

Chapter 7: The Schrödinger Equation in One Dimension

Comprehensive Notes

7.1 Introduction

- In **classical mechanics**, motion is determined by Newton's law:

$$F = m a = m \frac{d^2x}{dt^2}.$$

- In **quantum mechanics**, the state of motion is described by a **wavefunction** $\Psi(x, t)$.
- Its evolution is governed by the **time-dependent Schrödinger equation** (TDSE):

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi.$$

- For states of definite total energy E , Ψ separates into spatial and temporal parts:

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar},$$

reducing the TDSE to the simpler **time-independent Schrödinger equation** (TISE):

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

These $\psi(x)$ describe stationary (standing-wave) states.

7.2 Classical Standing Waves

For a string of length a fixed at both ends:

$$y(x, t) = A \sin(kx) \cos(\omega t),$$

where $k = 2\pi/\lambda$ and $\omega = 2\pi f$.

- Boundary conditions: $y(0, t) = y(a, t) = 0 \Rightarrow \lambda_n = 2a/n$, $n = 1, 2, 3, \dots$
- Only integer numbers of half-wavelengths fit between the ends.
- Quantization arises from the *boundary condition*, not from any discrete force.

7.3 Standing Waves in Quantum Mechanics: Stationary States

Connecting classical and quantum standing waves. In classical physics, a standing wave on a string can be written as:

$$y(x, t) = A \sin(kx) \cos(\omega t),$$

a product of a spatial function and a temporal function. The points where the wave is always zero are called **nodes**, and the string oscillates between them without net motion along x .

In quantum mechanics, a similar separation occurs for the wavefunction $\Psi(x, t)$:

$$\Psi(x, t) = \psi(x) T(t),$$

where $\psi(x)$ describes the spatial distribution and $T(t)$ the time evolution. However, unlike classical waves, Ψ is generally **complex-valued**.

Complex time dependence. In quantum mechanics the time factor naturally combines $\cos(\omega t)$ and $\sin(\omega t)$ into a single exponential using Euler's formula:

$$e^{-i\omega t} = \cos(\omega t) - i \sin(\omega t),$$

so that a quantum standing wave takes the form

$$\boxed{\Psi(x, t) = \psi(x)e^{-i\omega t}}.$$

This compact representation simplifies analysis, and the imaginary unit i does not imply any “imaginary” physical quantity—observable quantities come from real combinations such as $|\Psi|^2$.

Energy of a stationary state. From the Planck–de Broglie relation:

$$E = \hbar\omega,$$

each stationary state corresponds to a definite, quantized energy. A system in such a state has a fixed total energy and a wavefunction that oscillates in time with angular frequency ω but does not change its spatial probability distribution.

Time independence of probability density. The measurable quantity is the **probability density**:

$$|\Psi(x, t)|^2 = \Psi^*(x, t)\Psi(x, t) = \psi^*(x)\psi(x)|e^{-i\omega t}|^2 = |\psi(x)|^2.$$

Since $|e^{-i\omega t}| = 1$, the probability density is independent of time. Thus, in a stationary state the distribution of where the particle may be found does not vary with time—analogous to a classical standing wave with stationary nodes.

Interpretation and terminology.

- A **stationary state** (or energy eigenstate) is one whose probability density $|\Psi|^2$ is time-independent.
- These are the quantum analogue of classical standing waves: energy is fixed and the shape of the wave does not change in time.
- The spatial part $\psi(x)$ determines the allowed patterns of standing waves, which are quantized by the system's boundary conditions.
- The time-dependent factor $e^{-iEt/\hbar}$ merely adds a uniform phase rotation and carries no measurable effect on probabilities.

Superpositions and time dependence. If two stationary states of different energies are combined,

$$\Psi(x, t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar},$$

the cross-term in $|\Psi|^2$ introduces oscillations with frequency $(E_2 - E_1)/\hbar$. This interference causes the probability density to vary with time—these are **non-stationary states**.

