Quantum Mechanics in Medicine
Lecture 4

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For Third-year Students

Outline

Monochromatic Plane Wave

A free particle of mass m moving along $+x$ with momentum p and energy E may be represented by

$$\Psi(x,t) = A\, e^{i(kx-\omega t)}, \qquad E = \hbar\omega, \quad p = \hbar k.$$

Using $E = \dfrac{p^2}{2m}$ and the operator substitutions $\hat{E} = i\hbar\,\frac{\partial}{\partial t}$, $\hat{p} = -i\hbar\,\frac{\partial}{\partial x}$, we obtain the 1D free-particle TDSE:

$$i\hbar\,\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\,\frac{\partial^2\Psi}{\partial x^2}.$$

Three-Dimensional Form

In 3D the plane wave is

$$\Psi(\mathbf{r}, t) = A\, e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)},$$

with position-representation operators

$$\hat{\mathbf{p}} = -i\hbar\nabla, \qquad \hat{E} = i\hbar\,\frac{\partial}{\partial t}.$$

Therefore the TDSE becomes

$$i\hbar\,\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi.$$

Including a Potential

If the force derives from a potential $V(\mathbf{r}, t)$, classically $E = \dfrac{p^2}{2m} + V$. Promoting $E \to \hat{E}$ and $\mathbf{p} \to \hat{\mathbf{p}}$ gives

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi.$$

The Hamiltonian operator is

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t).$$

Born Interpretation and Normalization

Probability density: $\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2$. Normalization:

$$\int_{\mathbb{R}^3} |\Psi(\mathbf{r}, t)|^2 \, \mathrm{d}^3 r = 1, \quad \text{for all } t.$$

Physical (square-integrable) states vanish sufficiently fast as $r \to \infty$.

Continuity Equation and Probability Current Density

From the TDSE and its conjugate one derives

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0, \qquad \rho = |\Psi|^2,$$

with probability current density

$$\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2mi}\big(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*\big).$$

Using Gauss' theorem: $\mathrm{d}/\mathrm{d}t \int_V \rho \, \mathrm{d}^3 r = -\oint_S \mathbf{j} \cdot \mathrm{d}\mathbf{S} \to 0$ as S recedes to infinity for localized Ψ.

MCQs (1/10)

Q1. TDSE for a free particle in 1D is derived from:

A. Newton's second law

B. $E = \frac{p^2}{2m}$

C. Maxwell's equations

D. Planck's radiation law

Q2. General solution for a definite momentum is:

A. Wave packet

B. Plane wave

C. Standing wave

D. Spherical wave

MCQs (2/10)

Q3. $\Psi(x,t) = Ae^{i(kx-\omega t)}$ represents:

A. Plane wave solution

B. Gaussian packet

C. Bound state

D. Stationary wave

Q4. For $p = 2 \times 10^{-24}\,\mathrm{kg\,m\,s^{-1}}$, the de Broglie wavelength is:

A. 3.3 nm

B. 1.7 nm

C. 0.33 nm

D. 6.6 nm

MCQs (3/10)

Q5. The time-dependent Schrödinger equation is:

A. Linear and homogeneous

B. Nonlinear

C. Non-homogeneous

D. Non-differential

Q6. A wave packet is constructed by:

A. A single frequency wave

B. Superposition of plane waves

C. Delta function

D. Classical trajectory

MCQs (4/10)

Q7. The energy (Hamiltonian) operator in $V(x,t)$ is:

A. $-\frac{\hbar^2}{2m}\nabla^2 + V(x,t)$

B. $-i\hbar\,\partial_t$

C. $p^2/2m$ only

D. ∇^2

Q8. The Hamiltonian operator is named after:

A. Schrödinger

B. Hamilton

C. Born

D. Dirac

MCQs (5/10)

Q9. The statistical interpretation of $|\Psi(\mathbf{r}, t)|^2$ is:

A. Probability current density

B. Energy density

C. Probability density

D. Momentum density

Q10. The normalization condition of a wavefunction is:

A. $\int |\Psi|^2 \, \mathrm{d}\tau = 1$

B. $\int |\Psi|^2 \, \mathrm{d}\tau = 0$

C. $\int \Psi \, \mathrm{d}\tau = 1$

D. $\int \Psi \, \mathrm{d}\tau = 0$

Q11. If $\Psi(x) = Ae^{-ax^2}$, find A s.t. $\int |\Psi|^2 \, \mathrm{d}x = 1$:

A. $(a/\pi)^{1/4}$

B. $(\pi/a)^{1/2}$

C. $a^{1/2}$

D. $1/\pi$

Q12. Conservation of probability means:

A. $\int |\Psi|^2 \, \mathrm{d}\tau$ changes with time

B. Normalization integral is independent of time

C. Probability can vanish

D. Wavefunction disappears

MCQs (7/10)

Q13. Probability current density is:

A. $\frac{i\hbar}{2m}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right)$

B. $|\Psi|^2 v$

C. $\nabla|\Psi|^2$

D. $\hbar k/m$

Q14. The continuity equation in quantum mechanics ensures:

A. Conservation of mass

B. Conservation of charge

C. Conservation of probability

D. Conservation of momentum

MCQs (8/10)

Q15. For a square-integrable wavefunction, as $r \to \infty$, $\Psi \to$:

A. ∞

B. 0

C. 1

D. Constant

Q16. Electron with $E = 5\,\text{eV}$ and $V = 0$: the wave number k is

A. $1.1 \times 10^{10}\,\text{m}^{-1}$

B. $3.6 \times 10^{9}\,\text{m}^{-1}$

C. $5.2 \times 10^{10}\,\text{m}^{-1}$

D. $9.1 \times 10^{8}\,\text{m}^{-1}$

MCQs (9/10)

Q17. A wavefunction is square-integrable if:

A. It is continuous and differentiable

B. $\int |\Psi|^2 \, \mathrm{d}\tau < \infty$

C. It vanishes everywhere

D. It has discontinuities

Q18. Momentum operator in 3D:

A. $-i\hbar\nabla$

B. $-\hbar^2\nabla^2$

C. $-i\hbar\,\partial_t$

D. ∇V

Q19. 3D plane wave solution is:

A. $Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$

B. Ae^{ikx}

C. Ae^{-ax^2}

D. $\sin(kx)$

Q20. Probability conservation law:

A. $\partial_t\rho + \nabla\cdot\mathbf{j} = 0$

B. $\rho = |\Psi|^2$ only

C. $\nabla^2\rho = 0$

D. $\mathbf{j} = \nabla\rho$