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n-Identical Particle States

For the two-particle system, it was easy to make two-particle wavefunctions either symmetric or antisymmetric under exchange of particle indices. Moreover, it was easy to write the full two-particle wave functions as products of two-particle orbital and two-particle spin functions. For n-particle systems, however, it is in principle straightforward to make a totally symmetric or a totally antisymmetric wave function by acting on a product of n single-particle functions, with a symmetrizer or an antisymmetrizer operator, provided the single-particle functions include *all* variables, orbital and spin variables (and perhaps other internal variables, if they exist), appropriate for the n-particle system. We will denote the symmetrizer by $\mathcal{S}$ and the antisymmetrizer by $\mathcal{A}$. For the two-particle system, we can construct symmetric and antisymmetric 2-particle functions via

$$\psi^{(s)}(\vec{r}_1, \sigma_1; \vec{r}_2, \vec{\sigma}_2) = \left[\mathcal{S} = (1 + P_{(12)})\right]\psi_a(\vec{r}_1, \vec{\sigma}_1)\psi_b(\vec{r}_2, \vec{\sigma}_2),$$
$$\psi^{(a)}(\vec{r}_1, \vec{\sigma}_1; \vec{r}_2, \vec{\sigma}_2) = \left[\mathcal{A} = (1 - P_{(12)})\right]\psi_a(\vec{r}_1, \vec{\sigma}_1)\psi_b(\vec{r}_2, \vec{\sigma}_2), \quad (1)$$

where a and b now stand for all single-particle quantum numbers, e.g., $a \equiv n_a l_a m_{l_a} m_{s_a}$. To generalize this to n-particle systems, the symmetrizer must include, besides the identity operation, a sum over all possible permutation operators for the n-particle system. That is,

$$\mathcal{S} = \sum_P P, \quad (2)$$

where the sum includes all $n!$ possible permutation operators, P, including the identity operation, 1. For example, for $n = 3$,

$$\mathcal{S} = (1 + P_{(12)} + P_{(13)} + P_{(23)} + P_{(123)} + P_{(132)}), \quad (3)$$

where $P_{(ij)}$ are pair exchange operators, which exchange the indices i and j on both orbital and spin variables. The permutation operator $P_{(123)}$ designates the cyclic interchange of labels (123) in the order $1 \to 2, 2 \to 3, 3 \to 1$. This interchange could be achieved by first making the pair exchange $1 \leftrightarrow 3$ followed by the pair exchange $2 \leftrightarrow 3$; i.e., $P_{(123)} = P_{(23)}P_{(13)}$. We could just as well have expressed $P_{(123)}$ by $P_{(123)} = P_{(13)}P_{(12)}$, or in many other ways, e.g., $P_{(123)} = P_{(13)}P_{(23)}P_{(12)}P_{(13)}$. $P_{(123)}$ will, however, always involve a product of an even number of pair exchanges. In general, the $n!$ permutations of n labels involve $\frac{1}{2}n!$ even permutations, including the identity operation, and $\frac{1}{2}n!$ odd permutations. All even permutations can be expressed in terms of products of an even number of pair exchanges, and all odd permutations can be expressed in terms of products of an odd number of pair exchanges. For $n = 4$, the 24 permutation operators include the identity operation, six pair exchanges of type $P_{(ij)}$, three double pair exchanges of type $P_{(ij)}P_{(kl)}$, eight cyclic interchanges of type $P_{(ijk)}$ in which one label remains invariant, and six cyclic interchanges of all four labels of type $P_{(ijkl)}$, where the latter are odd permutations.

To build a totally symmetric n-particle state, for an n-boson system, we simply act with the symmetrizer, $\mathcal{S}$, on a product of n single particle states. If the latter are given in Dirac ket notation, e.g.,

$$|aaaaabbccc\cdots\rangle,$$

where $a \equiv n_a l_a m_{l_a} m_{s_a}$; i.e., the quantum numbers for a include all orbital and all other (internal) quantum numbers, such as the spin quantum number m_s. In this example, the particles labeled 1, 2, 3, 4, 5 are all in the same quantum state, a, whereas particles labeled 6 and 7 are in quantum state, b, and particles labeled 8, 9, 10 are in quantum state, c, and so on. The operator $\mathcal{S}$ acting on such a state does not give a normalized state vector, but it is straightforward to construct the normalized totally symmetric state vector,

$$\sqrt{\frac{(n_1!n_2!n_3!\cdots)}{n!}}\mathcal{S}|aaaaabbccc\cdots\rangle, \qquad (4)$$

where we have assumed n_1 particles exist in quantum state a, n_2 particles exist in quantum state b, n_3 particles exist in quantum state c, and on on. Note, in particular, that all n bosons could be in the same quantum state. Also, in eq. (4) the symmetrizer, $\mathcal{S}$, now includes only permutations that exchange particles in different quantum states, e.g., $P_{(16)}$ but not $P_{(12)}$.