7.4 Particle in a Rigid Box (Infinite Square Well)

Physical model. Consider a particle of mass m confined to move along the x -axis between two perfectly rigid walls at $x = 0$ and $x = a$.

$$U(x) = \begin{cases} 0, & 0 < x < a, \\ \infty, & x \leq 0 \text{ or } x \geq a. \end{cases}$$

Inside the box, the particle is free (no forces), while the infinite potential barriers prevent it from escaping. This model is often called the **infinite potential well** or **rigid box**.

Boundary conditions. Because the wavefunction must vanish wherever the potential is infinite:

$$\psi(0) = 0, \quad \psi(a) = 0.$$

The wavefunction must also be continuous within the well and cannot have discontinuities at the walls.

Solving the Schrödinger equation. Within the box ($U = 0$), the time-independent Schrödinger equation (TISE) becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0,$$

where $k = \sqrt{2mE}/\hbar$.

The general solution is

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

Applying the boundary conditions.

$$\begin{aligned}\psi(0) &= 0 \Rightarrow B = 0, \\ \psi(a) &= 0 \Rightarrow A \sin(ka) = 0.\end{aligned}$$

A nontrivial solution requires $\sin(ka) = 0$, which occurs only if

$$k = \frac{n\pi}{a}, \quad n = 1, 2, 3, \dots$$

Quantized energies. Substituting $k_n = n\pi/a$ into $E = \hbar^2 k^2 / 2m$ gives the discrete energy levels:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, \dots$$

These energies increase as n^2 and cannot be zero. The lowest level ($n = 1$) is the **ground-state energy**:

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}.$$

This nonzero minimum energy reflects the Heisenberg uncertainty principle — confinement prevents the particle from being truly at rest.

Normalized wavefunctions. Normalization requires that

$$\int_0^a |\psi(x)|^2 dx = 1.$$

Substituting $\psi(x) = A \sin(k_n x)$ yields $A = \sqrt{2/a}$, so

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)}.$$

Probability density and nodes.

$$|\psi_n(x)|^2 = \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right).$$

- Each state has $n - 1$ interior nodes where $\psi = 0$.
- Higher $n \rightarrow$ shorter wavelength \rightarrow larger momentum \rightarrow higher energy.
- For $n = 1$, the probability is largest at the center ($x = a/2$).

Interpretation.

- The quantization of energy arises from boundary conditions that restrict λ :

$$\lambda_n = \frac{2a}{n}.$$

- The wavefunction can be viewed as a **standing de Broglie wave** trapped between impenetrable walls.
- The particle's momentum is not single-valued: the state is an equal superposition of right- and left-moving waves with $p = \pm\hbar k_n$.

Complete time-dependent solution. Including the time factor $e^{-iE_nt/\hbar}$:

$$\boxed{\Psi_n(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-iE_nt/\hbar}}.$$

Each Ψ_n represents a stationary state: $|\Psi_n|^2 = |\psi_n|^2$ is constant in time.

Expectation values (summary). For each normalized state:

$$\langle x \rangle = \frac{a}{2}, \quad \langle p \rangle = 0, \quad \langle E \rangle = E_n.$$

The particle is equally likely to move left or right inside the well, and its average position is at the center.

Key results.

$$\text{Allowed wavelengths: } \lambda_n = \frac{2a}{n},$$

$$\text{Allowed energies: } E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},$$

$$\text{Normalized wavefunctions: } \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right).$$

Quantization therefore emerges naturally from the wave nature of matter and the boundary conditions of confinement.

7.5 The Time-Independent Schrödinger Equation (TISE)

Motivation. In the previous section, the particle-in-a-box model showed that allowed energies and wavefunctions arise from requiring that a “matter wave” fit an integer number of half-wavelengths within a confined region. This example hints at a deeper rule: the shape of $\psi(x)$ and the allowed energies E are always linked through a single fundamental equation — the **Schrödinger equation**.

