Checklist of Mathematics Formulae

Lecture 1 – Fundamental Concepts in Quantum Physics

1. Time-independent Schrödinger equation
$$\hat{H}\Psi = E\Psi$$
For one-dimensional system,
$$\left[-\frac{\hbar^2}{2m}\cdot\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\Psi(x)=E\Psi(x)$$
For three-dimensional system,
$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(x,y,z)\right]\Psi(x,y,z)=E\Psi(x,y,z)$$

2. Time-dependent Schrödinger equation
$$i\hbar\frac{\partial\Psi(\boldsymbol{r},t)}{\partial t}=\hat{H}(t)\Psi(\boldsymbol{r},\mathrm{t})$$

3. Normalization of wavefunction
$$\int_{-\infty}^{+\infty}|\Psi(x)|^2\mathrm{d}x=\int_{-\infty}^{+\infty}\Psi^*(x)\Psi(x)\mathrm{d}x=1$$
For an unnormalized wavefunction $\Psi'(x)$, it can be normalized as
$$\Psi(x)=\frac{\Psi'(x)}{\sqrt{\int_{-\infty}^{+\infty}|\Psi'(x)|^2\mathrm{d}x}}$$

4. Probability of locating a particle
Probability density $|\Psi(x)|^2$: the probability to find the particle between x and $x+\mathrm{d}x$ is $|\Psi(x)|^2\mathrm{d}x$.
Probability to find a particle between x_1 and x_2:
$$P=\int_{x_1}^{x_2}|\Psi(x)|^2\mathrm{d}x$$

5. Eigenequation, eigenfunction and eigenvalue
For any operator $\hat{\Omega}$, if there exist some values satisfy $\hat{\Omega}\psi=\Omega\psi$, ψ is then called eigen function of operator $\hat{\Omega}$.

6. Hermiticity
$$\int \mathrm{d}\tau\psi_j^*\hat{\Omega}\psi_i=\left(\int \mathrm{d}\tau\psi_i^*\hat{\Omega}\psi_j\right)^*$$
Any eigenvalue of Hermitian operator is a real number. Eigenfunctions of Hermitian operator with different eigenvalues are orthogonal.

7. Orthogonality
$\int \mathrm{d}\tau\psi_i^*\psi_j=0$ for $i\neq j$.

8. Expectation value

$$\langle\hat{\Omega}\rangle = \int \mathrm{d}\tau\, \psi^* \hat{\Omega}\psi$$

9. Commutator of two operators

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Special case: $[\hat{x}, \hat{p}_x] = i\hbar$. The observables are complementary if $[\hat{A}, \hat{B}] \neq 0$.

10. Heisenberg uncertainty principle

$$\Delta A \cdot \Delta B \ \geq \frac{1}{2}\left|\langle[\hat{A}, \hat{B}]\rangle\right|$$

Special case: $\Delta x \cdot \Delta p_x \geq \hbar/2$.

Lecture 2 – Translational Motion

1. Free particle wavefunctions and energies

$$\psi_k(x) = Ae^{ikx} + Be^{-ikx}$$

$$E_k = \frac{k^2\hbar^2}{2m}$$

2. Particle in a one-dimensional box

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right), 0 \leq x \leq L \\ 0,\ \ x < 0 \text{ and } x > L \end{cases}$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Quantum number $n = 1,2, \ldots$

3. Particle in a two-dimensional box

$$\psi_{n_1,n_2}(x,y) = \begin{cases} \frac{2}{\sqrt{L_1L_2}}\sin\frac{n_1\pi x}{L_1}\sin\frac{n_2\pi y}{L_2},\ \text{within 2D box} \\ 0,\ \text{outside box} \end{cases}$$

$$E_{n_1,n_2} = \frac{n_1^2\pi^2\hbar^2}{2mL_1^2} + \frac{n_2^2\pi^2\hbar^2}{2mL_2^2}$$

Quantum number $n_1, n_2 = 1,2,3, \ldots.$

4. Particle in a three-dimensional box

$$\psi_{n_1,n_2,n_3}(x,y,z) = \begin{cases} \sqrt{\frac{8}{L_1L_2L_3}}\sin\frac{n_1\pi x}{L_1}\sin\frac{n_2\pi y}{L_2}\sin\frac{n_3\pi z}{L_3},\ \text{within 3D box} \\ 0,\ \text{outside box} \end{cases}$$

$$E_{n_1,n_2,n_3} = \frac{n_1^2\pi^2\hbar^2}{2mL_1^2} + \frac{n_2^2\pi^2\hbar^2}{2mL_2^2} + \frac{n_3^2\pi^2\hbar^2}{2mL_3^2}$$

Quantum number $n_1, n_2, n_3 = 1,2,3, \ldots.$

5. Tunnelling

Transmission coefficient

$$T = \left|\frac{A'}{A}\right| = \left[1 + \frac{(e^{-\kappa L} - e^{\kappa L})^2}{16\epsilon(1-\epsilon)}\right]^{-1/2}$$

- If $\epsilon \ll 1$, i.e. $E \ll V$: $T \approx \frac{4\sqrt{\epsilon(1-\epsilon)}}{e^{\kappa L} - e^{-\kappa L}} \approx 0$.
- If $\kappa L \gg 1$, i.e. high, wide barrier: $T \approx 4\sqrt{\epsilon(1-\epsilon)}e^{-\kappa L}$.