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REPRESENTATIONS OF $S_N$ GENERATED BY SPIN EIGENFUNCTIONS

7.1 REPRESENTATIONS OF THE SYMMETRIC GROUP GENERATED BY THE BRANCHING DIAGRAM FUNCTIONS

Let us start with the spin eigenfunctions obtained by the branching diagram method, and denote an eigenfunction by $X(N,S,M; i), i = 1 \ldots f(N,S)$ or alternatively by $X(N,S,M; B_i)$, where $B_i$ is the branching diagram symbol.

Let us apply a permutation $\mathbf{P}$ to a spin eigenfunction $X(N,S,M;k)$.

$$Y(P) = \mathbf{P} \ X(N,S,M;k)$$

It is easy to show that the new function $Y(P)$ is also an eigenfunction of both $S_z$ and $S^2$ and it belongs to the same eigenvalues as $X(N,S,M;k)$. This follows from the fact that both $S_z$ and $S^2$ are symmetric in the spin coordinates of the $N$ electrons, and so they commute with $\mathbf{P}$.

$$S_z Y(P) = S_z \mathbf{P} X(N,S,M;k) = \mathbf{P} S_z X(N,S,M;k) = \mathbf{P} M X(N,S,M;k) = MY(P)$$

$$S^2 Y(P) = S^2 \mathbf{P} X(N,S,M;k) = \mathbf{P} S^2 X(N,S,M;k) = \mathbf{P} S (S + 1) X(N,S,M;k) = S(S + 1) Y(P)$$

We used also the fact that the permutation operator is a linear operator, so we can take out the constants, $M$ and $S(S + 1)$. The meaning of the above equalities is that $Y(P)$ lies in the space spanned by the eigenfunctions $X(N,S,M;k), (k = 1, \ldots, f(N,S))$. 

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\[ \mathbf{P} X(N, S, M; k) = \sum_{l=1}^{f(N, S)} X(N, S, M; l) U(P)_{lk} \quad k = 1, \ldots, f(N, S) \quad (7.1) \]

Let us abbreviate \( X(N, S, M; k) \) by \( X(k) \) and \( f(N, S) \) by \( f \) as the number of electrons \( N \), the spin quantum number \( S \) and the \( S_z \) quantum number \( M \) remain the same.

The expansion coefficient \( U(P)_{rk} \) can be obtained from Eq. (7.1) by forming the scalar product with \( X(r) \) and using the fact that the spin functions form an orthonormal system:

\[ \langle X(r)|\mathbf{P}|X(k) \rangle = \sum_{l=1}^{f} \langle X(r)|X(l) \rangle U(P)_{lk} = \sum_{l=1}^{f} \delta_{rl} U(P)_{lk} = U(P)_{rk} \quad (7.2) \]

Let us apply another permutation \( \mathbf{R} \) to the result of the first permutation:

\[ \mathbf{RP} X(k) = \sum_{l=1}^{f} \mathbf{R} X(l) U(P)_{lk} = \sum_{m=1}^{f} \sum_{k=1}^{f} X(m) U(R)_{ml} U(P)_{lk} \]

The product of two permutations \( \mathbf{R} \) and \( \mathbf{P} \) is another permutation \( \mathbf{Q} \). Let us apply \( \mathbf{Q} \) directly to \( X(k) \):

\[ \mathbf{Q} X(k) = \sum_{m=1}^{f} X(m) U(Q)_{mk} \]

The spin eigenfunctions are linearly independent and they form an orthonormal system. The two equations give the same result, and from the independence of the spin eigenfunctions follows that the coefficient of each \( X(m) \) should be the same:

\[ U(RP)_{mk} = \sum_{l=1}^{f} U(R)_{ml} U(P)_{lk} \]

The expansion coefficients \( U(P)_{lk} \) can be arranged in an \( f \) dimensional matrix form. The meaning of the last equation is that the matrix associated with the product \( \mathbf{RP} \) is the matrix product of the matrices associated with \( \mathbf{R} \) and \( \mathbf{P} \) respectively. In other words we have a representation of the symmetric group.

Kotani et al.\(^1\) showed that this representation is irreducible, i.e., we cannot find a subspace which is invariant under the permutation operators.

**Exercise 7.1**
Evaluate the representation matrices of the elementary transpositions generated by the spin eigenfunctions for \( N = 3 \) and \( S = 1/2, M = 1/2 \).