From wave motion to energy. For a free particle ($U(x) = 0$), the de Broglie relations give

$$p = \hbar k, \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}.$$

A sinusoidal wave $\psi(x) = A \sin(kx)$ satisfies

$$\frac{d^2\psi}{dx^2} = -k^2\psi.$$

Combining these two equations, we can rewrite the curvature of the wave in terms of its energy:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi.$$

Including potential energy. When the particle moves in a potential $U(x)$, its total energy is

$$E = K + U(x),$$

so the kinetic energy becomes $K = E - U(x)$. Replacing E by $E - U(x)$ in the previous relation gives

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}[E - U(x)]\psi(x).$$

Rearranging yields the **time-independent Schrödinger equation**:

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

Physical meaning of each term.

- $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$ — represents the **kinetic energy operator** acting on the wavefunction; the second derivative measures how rapidly ψ bends or curves in space. A larger curvature corresponds to higher kinetic energy.
- $U(x)\psi(x)$ — potential energy contribution at each point in space.
- $E\psi(x)$ — total energy times the wavefunction.

Thus the equation simply states: *total energy = kinetic + potential*, expressed in waveform language.

Operator form (Hamiltonian). The operator acting on $\psi(x)$ is called the **Hamiltonian operator**:

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x)}.$$

The Schrödinger equation can therefore be written compactly as the **eigenvalue equation**:

$$\hat{H}\psi(x) = E\psi(x),$$

where E is the eigenvalue (a measurable energy) and $\psi(x)$ is the corresponding eigenfunction (the stationary state).

Interpreting the solutions.

- Only specific values of E yield wavefunctions that are physically acceptable (continuous, finite, and normalizable). These allowed E values are the **quantized energy levels**.
- The function $\psi(x)$ gives the **probability amplitude** for finding the particle near position x . The measurable probability density is

$$P(x) = |\psi(x)|^2.$$

- The normalization condition ensures total probability equals one:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1.$$

Connection to classical ideas. In classical mechanics, Newton's second law

$$m \frac{d^2x}{dt^2} = \sum F$$

links acceleration to force. In quantum mechanics, the Schrödinger equation plays a similar role: it links the spatial curvature of the wavefunction (which encodes kinetic energy) to the potential energy landscape $U(x)$. Thus, it serves as the *quantum analogue of Newton's second law*.

Examples of potentials and their solutions.

- **Infinite square well:** $U(x) = 0$ for $0 < x < a$, $U = \infty$ elsewhere \rightarrow discrete energies $E_n \propto n^2$.
- **Harmonic oscillator:** $U(x) = \frac{1}{2}kx^2$ \rightarrow equally spaced energy levels.
- **Hydrogen atom:** $U(r) = -\frac{k_e e^2}{r}$ \rightarrow energy levels $E_n \propto -1/n^2$.

Each potential gives rise to its own characteristic set of quantized energies and spatial wavefunctions.

7.6 Operators and Observables

Motivation. The Schrödinger equation gives us $\psi(x)$, but how do we extract physical quantities — such as position, momentum, or energy — from it? In quantum mechanics, **every measurable quantity (observable)** is represented not by a number, but by a **mathematical operator** that acts on the wavefunction.

Operators in quantum mechanics. An **operator** is a rule that transforms one function into another, e.g.

$$\hat{A}f(x) = g(x).$$

If applying an operator \hat{A} to $\psi(x)$ returns the same function multiplied by a constant,

$$\hat{A}\psi(x) = a\psi(x),$$

then $\psi(x)$ is called an **eigenfunction** of \hat{A} , and a is its **eigenvalue**. That eigenvalue represents a definite, measurable value of the observable associated with \hat{A} .

The Hamiltonian operator. The Schrödinger equation itself is an eigenvalue equation where the operator is the Hamiltonian \hat{H} :

$$\boxed{\hat{H}\psi(x) = E\psi(x)},$$

where

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x)}.$$

Here:

- \hat{H} — total energy operator,
- E — eigenvalue (the measurable total energy),
- $\psi(x)$ — eigenfunction (stationary state).

Common one-dimensional operators.

