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2.6 Diagonalization of invariant blocks using the Slater-Condon rules3. EXAMPLES FROM QUANTUM CHEMISTRY; 3.1 The Hartree-Fock-Roothaan method applied to molecules; 3.2 Construction of invariant subsets; 3.3 The trigonal group C3v; the NH3 molecule; 4. GENERALIZED STURMIANS APPLIED TO ATOMS; 4.1 Goscinskian configurations; 4.2 Relativistic corrections; 4.3 The large-Z approximation: Restriction of the basis set to an R-block; 4.4 Electronic potential at the nucleus in the large-Z approximation; 4.5 Core ionization energies; 4.6 Advantages and disadvantages of Goscinskian configurations
4.7 R-blocks, invariant subsets and invariant blocks4.8 Invariant subsets based on subshells; Classification according to ML and Ms; 4.9 An atom surrounded by point charges; 5. MOLECULAR ORBITALS BASED ON STURMIANS; 5.1 The one-electron secular equation; 5.2 Shibuya-Wulfman integrals and Sturmian overlap integrals evaluated in terms of hyperpherical harmonics; 5.3 Molecular calculations using the isoenergetic configurations; 5.4 Building Tvv(N) and vv(N) from 1-electron components; 5.5 Interelectron repulsion integrals for molecular Sturmians from hyperspherical harmonics
5.6 Many-center integrals treated by Gaussian expansions (Appendix E) 5.7 A pilot calculation; 5.8 Automatic generation of symmetry-adapted basis functions; 6. AN EXAMPLE FROM ACOUSTICS; 6.1 The Helmholtz equation for a non-uniform medium; 6.2 Homogeneous boundary conditions at the surface of a cube; 6.3 Spherical symmetry of v(x); nonseparability of the Helmholtz equation; 6.4 Diagonalization of invariant blocks; 7. AN EXAMPLE FROM HEAT CONDUCTION; 7.1 Inhomogeneous media; 7.2 A 1-dimensional example; 7.3 Heat conduction in a 3-dimensional inhomogeneous medium
8. SYMMETRY-ADAPTED SOLUTIONS BY ITERATION8.1 Conservation of symmetry under Fourier transformation; 8.2 The operator - + p2k and its Green's function; 8.3 Conservation of symmetry under iteration of the Schrodinger equation; 8.4 Evaluation of the integrals; 8.5 Generation of symmetry-adapted basis functions by iteration; 8.6 A simple example; 8.7 An alternative expansion of the Green's function that applies to the Hamiltonian formulation of physics; Appendix A REPRESENTATION THEORY OF FINITE GROUPS; A.1 Basic definitions; A.2 Representations of geometrical symmetry groups
A.3 Similarity transformations

Sommario/riassunto

In theoretical physics, theoretical chemistry and engineering, one often wishes to solve partial differential equations subject to a set of boundary conditions. This gives rise to eigenvalue problems of which some solutions may be very difficult to find. For example, the problem of finding eigenfunctions and eigenvalues for the Hamiltonian of a many-particle system is usually so difficult that it requires approximate methods, the most common of which is expansion of the eigenfunctions in terms of basis functions that obey the boundary conditions of the problem. The computational effort needed