Quantum Mechanics in Medicine
Lecture 6

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For Third-year Students

Outline

Time-Independent Schrödinger Equation

In many physically interesting cases, the potential energy V is time-independent: $V = V(\mathbf{r})$.

In such cases, we may apply the **method of separation of variables**.

Assume that the total wave function can be written as a product:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) f(t).$$

Substituting into the Schrödinger equation yields separate equations for space and time, each equal to a constant.

Derivation and Energy Constant

Starting from the time-dependent Schrödinger equation:

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

and using the separable form $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})f(t)$, we obtain:

$$i\hbar\,\psi(\mathbf{r})\frac{df(t)}{dt} = f(t)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r})$$

which separates the time and spatial parts. Dividing by $\psi(\mathbf{r})f(t)$ gives

$$\frac{1}{f}\frac{df}{dt} = -\frac{iE}{\hbar}, \qquad \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi = E\psi.$$

Integrating yields $f(t) = e^{-iEt/\hbar}$; the second equation is the **time-independent Schrödinger equation (TISE)**.

Eigenvalue Equation Form

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

$\hat{H}$ acting on ψ multiplies it by E; such an equation is an **eigenvalue equation**.

ψ is an **eigenfunction**, E an **eigenvalue**.

The set of all E is the **eigenvalue spectrum**.

The problem of solving the Schrödinger equation reduces to finding eigenvalues and eigenfunctions of $\hat{H}$.

Degeneracy

Sometimes more than one linearly independent eigenfunction corresponds to the same eigenvalue.

Such an eigenvalue is **degenerate**.

If there are k independent eigenfunctions for the same E, the eigenvalue is k-**fold degenerate**.

Any linear combination of degenerate eigenfunctions is also an eigenfunction:

$$\Psi = c_1\Psi_1 + c_2\Psi_2 + \cdots + c_k\Psi_k.$$

Reality of Eigenvalues

Let E be the eigenvalue corresponding to eigenfunction Ψ:

$$\hat{H}\Psi = E\Psi.$$

The Hamiltonian $\hat{H}$ is a **Hermitian operator**.

Therefore, all energy eigenvalues are **real**.

Stationary States

For a separable wavefunction, the probability density is

$$|\Psi(\mathbf{r},t)|^2 = |\psi(\mathbf{r})|^2 \, |f(t)|^2 = |\psi(\mathbf{r})|^2,$$

which is independent of time.

These are called **stationary states**.

The expectation value of total energy equals the eigenvalue E for all time if the wavefunction is normalized.

Orthogonality and Orthonormality

Eigenfunctions corresponding to distinct eigenvalues are **orthogonal**.

If normalized, we combine orthogonality with normalization:

$$\int \psi_k^* \psi_n \, d\tau = \begin{cases} 1, & k = n, \\ 0, & k \neq n. \end{cases}$$

This is the **orthonormality condition**.

Parity in One Dimension

Suppose the potential is symmetric: $V(-x) = V(x)$.

Under the reflection $x \to -x$ (parity operation), Schrödinger's equation is invariant.

If $\psi(x)$ is an eigenfunction, $\psi(-x)$ is another eigenfunction with the same eigenvalue E.

Even and Odd Wavefunctions

If the eigenvalue is nondegenerate, $\psi(-x)$ and $\psi(x)$ differ only by a constant.
Hence, eigenfunctions can be classified as:

$$\psi(-x) = +\psi(x) \quad \text{(even)}, \qquad \psi(-x) = -\psi(x) \quad \text{(odd)}.$$

MCQs (1–2)

Q1. For a time-independent potential $V(\mathbf{r})$, the wavefunction can be written as:

A. $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) + f(t)$

B. $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) f(t)$

C. $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) t$

D. $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) - f(t)$

Q2. The separation constant appearing after separation of variables equals:

A. Momentum

B. Normalization constant

C. Energy E

D. Parity

MCQs (3–4)

Q3. The time part of an energy eigenfunction is proportional to:

A. $e^{-iEt/\hbar}$

B. $e^{+iEt/\hbar}$

C. $e^{-Et/\hbar}$

D. $e^{+Et/\hbar}$

Q4. The time-independent Schrödinger equation is expressed as:

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

B. $\hat{p}\psi = i\hbar\partial_x\psi$

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

D. $\hat{H}\psi = iE$

MCQs (5–6)

Q5. The complete set of all eigenvalues of $\hat{H}$ is the:

A. State space

B. Eigenvalue spectrum

C. Configuration space

D. Momentum space

Q6. More than one independent eigenfunction with the same E means the level is:

A. Normalized

B. Stationary

C. Degenerate

D. Orthogonal

MCQs (7–8)

Q7. A linear combination of degenerate eigenfunctions is:

A. Not an eigenfunction

B. An eigenfunction with the same eigenvalue

C. An eigenfunction with a different eigenvalue

D. Only approximately an eigenfunction

Q8. Hermiticity of $\hat{H}$ ensures that:

A. Energy eigenvalues are always complex

B. Energy eigenvalues are always real

C. Energy eigenvalues are imaginary

D. Energy eigenvalues are arbitrary

MCQs (9–10)

Q9. For $\Psi = \psi e^{-iEt/\hbar}$, the probability density is:

A. Time-dependent

B. Constant in time

C. Exponentially decaying

D. Oscillatory

Q10. The expectation value of $\hat{H}$ for a normalized eigenstate equals:

A. $\hbar$

B. 0

C. The eigenvalue E

D. Only kinetic energy

MCQs (11–12)

Q11. Eigenfunctions of distinct eigenvalues are:

A. Orthogonal

B. Parallel

C. Equal

D. Arbitrary

Q12. The orthonormality condition is:

A. $\int \psi_k^* \psi_n \, d\tau = \delta_{kn}$

B. $\int \psi_k \psi_n \, d\tau = 1$

C. $\int |\psi_n|^2 \, d\tau = 0$

D. $\psi_k = \psi_n$

MCQs (13–14)

Q13. For $V(-x) = V(x)$, the system is symmetric under:

A. Time reversal

B. Parity operation

C. Translation

D. Scaling

Q14. Nondegenerate energy levels in even potentials correspond to eigenfunctions that are:

A. Even or odd

B. Only even

C. Only odd

D. Neither even nor odd

Q15. The parity relation for even and odd functions is:

A. $\psi(-x) = +\psi(x)$ or $\psi(-x) = -\psi(x)$

B. $\psi(-x) = i\psi(x)$

C. $\psi(-x) = \psi^*(x)$

D. $\psi(-x) = 0$

Q16. The one-dimensional Schrödinger equation is:

A. $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$

B. $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$

C. $\hat{p}\psi = -i\hbar\frac{d\psi}{dx}$

D. $\nabla^2\psi = 0$

Q17. If ψ_1, ψ_2 are orthogonal eigenfunctions with the same E, $c_1\psi_1 + c_2\psi_2$ is:

A. Not normalizable

B. An eigenfunction with eigenvalue E

C. An eigenfunction with eigenvalue $E_1 + E_2$

D. Purely imaginary

Q18. The 3D Hamiltonian operator is:

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

B. $\hat{H} = i\hbar\frac{\partial}{\partial t}$

C. $\hat{H} = \nabla + V$

D. $\hat{H} = \mathbf{r}$

MCQs (19–20)

Q19. Hermiticity of $\hat{H}$ implies:

A. Real measurable energies

B. Imaginary eigenvalues

C. Infinite degeneracy

D. Random phases

Q20. Stationary states have:

A. Constant probability density

B. Decaying probability density

C. Increasing momentum

D. Nonconserved energy