Observable	Operator form	Interpretation
Position	$\hat{x} = x$	Acts by multiplication (returns $x\psi$)
Momentum	$\hat{p} = -i\hbar \frac{d}{dx}$	Measures spatial change in ψ ; related to λ .
Kinetic energy	$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$	Derived from momentum operator.
Potential energy	$\hat{U} = U(x)$	Acts by multiplication.
Total energy (Hamiltonian)	$\hat{H} = \hat{T} + \hat{U}$	Defines the full system's energy.

Interpretation of eigenvalue equations.

- When $\psi(x)$ is an eigenfunction of \hat{A} , measurement of that observable always yields the eigenvalue a .
- When $\psi(x)$ is not an eigenfunction, the measurement outcomes vary — only the **average** (expectation value) can be predicted.
- Thus, operators connect the wavefunction's mathematical form to experimentally measurable results.

Analogy with linear algebra. In linear algebra, eigenvalue equations have the form

$$A\vec{v} = \lambda\vec{v}.$$

Here A is a matrix (operator), \vec{v} is an eigenvector (state), and λ is an eigenvalue (measured value). Quantum mechanics generalizes this concept: $\psi(x)$ plays the role of \vec{v} , and operators replace matrices.

Example: Applying operators. For a harmonic potential $U(x) = \frac{1}{2}kx^2$ and trial wavefunction $\psi(x) = e^{-\alpha x^2}$:

$$\begin{aligned}\hat{x}\psi(x) &= xe^{-\alpha x^2}, \\ \hat{p}\psi(x) &= -i\hbar \frac{d}{dx}(e^{-\alpha x^2}) = 2i\hbar\alpha x e^{-\alpha x^2}, \\ \hat{H}\psi(x) &= \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2\right] e^{-\alpha x^2}.\end{aligned}$$

Each operator transforms the wavefunction in a way that corresponds to the physical operation of “measuring” the associated quantity.

Eigenvalues and physical meaning.

- The eigenvalue E of \hat{H} gives the measurable energy of a stationary state.
- The eigenvalue p of \hat{p} gives a definite momentum state.
- In general, two observables can be simultaneously known with precision only if their operators **commute**:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0.$$

- For example, position and momentum do not commute, leading to the Heisenberg uncertainty principle.

7.7 Expectation Values

Motivation. In quantum mechanics, measurements are inherently probabilistic. When an observable does not have a definite value (i.e., ψ is not an eigenfunction of its operator), we can still predict the **average result** obtained from many identical measurements. This average is called the **expectation value**.

Classical analogy. In probability theory, if a quantity x can take values with probabilities $P(x)$, the average or expected value is

$$\langle x \rangle = \int x P(x) dx.$$

In quantum mechanics, the probability density is given by the wavefunction:

$$P(x) = |\psi(x)|^2 = \psi^*(x)\psi(x).$$

Thus, the same concept applies — but with $\psi(x)$ replacing $P(x)$.

Definition (position expectation value). The expectation value of position is:

$$\boxed{\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx.}$$

This gives the average position you would find the particle if many measurements were made on identically prepared systems.

General definition (any observable). Every measurable quantity (observable) is represented by an operator \hat{A} . The general expression for its expectation value is:

$$\boxed{\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{A} \psi(x) dx.}$$

Here:

- $\psi(x)$ — normalized wavefunction, satisfying $\int |\psi|^2 dx = 1$,
- $\psi^*(x)$ — its complex conjugate,
- \hat{A} — operator representing the observable.

Key examples.

$$\text{Position: } \langle x \rangle = \int \psi^* x \psi dx,$$

$$\text{Momentum: } \langle p \rangle = \int \psi^* \left(-i\hbar \frac{d}{dx} \right) \psi dx,$$

$$\text{Kinetic energy: } \langle T \rangle = \int \psi^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi dx,$$

$$\text{Potential energy: } \langle U \rangle = \int \psi^* U(x) \psi dx,$$

$$\text{Total energy: } \langle E \rangle = \int \psi^* \hat{H} \psi dx.$$

Interpretation.

