SYMMETRY OF THE COORDINATE WAVE FUNCTION OF A MANY-ELECTRON SYSTEM

Iu. N. DEMKOV

Leningrad State University

Submitted to JETP editor October 14, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 714-716 (March, 1958)

The relation between the two main methods for constructing the wave function of a many-electron system, the group-theoretical method and Fock's method, is considered. It is shown that the coordinate function obtained from the first method satisfies Fock's condition of cyclic symmetry.

ASSUME that the coordinate and spin variables separate in the energy operator of an n-electron system and, in addition, that the spin part H_s of the energy operator is spherically symmetric:

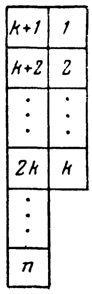
$$H = H_0(1, 2, \ldots, n) + H_s(\sigma_1, \sigma_2, \ldots, \sigma_n).$$

Then we construct a total wave function, which satisfies the Pauli principle and is an eigenfunction of the square of the total spin $\mathbf{S}^2$, if we know the coordinate eigenfunction $\psi(1, 2, \ldots, n)$ of the operator H_0 and the spin eigenfunction $\chi(\sigma_1, \sigma_2, \ldots, \sigma_n)$ of the operator H_s. This construction can be done either by using the methods of group theory[1] or by the method proposed by Fock.[2] In both methods, both the coordinate and the spin functions must satisfy definite symmetry conditions with respect to permutation of their arguments. It is obvious that the two methods of construction must be equivalent, so there should be a connection between the two kinds of symmetry conditions. We shall treat this relation.

It follows from group theory that the symmetry of the coordinate wave function must be defined by a Young tableau having two columns (see figure). This means that a function of the required symmetry can be obtained from an arbitrary function if we first symmetrize with respect to the pairs of variables in each row of the tableau, i.e., $(1, k+1)$, $(2, k+2)$, $\ldots$, $(k, 2k)$, and then antisymmetrize with respect to the columns, i.e., with respect to the variables $(1, 2, \ldots, k)$ and $(k+1, k+2, \ldots, n)$. If we denote the symmetrizer and antisymmetrizer in the set of variables $(\alpha_1, \alpha_2, \ldots, \alpha_m)$ by $S(\alpha_1, \alpha_2, \ldots, \alpha_m)$ and $A(\alpha_1, \alpha_2, \ldots, \alpha_m)$ respectively, the Young operator can be written as

$$J(1, 2, \ldots, k \mid k+1, k+2, \ldots, n) = A(1, 2, \ldots, k) \times A(k+1, k+2, \ldots, n) \sum_{i=1}^{k} S(i, k+i) = A_1 A_2 S.$$

(Obviously the sequence of variables in the Young tableau may be different; we would then get different operators; the number of linearly independent operators determines the dimensionality of the representation of the symmetric group which is related to the given Young pattern.) The symmetry of the corresponding spin function must be determined by the transposed Young tableau. It is obvious that $k \le n/2$. The total spin is $n/2 - k$.



In Fock's method, the coordinate wave function must satisfy the following three conditions: (a) antisymmetry in the variables $1, 2, \ldots, k$, (b) antisymmetry in the variables $k+1, k+2, \ldots, n$, (c) cyclic symmetry: the operator

$$\Phi = 1 - P_{k,k+1} - P_{k,k+2} - \ldots - P_{k,n},$$

must annihilate the coordinate wave function. P_{ij} is the operator for transposition of the variables i and j.

A function which is symmetrized according to the Young scheme obviously satisfies conditions (a) and (b). We shall show that such a function also satisfies the cyclic symmetry condition (c), i.e., that the identity

$$\Phi J = 0.$$

is satisfied. We shall verify this by showing that all the terms in the product $\Phi A_1 A_2 S$ cancel in pairs. Consider one of the $k!(n-k)!$ terms in the product A_1A_2. It can be written as a permutation

$$\pm\begin{pmatrix} 1, 2, \ldots, k & \Big| & k+1, k+2, \ldots, n \\ \alpha_1, \alpha_2, \ldots, \alpha_k & \Big| & \alpha_{k+1}, \alpha_{k+2}, \ldots, \alpha_n \end{pmatrix},$$

where $\alpha_1, \alpha_2, \ldots, \alpha_k$ is a permutation of the sequence 1, 2, ..., k; $\alpha_{k+1}, \alpha_{k+2}, \ldots, \alpha_n$ is a permutation of the sequence k + 1, k + 2, ..., n; the sign is determined by the parity of the permutation.

