B.Sc. Physics

Detailed Lecture Note

Schrödinger Wave Equation and Normalisation of Wave Functions

Quantum Mechanics — undergraduate level

Learning Objectives

• Understand the physical meaning of the wave function ψ.

• Derive the time-dependent and time-independent Schrödinger equations.

• Understand operators, eigenvalues and energy eigenfunctions.

• Apply the equation to a free particle and a particle in a one-dimensional box.

• Understand probability density and normalisation.

• Normalise common wave functions and test physical acceptability.

Notation: $\hbar = h/(2\pi)$, m = particle mass, V = potential energy, E = total energy, $i = \sqrt{(-1)}$.

1. Introduction to Quantum Mechanics

Classical mechanics describes macroscopic particles using position, velocity and momentum. At atomic and subatomic scales, particles such as electrons, neutrons and photons show wave-like behaviour. Quantum mechanics represents the state of a particle by a mathematical wave function, usually written as $\psi(x,t)$ or $\psi(r,t)$.

The Schrödinger equation is the fundamental dynamical equation of non-relativistic quantum mechanics. Its solutions are wave functions rather than classical trajectories.

Matter Waves

According to de Broglie, a particle having momentum p has an associated wavelength:

$$\lambda = h/p = 2\pi\hbar/p$$

A plane matter wave may be written:

$$\psi(x,t) = A \exp[i(kx - \omega t)]$$

where $k = 2\pi/\lambda$. The relations $p = \hbar k$ and $E = \hbar\omega$ connect wave properties with particle momentum and energy.

2. Meaning of the Wave Function

The wave function ψ is generally not itself a directly measurable quantity. Born's interpretation gives:

$$\text{Probability density} = |\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t)$$

$|\psi|^2 dx$ is the probability of finding the particle between x and x+dx. In three dimensions, the probability in a volume element $d\tau$ is $|\psi(r,t)|^2 d\tau$.

Conditions for a Physically Acceptable Wave Function

3. From Classical Energy to the Schrödinger Equation

For a non-relativistic particle, the classical total energy is

$$E = p^2/(2m) + V$$

Quantum mechanics associates operators with energy and momentum:

$$\hat{E} = i\hbar\, \partial/\partial t$$

$$\hat{p} = -i\hbar\, \partial/\partial x$$

Hence the kinetic-energy operator is

$$\hat{T} = \hat{p}^2/(2m) = -(\hbar^2/2m)\, \partial^2/\partial x^2$$

Applying the energy operator to ψ gives the time-dependent Schrödinger equation.

4. Time-Dependent Schrödinger Wave Equation

One-Dimensional Form

$$i\hbar\, \partial\psi/\partial t = [-(\hbar^2/2m)\, \partial^2/\partial x^2 + V(x,t)]\psi$$

This is the time-dependent Schrödinger equation (TDSE) in one dimension.

Three-Dimensional Form

$$i\hbar\,\partial\psi(r,t)/\partial t = [-(\hbar^2/2m)\nabla^2 + V(r,t)]\psi(r,t)$$

Here $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ is the Laplacian.

5. Time-Independent Schrödinger Equation

When V does not depend explicitly on time, use separation of variables:

$$\psi(r,t) = \psi(r)T(t)$$

The separation constant is identified with the energy E. The time-dependent factor is

$$T(t) = \exp(-iEt/\hbar)$$

The spatial equation becomes

$$-(\hbar^2/2m)\nabla^2\psi + V\psi = E\psi$$

In one dimension:

$$-(\hbar^2/2m)d^2\psi/dx^2 + V(x)\psi = E\psi$$

$$d^2\psi/dx^2 + (2m/\hbar^2)[E-V(x)]\psi = 0$$

Operator Form

$$\hat{H}\psi = E\psi$$

where $\hat{H} = -(\hbar^2/2m)\nabla^2 + V$ is the Hamiltonian operator. ψ is an energy eigenfunction and E is its energy eigenvalue.

6. Separation of Variables — Step-by-Step

Put $\psi(x,t)=\varphi(x)T(t)$ into the TDSE:

$$i\hbar\varphi\, dT/dt = T[-(\hbar^2/2m)d^2\varphi/dx^2 + V\varphi]$$

Divide by φT:

$$i\hbar(1/T)dT/dt = -(\hbar^2/2m)(1/\varphi)d^2\varphi/dx^2 + V$$

The left side depends only on t and the right side only on x. Both therefore equal E:

$$i\hbar(1/T)dT/dt = E$$

$$-(\hbar^2/2m)d^2\varphi/dx^2 + V\varphi = E\varphi$$

The time equation gives

$$T(t)=C\exp(-iEt/\hbar)$$

Thus a stationary-state wave function is $\psi(x,t)=\varphi(x)\exp(-iEt/\hbar)$, apart from an overall constant.