- $\langle A \rangle$ gives the mean result of measuring observable A over many identically prepared systems.
- If ψ is an eigenfunction of \hat{A} with eigenvalue a , then $\hat{A}\psi = a\psi$, and

$$\langle A \rangle = a.$$

This corresponds to a definite (non-random) outcome.

- If ψ is a superposition of multiple eigenstates of \hat{A} , $\langle A \rangle$ represents a weighted average of their eigenvalues.

Expectation value of powers. Sometimes it is useful to compute $\langle A^2 \rangle$ as well:

$$\langle A^2 \rangle = \int \psi^*(x) \hat{A}^2 \psi(x) dx.$$

This helps quantify the spread (uncertainty) of possible measurements of A .

Uncertainty (standard deviation). The uncertainty or standard deviation in a measurement of observable A is:

$$\sigma_A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}.$$

The smaller σ_A , the more precisely A is known. For position and momentum, these uncertainties obey the Heisenberg uncertainty principle:

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}.}$$

Example. For a particle in a normalized wavefunction $\psi(x) = Ae^{-x/L}$ defined for $x \geq 0$:

$$\begin{aligned}\langle x \rangle &= \int_0^\infty x |\psi(x)|^2 dx = \frac{L}{2}, \\ \langle p \rangle &= \int_0^\infty \psi^*(-i\hbar \frac{d\psi}{dx}) dx = i\hbar/(2L) \text{ (complex} \rightarrow \text{not physical since } \psi(0) \neq 0), \\ \langle E \rangle &= \int_0^\infty \psi^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi dx.\end{aligned}$$

This illustrates the importance of using properly normalized, physically valid wavefunctions that satisfy boundary conditions.

Summary.

- Every measurement corresponds to an operator \hat{A} acting on ψ .
- The expectation value $\langle A \rangle$ is the average measurement outcome:

$$\langle A \rangle = \int \psi^* \hat{A} \psi dx.$$

- If ψ is an eigenstate of \hat{A} , the expectation value equals the eigenvalue (a definite result).
- If not, the result is probabilistic, characterized by $\langle A \rangle$ and the uncertainty σ_A .

7.10 Barrier Penetration and Quantum Tunneling

Overview. In classical physics, a particle encountering a potential barrier higher than its total energy cannot cross — it is reflected entirely. Quantum mechanics, however, predicts that a particle has a finite probability to “tunnel” through the barrier due to the wave-like nature of matter. This phenomenon is called **quantum tunneling** or **barrier penetration**.

The setup. Consider a one-dimensional potential barrier of height U_0 extending from $x = 0$ to $x = L$:

$$U(x) = \begin{cases} 0, & x < 0, \\ U_0, & 0 \leq x \leq L, \\ 0, & x > L. \end{cases}$$

A particle with total energy $E < U_0$ is incident from the left.

Regions and wavefunctions. The time-independent Schrödinger equation (TISE) in each region is

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

Region I ($x < 0$, free space):

$$U = 0 \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}.$$

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

Ae^{ikx} represents the incident wave; Be^{-ikx} represents the reflected wave.

Region II ($0 < x < L$, barrier):

$$U = U_0 > E \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} - \kappa^2\psi = 0, \quad \text{where } \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}.$$

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}.$$

The exponential form shows that the wave decays inside the barrier rather than oscillates.

Region III ($x > L$, free space):

$$U = 0 \quad \Rightarrow \quad \psi_{III}(x) = Fe^{ikx}.$$

Only a transmitted (right-moving) wave exists beyond the barrier.

Boundary conditions. The wavefunction and its first derivative must be continuous at $x = 0$ and $x = L$:

$$\begin{aligned} \psi_I(0) &= \psi_{II}(0), & \psi_{II}(L) &= \psi_{III}(L), \\ \psi'_I(0) &= \psi'_{II}(0), & \psi'_{II}(L) &= \psi'_{III}(L). \end{aligned}$$

Solving these four equations determines the ratios between the amplitudes A, B, C, D, F and allows us to compute the **transmission** and **reflection** probabilities.

