Fundamental Equations

Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$$

Time-independent Schrödinger equation:

$$H\psi = E\psi, \qquad \Psi = \psi e^{-iEt/\hbar}$$

Hamiltonian operator:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V$$

Momentum operator:

$$\mathbf{p} = -i\hbar\nabla$$

Time dependence of an expectation value:

$$\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\langle[H,Q]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle$$

Generalized uncertainty principle:

$$\sigma_A\sigma_B \geq \left|\frac{1}{2i}\langle[A,B]\rangle\right|$$

Heisenberg uncertainty principle:

$$\sigma_x\sigma_p \geq \hbar/2$$

Canonical commutator:

$$[x,p] = i\hbar$$

Angular momentum:

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y$$

Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Fundamental Constants

Planck's constant: $\hbar = 1.05457 \times 10^{-34}$ Js

Speed of light: $c = 2.99792 \times 10^{8}$ m/s

Mass of electron: $m_e = 9.10938 \times 10^{-31}$ kg

Mass of proton: $m_p = 1.67262 \times 10^{-27}$ kg

Charge of proton: $e = 1.60218 \times 10^{-19}$ C

Charge of electron: $-e = -1.60218 \times 10^{-19}$ C

Permittivity of space: $\epsilon_0 = 8.85419 \times 10^{-12}\ \mathrm{C^2/Jm}$

Boltzmann constant: $k_B = 1.38065 \times 10^{-23}$ J/K

Hydrogen Atom

Fine structure constant: $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} = 1/137.036$

Bohr radius: $a = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = \frac{\hbar}{\alpha m_e c} = 5.29177 \times 10^{-11}$ m

Bohr energies: $E_n = -\frac{m_e e^4}{2(4\pi\epsilon_0)^2\hbar^2 n^2} = \frac{E_1}{n^2}$ $(n = 1,2,3,\dots)$

Binding energy: $-E_1 = \frac{\hbar^2}{2m_e a^2} = \frac{\alpha^2 m_e c^2}{2} = 13.6057$ eV

Ground state: $\psi_0 = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$

Rydberg formula: $\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

Rydberg constant: $R = -\frac{E_1}{2\pi\hbar c} = 1.09737$ /m

Mathematical Formulas

Trigonometry:

$$\sin(a \pm b) = \sin a \cos b \pm \cos a \sin b$$
$$\cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$$

Law of cosines:

$$c^2 = a^2 + b^2 - 2ab\cos\theta$$

Integrals:

$$\int x\sin(ax)\,dx = \frac{1}{a^2}\sin(ax) - \frac{x}{a}\cos(ax)$$
$$\int x\cos(ax)\,dx = \frac{1}{a^2}\cos(ax) + \frac{x}{a}\sin(ax)$$

Exponential integrals:

$$\int_0^\infty x^n e^{-x/a}dx = n!\,a^{n+1}$$

Gaussian integrals:

$$\int_0^\infty x^{2n} e^{-x^2/a^2}dx = \sqrt{\pi}\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}$$
$$\int_0^\infty x^{2n+1} e^{-x^2/a^2}dx = \frac{n!}{2}a^{2n+2}$$

Integration by parts:

$$\int_a^b f\frac{dg}{dx}dx = -\int_a^b \frac{df}{dx}g\,dx + [fg]_a^b$$