For n-fermion states, we construct the n-particle states in the same way using an n-particle antisymmetrizer, $\mathcal{A}$,

$$\mathcal{A} = \sum_P (-1)^{\sigma(P)} P, \qquad \text{with} \qquad \sigma(P) = \text{even (odd)}$$

$$\text{for } P = \text{even (odd)}. \qquad (5)$$

For $n = 3$, e.g.,

$$\mathcal{A} = [1 - P_{(12)} - P_{(13)} - P_{(23)} + P_{(123)} + P_{132)}]. \qquad (6)$$

Now, normalized states are constructed via

$$\frac{1}{\sqrt{n!}}\mathcal{A}|abc\cdots\rangle. \tag{7}$$

In particular, all single-particle quantum states must now be different; i.e. $a \neq b \neq c \neq \cdots$. Otherwise, the state vector would be annihilated by the antisymmetrizer $\mathcal{A}$. In coordinate representation, the totally antisymmetric state can also be expressed through an $n \times n$ determinant, the so-called Slater determinant,

$$\psi^{(a)} = \frac{1}{\sqrt{n!}}\begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) & \cdots & \psi_k(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) & \cdots & \psi_k(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) & \cdots & \psi_k(3) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \psi_a(n) & \psi_b(n) & \psi_c(n) & \cdots & \psi_k(n) \end{vmatrix}, \tag{8}$$

where the particle indices, (i), are shorthand for $(\vec{r}_i, \vec{\sigma}_i)$. This n-particle wave function is totally antisymmetric. An odd permutation of particle indices corresponds to an odd permutation of rows of the determinant and therefore changes the sign of the determinant. Similarly, an even permutation of indices corresponds to an even permutation of rows of the determinant and does not change the sign of the determinant.

Even though we have succeeded in constructing n-particle wave functions of the appropriate totally symmetric or totally antisymmetric character, these functions may not be easy to work with. Later in the course (Chapters 78 and 79) we shall develop special techniques to deal with n-boson or n-fermion systems, involving single-boson or single-fermion creation and annihilation operators, with special commutation or anticommutation relations, respectively. The boson creation and annihilation operators are very similar to harmonic oscillator creation and annihilation operators. The fermion creation and annihilation operators will be particularly useful in quantum field theory, and we shall meet them there.

A final remark: For the n-electron atom, we would find it very convenient to separate the n-particle wave function into a product of an n-particle orbital function and an n-particle spin function because our Hamiltonian has only a very weak dependence on spin. For $n = 2$, this separation was trivial and led to orbitally symmetric spin singlet states and orbitally antisymmetric spin triplet states. For $n = 3$, this separation is already much more complicated. States with $S = \frac{3}{2}$ have totally symmetric three-particle spin functions. This fact is immediately apparent for the three-particle spin state with $S = \frac{3}{2}$ and $M_S = \frac{3}{2}$. It follows for the states with lower values of M_S because the three-particle M_S-lowering operator, $S_- = S_-(1)+S_-(2)+S_-(3)$, is totally symmetric, i.e., invariant under any permutation of particle indices. For these three-particle quartet spin states with $S = \frac{3}{2}$, it is trivial to combine this totally symmetric spin state with a totally antisymmetric orbital state. The three orbital quantum numbers $n_a l_a m_{l_a}$, n_b, l_b, m_{l_b}, and $n_c l_c m_{l_c}$ must differ in at least one of the three quantum numbers, in this totally antisymmetric orbital state. Next, it is impossible to make a totally antisymmetric three-particle spin state, because the single-particle spin states have only two available quantum states, $m_s = \pm\frac{1}{2}$. We would require three different single-particle spin states to make a totally antisymmetric three-particle spin function. Three-particle spin functions, with $S = \frac{1}{2}$, thus, must have a mixed intermediate symmetry, neither totally antisymmetric nor totally symmmetric. They must be combined with three-particle orbital functions also of such a mixed symmetry. Actually two types of intermediate-symmetry three-particle functions exist, and the two orbital and two spin functions must be combined in proper linear combination to make a totally antisymmetric total three-particle function. Already, for $n = 3$, this is no longer a completely trivial problem. For elegant techniques of handling such problems, we will find it advantageous to use the detailed properties of the permutation group of n objects. For a more detailed description of the possible intermediate symmetries for $n = 3$ and $n = 4$ in terms of the so-called Young tableaux, see the introductory part of Chapter 78.