uparrow S_N \).

The rules for decomposing such representations which have been given by Littlewood [14], are as follows: After writing the Young diagram for the irreducible representation \([\lambda]\), one adds the boxes of the (single row) diagram \([N-n]\) one by one to the boundary of \([\lambda]\) so that:

(i) the augmented diagram remains a proper Young diagram,

(ii) not more than one box is added to each column of \([\lambda]\).

For example, let us treat the two-electron operators again (\( n = 2 \)). If they are symmetric, \([\lambda] = [2]\) and the decomposition reads:

\[ \Gamma^2 \text{sym} = [2] \otimes [N-2] \uparrow S_N = [N] \oplus [N-1,1] \oplus [N-2,2]. \]

For antisymmetric operators with \([\lambda] = [1^2]\), we find:

\[ \Gamma^2 \text{anti} = [1^2] \otimes [N-2] \uparrow S_N = [N-1,1] \oplus [N-2,1^2]. \]
4. Conclusion

We have derived two methods for decomposing the representation spanned by the $n$-particle operators in $N$-particle Hilbert space into irreducible representations of $S_N$. The second method using Young diagrams is much easier to handle than the first one, based on character relations. Since this decomposition can be applied to both the space and spin operators separately, general spin-dependent operators can be decomposed and their matrix elements simplified by the techniques described in the introduction.

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