We now apply to this term one of the transpositions in the operator Φ. The following identity is easily shown:

$$\begin{pmatrix} k, a \\ a, k \end{pmatrix}\begin{pmatrix} \ldots b \ldots & \Big| & \ldots b+k \ldots d \ldots \\ \ldots k \ldots & \Big| & \ldots \ c \ \ \ldots a \ldots \end{pmatrix}$$

$$= \begin{pmatrix} k, c \\ c, k \end{pmatrix}\begin{pmatrix} \ldots b \ldots & \Big| & \ldots b+k \ldots d \ldots \\ \ldots k \ldots & \Big| & \ldots \ a \ \ \ldots c \ldots \end{pmatrix}\begin{pmatrix} b, & b+k \\ b+k, & b \end{pmatrix};$$

where

$$1 \leqslant b \leqslant k,\ k+1 \leqslant a \leqslant n,\ k+1 \leqslant c \leqslant n,\ k+1 \leqslant d \leqslant n.$$

The second factors on both sides of the identity are contained in the product A_1A_2, and differ only in a single transposition, so that they appear in the product with opposite signs. The first factors on each side are contained in the operator Φ. Finally, the operator

$$P_{b,\,b+k} = \begin{pmatrix} b, & b+k \\ b+k, & b \end{pmatrix},$$

does not change the operator S. It follows that the corresponding terms in the product ΦA_1A_2S cancel against one another.

A special case occurs when a = c, and consequently b + k = d. Then we can use the identity

$$\begin{pmatrix} k, a \\ a, k \end{pmatrix}\begin{pmatrix} \ldots b \ldots & \Big| & \ldots b+k \ldots \\ \ldots k \ldots & \Big| & \ldots \ a \ \ \ldots \end{pmatrix}$$

$$= \begin{pmatrix} \ldots b \ldots & \Big| & \ldots b+k \ldots \\ \ldots k \ldots & \Big| & \ldots \ a \ \ \ldots \end{pmatrix}\begin{pmatrix} b, & b+k \\ b+k, & b \end{pmatrix},$$

from which it follows that such a term in the product cancels against the product of the first term in the operator Φ (the identity operator) with the same term in the product A_1A_2. We have thus proven our assertion. So every function which is symmetrized by using the Young operator satisfies Fock's conditions.

The reverse relation is obviously more complicated since a function which satisfies conditions (a), (b), and (c) corresponds in general to a set of Young tableaus with all possible permutations of the variables k + 1, k + 2, ..., n. Any linear combination of the corresponding operators (among which there may be a linear dependence), when acting on an arbitrary function, gives a function which satisfies Fock's three conditions.

In comparing the two methods we note that symmetrization by means of the Young operator is convenient when we have to construct a function with particular symmetry properties from some unsymmetric function. But if the function is already known, it is easier to check whether or not it satisfies Fock's symmetry conditions than to make the analogous check using the Young operator. Fock's conditions do not give us a specific recipe for constructing a function which satisfies them; recipes for various special cases have been given.[2,3] From our proof it follows that the general recipe is to symmetrize by using the Young operator.

Thus the two methods, which are basically equivalent, supplement one another in various cases.

The methods for constructing the total wave function from the coordinate and spin functions using the method of Fock or the group theory method are also different. The relation between these methods requires further consideration.

In conclusion I thank G. F. Drukarev; the present note was written as a result of discussions with him about this class of problems.

[1] H. Weyl, Theory of Groups and Quantum Mechanics (Dover). E. Wigner, Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren, Braunschweig, 1931. L. D. Landau and E. M. Lifshitz, Квантовая механика (Quantum Mechanics), Vol. 1, §61, Gostekhizdat, 1948.

[2] V. A. Fock, J. Exptl. Theoret. Phys. (U.S.S.R.) **10**, 961 (1940).

[3] I. V. Abrenkov, Вестн. ЛГУ (Bulletin, Leningrad State University) No. 10, 43 (1956). G. F. Drukarev, J. Exptl. Theoret. Phys. (U.S.S.R.) **31**, 288 (1956), Soviet Phys. JETP **4**, 309 (1957).

Translated by M. Hamermesh
134