Transmission and reflection coefficients. The **transmission coefficient T** (fraction of the wave that passes through) is defined as

$$T = \frac{\text{Transmitted current}}{\text{Incident current}} = \frac{|F|^2}{|A|^2}.$$

The **reflection coefficient R** is

$$R = \frac{|B|^2}{|A|^2}.$$

Since total probability must be conserved, $R + T = 1$.

Approximate transmission probability. For $E < U_0$ and a sufficiently thick barrier ($\kappa L \gg 1$), the transmission coefficient is approximately

$$T \approx e^{-2\kappa L}, \quad \text{where } \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}.$$

This exponential dependence means that the tunneling probability decreases rapidly with:

- increasing barrier width L ,
- increasing barrier height U_0 ,
- increasing particle mass m .

Physical interpretation.

- Inside the barrier, where $E < U(x)$, the classical particle would have negative kinetic energy — forbidden in classical mechanics. But quantum mechanically, $\psi(x)$ does not vanish; it merely decays exponentially.
- If the barrier is not infinitely wide, some of the wave “leaks” through, emerging as a transmitted wave on the other side.
- This leakage gives a non-zero probability of finding the particle beyond the barrier, even when $E < U_0$.

Examples of tunneling in nature.

- **Alpha decay:** An alpha particle escapes from a nucleus by tunneling through the nuclear potential barrier.
- **Field emission:** Electrons tunnel from a metal surface under strong electric fields.
- **Scanning tunneling microscope (STM):** Measures the tunneling current between a sharp metal tip and a conducting surface to map atomic-scale features.
- **Semiconductors:** Electron tunneling underlies diode and transistor behavior (e.g., tunnel diodes, Josephson junctions).

Key results.

$$\text{Barrier region decay constant: } \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar},$$

$$\text{Transmission probability: } T \approx e^{-2\kappa L},$$

$$\text{Condition for significant tunneling: } \kappa L \lesssim 1.$$

7.11 The Time-Dependent Schrödinger Equation (TDSE)

Motivation. The time-independent Schrödinger equation (TISE) determines the **allowed stationary states** and their corresponding energies for systems whose potential $U(x)$ does not vary with time. However, to describe how a quantum state evolves or changes in time — especially if it is a superposition of stationary states — we must use the more general **time-dependent Schrödinger equation (TDSE)**.

Derivation from the stationary solution. For a stationary (single-energy) state, we found that

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar},$$

where $\psi(x)$ satisfies the TISE:

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

Differentiating $\Psi(x, t)$ with respect to time:

$$\frac{\partial\Psi}{\partial t} = -\frac{iE}{\hbar}\Psi.$$

Multiplying both sides by $i\hbar$ gives:

$$i\hbar \frac{\partial\Psi}{\partial t} = E\Psi.$$

Now substitute $E\Psi$ from the TISE:

$$E\Psi = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \Psi.$$

Combining both results yields the **time-dependent Schrödinger equation**:

$$i\hbar \frac{\partial\Psi(x, t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi(x, t).$$

Interpretation.

- The TDSE governs how the wavefunction $\Psi(x, t)$ evolves in time.
- The Hamiltonian operator \hat{H} (in brackets) represents the total energy operator.
- The TDSE is a first-order differential equation in time but a second-order equation in space.
- It ensures that probability is conserved:

$$\frac{d}{dt} \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 0.$$

Stationary states revisited. When the potential $U(x)$ is constant in time, solutions can be separated into spatial and temporal parts:

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}.$$

Each stationary state $\psi(x)$ oscillates in phase at frequency $\omega = E/\hbar$, but its probability density

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

remains constant in time. Such states are called **stationary states** because all measurable quantities (like $\langle x \rangle$, $\langle p \rangle$, $\langle E \rangle$) are time-independent.

