Quantum Mechanics Formulas

Constants

$$\hbar \equiv \frac{h}{2\pi}$$

De Broglie–Einstein Relations

$$\mathcal{E} = \hbar\omega$$
$$\mathbf{p} = \hbar\mathbf{k}$$

Dispersion Relations

$$\omega_{\text{light}}(\mathbf{k}) = ck$$
$$\omega_{\text{electron}}(\mathbf{k}) = \frac{\hbar k^2}{2M}$$

Heisenberg Uncertainty Principle

$$\Delta p_x \Delta x \geq \hbar/2$$
$$\Delta\mathcal{E}\Delta t \geq \hbar/2$$
$$\Delta x = \left\langle x^2 \right\rangle - \langle x \rangle^2$$

Schroedinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r},t)\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}$$

Time-Independant SWE

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r})\varphi(t)$$
$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = \mathcal{E}\psi(\mathbf{r})$$
$$\varphi(t) = e^{-i\mathcal{E}t/\hbar}$$

Probability Current Density

$$\mathbf{j} = -\frac{i\hbar}{2m}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right)$$

Free Electron Beam

$$\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx};\;\; k = \sqrt{\frac{2m_e(\mathcal{E} - V_0)}{\hbar^2}}$$
$$R = \frac{A_2^* A_2}{A_1^* A_1}$$

Expectation Values and Operators

$$\hat{\mathbf{p}} = -i\hbar\nabla$$
$$\hat{\mathcal{E}} = i\hbar\frac{\partial}{\partial t}$$
$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$$
$$\rho(\mathbf{r},t) = |\Psi|^2 = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t)$$
$$\langle f \rangle = \int_{\forall V} \Psi^*(\mathbf{r},t)\,\hat{f}\,\Psi(\mathbf{r},t)\,dV = \langle\Psi|\hat{f}|\Psi\rangle$$

Harmonic Oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2$$
$$\psi_0(x) = \frac{m\omega}{\pi\hbar}^{1/4} e^{-x^2/2L^2} \quad \psi_0(Q) = \frac{1}{\pi}^{1/4} e^{-Q^2}$$
$$L = \sqrt{\frac{\hbar}{m\omega}}$$
$$\mathcal{E}_0 = \frac{\hbar\omega}{2}$$
$$\mathcal{E}_n = \left(n + \frac{1}{2}\right)\hbar$$
$$Q \equiv x/L$$
$$\left(-\frac{d^2}{dQ^2} + Q^2\right)\psi = \frac{\mathcal{E}}{\mathcal{E}_0}\psi = \hat{h}\psi$$
$$\hat{a}^+ \equiv \frac{1}{\sqrt{2}}\left(-\frac{d}{dQ} + Q\right)$$
$$\hat{a}^- \equiv \frac{1}{\sqrt{2}}\left(\frac{d}{dQ} + Q\right)$$
$$H_n(Q) = 2QH_{n-1}(Q) - 2(n-1)H_{n-2}(Q)$$
$$\psi_n(Q) = A_n H_n(Q) e^{-Q^{2/2}}$$
$$A_n^2 = \frac{A_{n-1}^2}{2n}$$
$$\psi_n(Q) = \sqrt{\frac{2}{n}}\left[Q\psi_{n-1}(Q) - \sqrt{\frac{n-1}{2}}\psi_{n-2}(Q)\right]$$

Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

$$\mathcal{E}_n = -\frac{R_\infty}{n^2}$$

Quasi Classical Approximation

$$\psi = e^{-i/\hbar \int p(x)\,dx}$$

$$T_{QC} = e^{-2/\hbar \int_a^b |p(x)|\,dx} = e^{-2/\hbar}$$

Wave Packets

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a(k)\,\exp[i(kx-\omega t)]\,dk$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} A(k,t) e^{ikx}\,dk$$

$$A(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,t) e^{-ikx}\,dx$$

$$\Phi(p,t) = \frac{1}{\sqrt{\hbar}} A(k,t); \quad p = \hbar k$$

Expansion Principle and Hilbert Space

$$|\Psi\rangle = \sum_{n=1}^{\infty} a_n |n\rangle$$
$$a_n = \langle n|\Psi\rangle, \quad \hat{H}|n\rangle = \mathcal{E}_n|n\rangle$$

$$\langle\Psi|\Psi\rangle = \sum_{n=1}^{\infty} |a_n|^2 = 1$$

$$\langle A\rangle = \sum_n |a_n|^2 A_n$$

$$|\Psi\rangle = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}$$

$$\sum_n |n\rangle\langle n| = \sum_n \hat{P}_{nn} = \hat{1}$$

Stationary Perturbation Theory

Degenerate

$$\hat{H} = \hat{H}^{(0)} + \hat{W}$$
$$\hat{H}^{(0)}|n\rangle = \mathcal{E}_n^{(0)}|n\rangle$$
$$|\psi\rangle \approx \sum_{n=1}^{N} a_n|n\rangle$$
$$\begin{bmatrix} H_{11} & H_{12} & \dots & H_{1N} \\ H_{21} & H_{22} & \dots & H_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & \dots & H_{NN} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \mathcal{E} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}$$
$$H_{mn} = \langle m|\hat{H}|n\rangle$$
$$\begin{vmatrix} H_{11}-\mathcal{E} & H_{12} & \dots & H_{1N} \\ H_{21} & H_{22}-\mathcal{E} & \dots & H_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & \dots & H_{NN}-\mathcal{E} \end{vmatrix} = 0$$

Nondegenerate

$$|\psi\rangle = |u\rangle + |\phi\rangle$$
$$\langle\phi|u\rangle = 0, \quad \langle\psi|u\rangle = 1$$

$$\mathcal{E}'_n = \mathcal{E}_n + \langle n|\hat{W}|n\rangle$$
$$\mathcal{E} = \mathcal{E}'_u + \langle u|\hat{W}|\phi\rangle$$
$$|\psi\rangle = |u\rangle + \sum_{m\neq u}\sum_{n\neq m} |m\rangle \frac{\langle m|\hat{W}|n\rangle}{\mathcal{E}-\mathcal{E}'_m} \langle n|\psi\rangle$$
$$\mathcal{E} \approx \mathcal{E}'_u + \Delta\mathcal{E}^{(2)}$$
$$\Delta\mathcal{E}^{(2)} = \sum_{m\neq u} \frac{|\langle m|\hat{W}|u\rangle|^2}{\mathcal{E}_u - \mathcal{E}_m}$$