

Things You Should Know

Chapters 8: Many Electron Atoms

Be able to define the following terms (using words, equations, or figures):

Perturbation Theory
Zeroth-order wave function
First-order correction
Variational principle
Trial function
Secular determinant
Koopman's theorem
Hartree-Fock method

Zeroth-order energy
Zeroth-order Hamiltonian
Second-order correction
Variational function
Secular equation
Inter-electronic repulsion
Ionization Energy

Concepts and Exercises:

1. Be able to explain (not memorize) atomic units.
2. Be able to interpret the results of the calculations using approximation methods for the helium atom.
3. Understand the reasoning behind using products of one-electron functions for many electron atoms. Be able to describe the basic procedure of the Hartree-Fock SCF method. Know the physical basis behind it.