Superpositions and time dependence. A general wavefunction can be a linear combination of stationary states:

$$\Psi(x, t) = \sum_n c_n \psi_n(x)e^{-iE_n t/\hbar}.$$

The corresponding probability density is

$$|\Psi(x, t)|^2 = \sum_n |c_n|^2 |\psi_n(x)|^2 + \sum_{m \neq n} c_m^* c_n \psi_m^*(x) \psi_n(x) e^{-i(E_n - E_m)t/\hbar}.$$

The cross-terms (interference terms) oscillate in time with frequencies determined by energy differences $(E_n - E_m)/\hbar$. This makes the overall probability density time-dependent — such states are **non-stationary**.

Example: Superposition of two stationary states. For two energy eigenstates ψ_1 and ψ_2 :

$$\Psi(x, t) = c_1 \psi_1(x)e^{-iE_1 t/\hbar} + c_2 \psi_2(x)e^{-iE_2 t/\hbar}.$$

The resulting probability density is

$$|\Psi|^2 = |c_1|^2 |\psi_1|^2 + |c_2|^2 |\psi_2|^2 + 2 \operatorname{Re}[c_1^* c_2 \psi_1^*(x) \psi_2(x) e^{-i(E_2 - E_1)t/\hbar}].$$

The oscillating interference term shows that the system's spatial probability distribution changes with time — a direct signature of quantum superposition.

Probability current and conservation. The TDSE ensures local conservation of probability, described by the **continuity equation**:

$$\frac{\partial}{\partial t} |\Psi|^2 + \frac{\partial j}{\partial x} = 0,$$

where the probability current density j is defined as

$$j = \frac{\hbar}{2mi} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right).$$

This equation expresses the conservation of probability — any change in total probability in a region results from flow across its boundaries.

Physical meaning.

- The TDSE is to quantum mechanics what Newton's second law is to classical mechanics: it determines the future evolution of a system from its present state.
- Given $\Psi(x, 0)$ at $t = 0$, the TDSE uniquely determines $\Psi(x, t)$ for all future times.
- Time evolution is **deterministic**, but measurement outcomes are probabilistic, governed by $|\Psi(x, t)|^2$.

Special case — free particle. For a free particle ($U = 0$):

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

Plane-wave solutions take the form:

$$\Psi(x, t) = A e^{i(kx - \omega t)},$$

with $E = \hbar\omega = \frac{\hbar^2 k^2}{2m}$, representing a particle of definite momentum $p = \hbar k$.

Summary.

- The TDSE is the fundamental equation of motion for quantum systems:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \hat{H}\Psi(x, t).$$

- Stationary states yield time-independent probabilities, while superpositions produce time-varying interference patterns.
- Probability is conserved through the continuity equation.
- The TDSE generalizes the TISE and fully describes the dynamical evolution of any quantum state.

Summary of Key Equations

Newton (classical): $F = m \ddot{x}$,

de Broglie: $\lambda = \frac{h}{p}$, $p = \hbar k$,

Planck / energy-frequency: $E = \hbar\omega$,

String standing waves: $\lambda_n = \frac{2a}{n}$, $n = 1, 2, 3, \dots$,

Stationary state form: $\Psi_n(x, t) = \psi_n(x) e^{-iE_n t/\hbar}$,

Infinite well potential: $U(x) = \begin{cases} 0, & 0 < x < a, \\ \infty, & \text{otherwise,} \end{cases}$

Infinite well energies: $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$, $n = 1, 2, 3, \dots$,

Infinite well wavefunctions: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$,

Time-independent Schrödinger (TISE): $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U(x)\psi = E\psi$,

Hamiltonian operator: $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x)$,

Basic operators: $\hat{x} = x$, $\hat{p} = -i\hbar \frac{d}{dx}$,

Expectation value (general): $\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{A} \psi(x) dx$,

Uncertainty (standard deviation): $\sigma_A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$,

Heisenberg uncertainty: $\sigma_x \sigma_p \geq \frac{\hbar}{2}$,

Barrier decay constant: $\kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$,

Tunneling (thick barrier approx.): $T \approx e^{-2\kappa L}$,

Time-dependent Schrödinger (TDSE): $i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi$.