7. Example: Free Particle

For a free particle, V=0:

$$-(\hbar^2/2m)d^2\psi/dx^2 = E\psi$$

$$d^2\psi/dx^2 + k^2\psi = 0,\ k = \sqrt{(2mE)}/\hbar$$

$$\psi(x)=Ae\hat{}(ikx)+Be\hat{}(-ikx)$$

Since $p=\hbar k$, the energy is $E=p^2/(2m)$. An ideal plane wave over infinite space is not normalisable by an ordinary finite integral; box or Dirac-delta normalisation is used instead.

8. Particle in a One-Dimensional Infinite Potential Box

Consider $0<x<L$ with $V=0$ inside and an effectively infinite potential outside. The boundary conditions are $\psi(0)=\psi(L)=0$.

$$d^2\psi/dx^2+k^2\psi=0$$

$$\psi=A\sin(kx)+B\cos(kx)$$

$\psi(0)=0$ gives $B=0$. Then $\psi(L)=0$ requires

$$\sin(kL)=0 \Rightarrow k=n\pi/L,\ n=1,2,3,\ldots$$

Therefore

$$E_n = n^2\pi^2\hbar^2/(2mL^2)$$

The unnormalised spatial eigenfunction is $\psi_n=A\sin(n\pi x/L)$.

9. Normalisation of Wave Functions

The total probability of finding the particle somewhere must be one:

$$\int |\psi(x,t)|^2\, dx = 1$$

The limits cover the complete physically accessible region. In three dimensions:

$$\iiint |\psi(r,t)|^2\, d\tau = 1$$

A wave function satisfying this condition is called normalised.

Finding the Normalisation Constant

If $\psi=A\,f(x)$, then

$$1=\int|Af(x)|^2dx=|A|^2\int|f(x)|^2dx$$

$$|A|=1/\sqrt{\left(\int|f(x)|^2dx\right)}$$

The overall phase of A has no effect on measurable probabilities, so A is commonly chosen real and positive.

10. Normalisation of the Particle-in-a-Box State

For $\psi_n=A\sin(n\pi x/L)$, normalisation requires

$$\int_0^L |A|^2\sin^2(n\pi x/L)dx=1$$

$$\int_0^L \sin^2(n\pi x/L)dx=L/2$$

$$|A|^2L/2=1$$

$$A=\sqrt{(2/L)}$$

Hence the normalised eigenfunction is

$$\psi_n(x)=\sqrt{(2/L)}\sin(n\pi x/L),\ 0<x<L$$

and $\psi_n(x)=0$ outside the box.

11. Probability in an Interval

For a normalised state, the probability of finding the particle between x=a and x=b is

$$P(a \le x \le b) = \int_a^b |\psi(x)|^2 dx$$

For the nth box state:

$$P = (2/L)\int_a^b \sin^2(n\pi x/L)dx$$

$$P = (b-a)/L - [\sin(2n\pi b/L) - \sin(2n\pi a/L)]/(2n\pi)$$

This shows that probability is determined by $|\psi|^2$, not by ψ alone.

12. Orthogonality and Orthonormality

Different energy eigenstates of a Hermitian Hamiltonian with different eigenvalues are orthogonal.
For the box:

$$\int_0^L \psi_n^*(x)\psi_m(x)dx = 0,\ n \ne m$$

After normalisation:

$$\int_0^L \psi_n^*(x)\psi_m(x)dx = \delta_{nm}$$

Here δ_{nm} is the Kronecker delta. A set satisfying both normalisation and orthogonality is orthonormal.

13. Normalisation Example: Exponential

Let $\psi(x) = Ae^{(-\alpha x)}$ for $x \ge 0$ and $\psi = 0$ for $x < 0$, where $\alpha > 0$.

$$\int_0^\infty |A|^2 e^{(-2\alpha x)}dx = 1$$

$$|A|^2/(2\alpha) = 1$$

$$A = \sqrt{(2\alpha)}$$

Thus $\psi(x) = \sqrt{(2\alpha)}e^{(-\alpha x)}$ for $x \ge 0$. The condition $\alpha > 0$ ensures convergence.

14. Normalisation Example: Gaussian

Let $\psi(x) = A \exp(-\alpha x^2/2)$, $\alpha > 0$.

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{(-\alpha x^2)}dx$$

$$\int_{-\infty}^{\infty} e^{(-\alpha x^2)}dx = \sqrt{(\pi/\alpha)}$$

$$A = (\alpha/\pi)^{(1/4)}$$

Therefore the normalised Gaussian is

$$\psi(x) = (\alpha/\pi)^{(1/4)}\exp(-\alpha x^2/2)$$

Gaussian wave packets are important examples of localised, square-integrable quantum states.

