Fundamental Equations

Schrodinger Equation	$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$
Time-independent Schrodinger Equation	$\hat{H}\psi = E\psi, \qquad \Psi(\vec{x},t) = \psi(\vec{x})e^{-iEt/\hbar}$
Hamiltonian operator	$\hat{H} = \frac{\hat{p}^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V$
Momentum operator	$\hat{p} = -i\hbar\nabla, \qquad \text{1D:} \quad \hat{p} = -i\hbar\frac{\partial}{\partial x}$
Time dependence expectation value	$\frac{d\langle\hat{Q}\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$
Generalized uncertainty principle	$\sigma_A\sigma_B \geq \left\lvert\frac{1}{2i}\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right\rvert$
Heisenberg uncertainty principle	$\sigma_x\sigma_p \geq \frac{\hbar}{2}$
Canonical commutator	$[\hat{x},\hat{p}] = i\hbar$
Angular momentum	$[\hat{L}_x,\hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y,\hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z,\hat{L}_x] = i\hbar\hat{L}_y$
Pauli matrices	$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$
Minimal coupling	$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}(\vec{p}-q\vec{A})^2 + qV\right]\Psi$
Pauli equation	$i\hbar\frac{\partial}{\partial t}\chi = \left[\frac{1}{2m_e}(\vec{p}-e\vec{A})^2\mathbb{1} + eV\mathbb{1} + \frac{g\mu_B}{2}\hat{\vec{\sigma}}\cdot\vec{B}\right]\chi$ with spinor $\chi = \begin{pmatrix}\varphi_\uparrow\\ \varphi_\downarrow\end{pmatrix}$

Operators & Dirac notation

Bra, ket in $\mathbb{R}^n$	$\langle\alpha\rvert = \lvert\alpha\rangle^\dagger = (a_1^*,\ldots,a_n^*), \qquad \lvert\alpha\rangle = \begin{pmatrix}b_1\\ \vdots\\ b_n\end{pmatrix}$
Inner product	$\text{in } \mathbb{R}^n : \langle\alpha\vert\beta\rangle = \sum_j a_j^* b_j, \qquad \text{in } \infty D : \langle f\vert g\rangle = \int_{\mathcal{D}} f^* g\, d$
Cauchy-Schwartz	$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Triangular inequality	$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Eigenstate expansion	$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
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Projection operator	$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Spectrum	$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Commutator	$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Anti-commutator	$\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

Fundamental Constants

Mass of an electron	$m_e = 9.11 \times 10^{-31}$ kg
Mass of a proton	$m_p \approx 1836\ m_e$
Charge of an electron	$e\ =\ 1.602 \times 10^{-19}$ C
Charge of a proton	$-e\ =\ -1.602 \times 10^{-19}$ C
Electronvolt	1 eV $=\ 1.602 \times 10^{-19}$ J
Atomic mass unit	$1\,\text{Dalton} = 1.66 \times 10^{-27}\ \text{kg} \approx \frac{5}{3} \times 10^{-27}\ \text{kg}$
Bohr magneton	$\mu_B = 9.3 \times 10^{-24}$ J/T $= 5.8 \times 10^{-5}$ eV/T
Joule in SI units	$[\text{J} = \text{kg m}^2/\text{s}^2]$
Boltzmann constant	$k_B = 1.38 \times 10^{-23}$ J/K $= 8.62 \times 10^{-5}$ eV/K
Planck's constant	$h = 6.63 \times 10^{-34}$ J s $= 4.14 \times 10^{-15}$ eV s
Reduced Planck's constant	$\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34}$ J s $= 6.582 \times 10^{-16}$ eV s
Speed of light	$c = 3 \times 10^8$m/s
Conversion $\quad E = hf = \frac{hc}{\lambda}$	$hc = 1240$ eV nm
Rest energy electron	$m_e c^2 = 0.511$ MeV

Bound States Common Potentials

1D Infinite well

$V(x) = 0$ if $0 < x < L$
$V(x) = \infty$ otherwise

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right),$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, \qquad n = 1, 2, 3, \ldots$$

3D Infinite well

$V = 0$ if $0 < x_i < L_i$,
$V = \infty$ otherwise

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right)$$

$$E_n = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right), \qquad n_x(n_y, n_z) = 1, 2, 3, \ldots$$

1D δ-function potential well
$V(x) = -\alpha\delta(x)$

$$\psi(x) = \sqrt{\kappa} e^{-\kappa|x|}, \qquad \kappa = \frac{m\alpha}{\hbar^2}, \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

1D Linear potential

$V(x) = e\tilde{E}x$ if $0 < x < L$
$V(x) = \infty$ otherwise

$$\psi_n(x) = C\,\mathrm{Ai}(z) + D\,\mathrm{Bi}(z), \quad \frac{D}{C} = -\frac{\mathrm{Bi}(\mathrm{z}_0)}{\mathrm{Ai}(\mathrm{z}_0)}$$

$$\varepsilon = \frac{E}{E_1^\infty}, \quad \nu_L = \frac{e\tilde{E}L}{E_1^\infty}, \quad z = \left(\frac{\pi}{\nu_L}\right)^{\frac{2}{3}} \left(\frac{x}{L}\nu_L - \varepsilon\right)$$

$$E_n \longleftarrow \mathrm{Ai}(z_0)\,\mathrm{Bi}(z_L) - \mathrm{Ai}(z_L)\,\mathrm{Bi}(z_0) = 0$$

$$z_0 = -\left(\frac{\pi}{\nu_L}\right)^{2/3} \varepsilon, \qquad z_L = \left(\frac{\pi}{\nu_L}\right)^{2/3} (\nu_L - \varepsilon)$$

1D Harmonic oscillator

$V(x) = \frac{1}{2} m\omega^2 x^2$

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n(\xi)\, e^{-\xi^2/2}, \quad \xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$H_0(\xi) = 1, \quad H_1(\xi) = 2\xi, \quad H_2(\xi) = 4\xi^2 - 2, \quad \ldots$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2, 3, \ldots$$

Scattering at Common Potentials

1D Infinite well

$V(x) = 0$ if $0 < x < L$
$V(x) = \infty$ otherwise

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right),$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, \qquad n = 1, 2, 3, \ldots$$

Hydrogen Atom

1D Infinite well

$V(x) = 0$ if $0 < x < L$
$V(x) = \infty$ otherwise

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right),$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, \qquad n = 1, 2, 3, \ldots$$

Rydberg energy unit: $\mathrm{Ry} = 13.6$ eV

Rydberg constant for hydrogen: $R_H = 1.0968 \times 10^7\ \mathrm{m}^{-1} \approx 1.1 \times 10^7\ \mathrm{m}^{-1}$

Rydberg constant for heavy atoms: $R_\infty = 1.0974 \times 10^7\ \mathrm{m}^{-1} \approx 1.1 \times 10^7\ \mathrm{m}^{-1}$