8.S: The Hydrogen Atom (Summary)

The Schrödinger equation for one-electron atoms and ions such as H, He^+, Li^{2+}, etc. is constructed using a Coulombic potential energy operator and the three-dimensional kinetic energy operator written in spherical coordinates. Because the radial and angular motions are separable, solutions to the Schrödinger equation consist of products $R(r)Y(\theta,\varphi)$ of radial functions $R(r)$ and angular functions $Y(\theta,\varphi)$ that are called atomic orbitals. Three quantum numbers, n, l, and m_l are associated with the orbitals. Numerous visualization methods are available to enhance our understanding of the orbital shapes and sizes represented by the modulus squared of the wavefunctions. The orbital energy eigenvalues depend only on the n quantum number and match the energies found using the Bohr model of the hydrogen atom. Because all orbitals with the same principal quantum number have the same energy in one-electron systems, each orbital energy level is n2-degenerate. For example, the n = 3 level contains 9 orbitals (one 3s, three 3p's and five 3d's.)

Atomic spectra measured in magnetic fields have more spectral lines than those measured in field-free environments. This Zeeman effect is caused by the interaction of the imposed magnetic field with the magnetic dipole moment of the electrons, which removes the m_l quantum number degeneracy.

In addition to the orbital wavefunctions obtained by solving the Schrödinger equation, electrons in atoms possess a quality called spin that has associated wavefunctions σ, quantum numbers s and ms, spin angular momentum S and spectroscopic selection rules. Interaction with a magnetic field removes the degeneracy of the two spin states, which are labeled α and β, and produces additional fine structure in atomic spectra. While spin does not appear during the solution of the hydrogen atom presented in this text, spin is presented as a postulate because it is necessary to explain experimental observations about atoms.

Single-electron wavefunctions that incorporate both the orbital (spatial) and spin wavefunctions are called spin-orbitals. The occupancy of spin-orbitals is called the electron configuration of an atom. The lowest energy configuration is called the ground state configuration and all other configurations are called excited state configurations. To fully understand atomic spectroscopy, it is necessary to specify the total electronic state of an atom, rather than simply specifying the orbital configuration. An electronic state, or term, is characterized by a specific energy, total angular momentum and coupling of the orbital and spin angular momenta, and can be represented by a term symbol of the form $^{2s+1}L_J$ where S is the total spin angular momentum quantum number, L is the total orbital angular momentum quantum number and J is the sum of L and S. One term may include several degenerate electron configurations. The degeneracy of a term is determined by the number of projections of the total angular momentum vector on the z-axis. The degeneracy of a term can be split by interaction with a magnetic field.

Overview of key concepts and equations for the hydrogen atom

- Potential energy
- Hamiltonian
- Wavefunctions
- Quantum Numbers
- Energies
- Spectroscopic Selection Rules
- Angular Momentum Properties

Contributors and Attributions

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