15. Normalisation and Time Evolution

For a stationary state $\psi(x,t) = \varphi(x)e^{(-iEt/\hbar)}$:

$$|e^{(-iEt/\hbar)}|^2 = 1$$

$$|\psi(x,t)|^2 = |\varphi(x)|^2$$

Thus the probability density of an energy eigenstate is time-independent even though the wave function acquires a time-dependent phase.

16. Superposition of Energy Eigenstates

A general state can be expanded as

$$\psi(x,t)=\Sigma_n\, c_n\psi_n(x)e^{(-iE_nt/\hbar)}$$

If the ψ_n are orthonormal, normalisation gives

$$\Sigma_n|c_n|^2=1$$

For an energy measurement, $|c_n|^2$ is the probability of obtaining E_n.

17. Important Mathematical Points

Complex Conjugation

If $\psi=a+ib$, then $\psi^*=a-ib$ and $|\psi|^2=\psi^*\psi=a^2+b^2$, which is real and non-negative.

Square Integrability

A bound-state wave function must have a finite integral of $|\psi|^2$ over all space so that it can be normalised to unity.

Probability Conservation

Schrödinger time evolution preserves total probability. A properly normalised state remains normalised.

Dimensions

In one dimension, $\int|\psi|^2dx=1$, so $[\psi]=L^{(-1/2)}$. In three dimensions, $[\psi]=L^{(-3/2)}$.

18. Common Examination Mistakes

- Confusing ψ with probability; probability density is $|\psi|^2$.
- Forgetting ψ^* when the wave function is complex.
- Using incomplete integration limits for normalisation.
- Trying to normalise an infinite plane wave with an ordinary finite integral.
- Ignoring boundary conditions.
- Forgetting $k=2\pi/\lambda$.
- Accepting any mathematical solution without checking finiteness, single-valuedness and square-integrability.

19. Examination-Oriented Derivations

Derivation of TDSE

Start from $E=p^2/(2m)+V$. Replace E by $i\hbar\partial/\partial t$ and p by $-i\hbar\partial/\partial x$. Applying the resulting operators to ψ gives $i\hbar\partial\psi/\partial t=[-(\hbar^2/2m)\partial^2/\partial x^2+V]\psi$.

Derivation of TISE

For a time-independent potential put $\psi(x,t)=\varphi(x)T(t)$, separate the variables, set the separation constant equal to E, and obtain $-(\hbar^2/2m)d^2\varphi/dx^2+V\varphi=E\varphi$.

Normalisation of Box Eigenfunction

Use $\int_0^L |\psi|^2 dx = 1$ for $\psi = A \sin(n\pi x/L)$. Since the sine-squared integral equals $L/2$, $A = \sqrt{(2/L)}$.

20. Practice Problems with Answers

Question	Answer
1. Normalise $\psi = Ae^{-ax}$ for $x \geq 0$, $a > 0$.	$A = \sqrt{(2a)}$.
2. For $\psi_1 = \sqrt{(2/L)}\sin(\pi x/L)$, find $P(0 < x < L/2)$.	$P = 1/2$.
3. Write the 1D Hamiltonian operator.	$\hat{H} = -(\hbar^2/2m)d^2/dx^2 + V(x)$.
4. Find $\lvert\psi\rvert^2$ for $\psi = Ae^{ikx}$.	$\lvert\psi\rvert^2 = \lvert A\rvert^2$, a constant.
5. Why must a bound-state wave function be square-integrable?	Because total probability must be finite and normalisable to one.
6. Evaluate $\int_0^L \psi_2^* \psi_3 dx$ for box eigenstates.	0, due to orthogonality.

21. Quick Revision Sheet

- de Broglie: $p = \hbar k$.
- Planck: $E = \hbar\omega$.
- Momentum operator: $\hat{p} = -i\hbar\nabla$.
- Energy operator: $\hat{E} = i\hbar\partial/\partial t$.
- Hamiltonian: $\hat{H} = -(\hbar^2/2m)\nabla^2 + V$.
- TDSE: $i\hbar\partial\psi/\partial t = \hat{H}\psi$.
- TISE: $\hat{H}\psi = E\psi$.
- Probability density: $\rho = |\psi|^2$.
- Normalisation: $\int |\psi|^2 d\tau = 1$.
- Probability in a region: $P = \int |\psi|^2 d\tau$.
- Orthonormality: $\int \psi_n^* \psi_m d\tau = \delta_{nm}$.
- 1D box: $\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$, $E_n = n^2\pi^2\hbar^2/(2mL^2)$.

22. Key Takeaways

The Schrödinger equation governs the evolution of a non-relativistic quantum state. The wave function is a probability amplitude, while $|\psi|^2$ is probability density. Normalisation ensures that the total probability is exactly one. Boundary conditions and square-integrability select physically meaningful solutions and, for bound systems, lead to discrete energy levels.