Chemistry

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1 Orbitals

Four quantum numbers can describe an electron in an atom completely:

- Principal quantum number (n)
- Azimuthal quantum number (l)
- Spin quantum number (s)
- Magnetic quantum number (ml)

Reference

An important problem in quantum mechanics is that of a particle in a spherically symmetric potential, i.e., a potential that depends only on the distance between the particle and a defined center point. In particular, if the particle in question is an electron and the potential is derived from Coulomb's law, then the problem can be used to describe a hydrogen-like (one-electron) atom (or ion).

In the general case, the dynamics of a particle in a spherically symmetric potential are governed by a Hamiltonian of the following form:

$$\hat{H} = \frac{\hat{p}}{2m_0} + V(r)$$

Where $\hat{p}$ is the momentum operator, m_0 is the mass of the particleand the potential $V(r)$ depends only on r, the length of the radius vector $\vec{r}$.

The quantum mechanical wavefunctions and energies (eigenvalues) are found by solving the Schrödinger equation with this Hamiltonian.

The eigenstates of the system have the form

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

in which the spherical polar angles θ and ϕ represent the colatitude and azimuthal angle, respectively. The last two factors of ψ are often grouped together as spherical harmonics, so that the eigenfunctions take the form:

$$\psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi)$$

The differential equation which characterizes the function $R(r)$ is called the radial equation.
Reference

In addition to l and m, a third integer $n > 0$, emerges from the boundary conditions placed on R. The functions R and Y that solve the equations above depend on the values of these integers, called quantum numbers.

$$\psi(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$$

$$R_{nl}(r) = \sqrt{\left(\frac{2Z}{na_\mu}\right)^3 \frac{(n-l-1)!}{2n(n+1)!}} e^{\frac{-Zr}{na_\mu}} \left(\frac{2Zr}{na_\mu}\right) L_{n-l-1}^{2l+1}\left(\frac{2Zr}{na_\mu}\right)$$

Where Z is the atomic number (number of protons in the nucleus),
e is the elementary charge (charge of an electron),
L_n^α is a Generalized Laguerre polynomial,
$\alpha_\mu = \frac{m_e}{\mu} a_0$
$\alpha_0 = 5.29177210903 \times 10^{-11} m$ is the Bohr radius
$\mu = \frac{m_N m_e}{m_N + m_e} \approx m_e = 9.1093837015(28) \times 10^{-31} kg$ which is the mass of an electron.
Where m_N is the mass of a nucleus.

Where $Y_{lm}(\theta, \phi)$ is a spherical harmonic.
Reference

1.1 Generalized Laguerre polynomial

For arbitrary real α the polynomial solutions of the following differential equation:

$$xy'' + (\alpha + 1 - x)y' + ny = 0$$

are called generalized Laguerre polynomials.
A Recursive formulation for the Generalized Laguerre polynomials is:

$$L_0^{(\alpha)}(x) = 1$$

$$L_1^{(\alpha)}(x) = 1 + \alpha - x$$

and then using the following recurrence relation for any k $\geq$ 1:

$$L_{k+1}^{(\alpha)}(x) = \frac{(2k + 1 + \alpha - x)L_k^{(\alpha)}(x) - (k + \alpha)L_{k-1}^{(\alpha)}(x)}{k + 1}$$

1.2 Spherical Harmonics

$$Y_{lm}(\theta, \phi) = \left\{ \begin{array}{cc} (-1)^m \sqrt{2} \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(cos(\theta)) sin(|m|\phi) & m < 0 \\ \sqrt{\frac{2l+1}{4\pi}} P_l^0(cos(\theta)) & m = 0 \\ (-1)^m \sqrt{2} \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(cos(\theta)) cos(m\phi) & m > 0 \end{array} \right\}$$

Where $P_l^m(x)$ is the Associated Legendre Polynomial.

$$P_l^m(x) = (-1)^m * 2^l * (1 - x^2)^{\frac{m}{2}} * \sum_{k=m}^{l} \frac{k!}{(k-m)!} * x^{k-m} * \binom{l}{k} \binom{l+k-1}{l}$$

Spherical Harmonics Reference
Associated Legendre polynomials Reference