



Spin Eigenfunctions: Construction and Use

Ruben Pauncz

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The aim of this book is to give a comprehensive treatment of the different methods for the construction of spin eigenfunctions and to show their interrelations. The ultimate goal is the construction of an antisymmetric many-electron wave function that has both spatial and spin parts and the calculation of the matrix elements of the Hamiltonian over the total wave function. The representations of the symmetric group play a central role both in the construction of spin functions and in the calculation of the matrix elements of the Hamiltonian, so this subject will be treated in detail. We shall restrict the treatment to spin-independent Hamiltonians; in this case the spin does not have a direct role in the energy expression, but the choice of spin functions influences the form of spatial functions through the antisymmetry principle; the spatial functions determine the energy of the system. We shall also present the "spin-free quantum chemistry" approach of Matsen and co-workers, in which one starts immediately with the construction of spatial functions that have the correct permutational symmetries. By presenting both the conventional and the spin-free approach, one gains a better understanding of certain aspects of the electronic correlation problem. The latest advance in the calculation of the matrix elements of the Hamiltonian is the use of the representations of the unitary group, so this will be the last subject. It is a pleasant task to thank all those who helped in writing this book.

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