Schrödinger's Wave Equation and Applications

The master equation of quantum mechanics, and what it predicts

A self-study guide for first-year engineering students

Why the Schrödinger equation?

IN CLASSICAL MECHANICS

Newton's law F = ma tells us how a particle's position changes with time. Give the starting position and velocity, and the whole path follows.

IN QUANTUM MECHANICS

The Schrödinger equation tells us how the wavefunction Ψ changes with time. Give the starting Ψ and the potential V, and Ψ at every later time follows.

ROADMAP

- Time-dependent and time-independent forms
- Free particle, particle in a box, tunnelling, harmonic oscillator
- Each application: set up V, solve for Ψ, read off the allowed energies

Form 1

Time-dependent equation

WHAT IT SAYS

The rate of change of Ψ is set by the total energy operator (kinetic + potential). It works for any potential V(x, t).

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

TERM BY TERM

First term on the right: kinetic energy. Second term: potential energy. Left side: how fast the state changes.

KEY FACTS

- Linear: sums of solutions are solutions (superposition)
- First order in time: Ψ(0) fixes the future
- Complex: the i is essential
- Needed when V changes with time

Form 2

Time-independent equation

WHAT IT SAYS

If V does not depend on time, we can separate Ψ(x,t) = ψ(x) e^(−iEt/ħ). The spatial part ψ satisfies an eigenvalue equation.

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

WHY IT IS USEFUL

Solving it gives the allowed energies E and their stationary states ψ. Most textbook applications use this form.

STEPS TO SOLVE

1. Write V(x) for the problem
2. Write the equation in each region
3. Solve the differential equation
4. Apply boundary conditions
5. Normalize: $\int |\psi|^2 dx = 1$

Rules a solution must obey

BOUNDARY CONDITIONS

- ψ must be finite everywhere
- ψ must be continuous
- $d\psi/dx$ must be continuous, unless V is infinite
- ψ must go to 0 as $x \to \pm\infty$ for bound states
- ψ must be normalizable

WHY ENERGY GETS QUANTIZED

Free particle: any energy is allowed.

Bound particle: the wave must fit the region, like a guitar string fixed at both ends. Only certain wavelengths fit, so only certain energies are allowed.

Quantization is a consequence of the boundary conditions, not an extra assumption.

V = 0

Application 1: Free particle

SET-UP

No force acts, so V = 0 everywhere. The equation becomes $\psi'' = -k^2\psi$.

$$\psi = A\, e^{ikx}, \quad E = \hbar^2 k^2 / 2m$$

WHAT WE LEARN

Every energy $E \geq 0$ is allowed: continuous spectrum, no quantization. Momentum $p = \hbar k$ is exactly known.

THINGS TO NOTICE

- Plane wave: $|\psi|^2 = |A|^2$, the same everywhere
- Position is completely unknown: not normalizable
- Real particles use wave packets (sums of plane waves)
- Link to de Broglie: $\lambda = 2\pi/k = h/p$

V = ∞ walls

Application 2: Particle in a 1D box

SET-UP

V = 0 for 0 < x < L, and V = ∞ outside. The particle cannot leave, so ψ(0) = ψ(L) = 0.

$$\psi_n = \sqrt{(2/L)}\sin(n\pi x/L)$$
$$E_n = n^2h^2 / 8mL^2$$

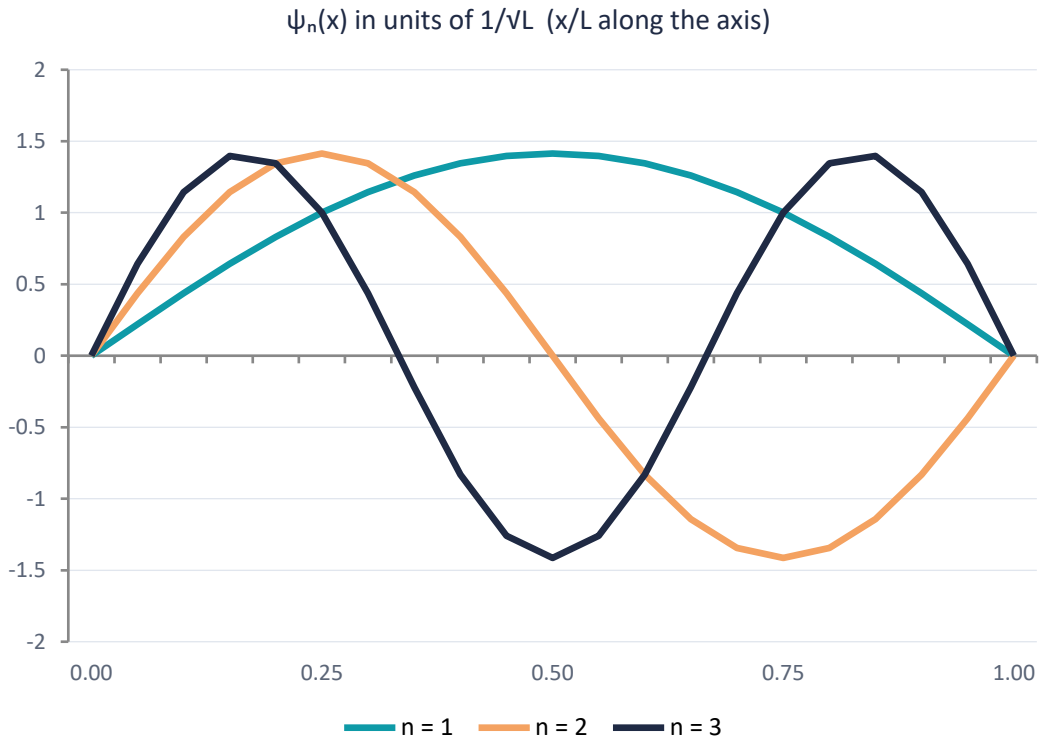
RESULT

Boundary conditions allow only whole numbers n = 1, 2, 3… The lowest energy is E_1, not zero.

DERIVATION IN 3 LINES

- Inside: $\psi'' = -k^2\psi$, so $\psi = A \sin kx + B \cos kx$
- $\psi(0) = 0$ gives $B = 0$
- $\psi(L) = 0$ gives $kL = n\pi$, so $k = n\pi/L$
- Normalizing gives $A = \sqrt{(2/L)}$

Box: wavefunctions and energy levels



WHAT TO NOTICE

- Energy grows as n^2: $E_2 = 4E_1$, $E_3 = 9E_1$
- Level n has n − 1 nodes (zero points)
- Higher n means shorter wavelength and higher energy
- Level spacing shrinks for a bigger box (large L)
- No n = 0 state: ψ would be zero everywhere

Worked example: electron in a 1 nm box

1 Ground energy

$E_1 = h^2/8mL^2 = 0.376$ eV (for L = 1 nm)

2 Higher levels

$E_2 = 4E_1 = 1.50$ eV
$E_3 = 9E_1 = 3.38$ eV

3 Transition 2 → 1

$\Delta E = E_2 - E_1 = 1.13$ eV

4 Photon emitted

$\lambda = hc/\Delta E = 1240$ eV·nm / 1.13 eV ≈ 1100 nm (infrared)

LINK TO TECHNOLOGY

Quantum dots and quantum wells work this way: smaller box, larger ΔE, bluer light.

V_0 barrier

Application 3: Barrier and tunnelling

SET-UP

A particle with energy E meets a barrier of height $V_0 > E$ and width a. Classically it bounces back. Quantum mechanically, ψ decays inside the barrier but does not become zero.

$$T \approx e^{(-2\kappa a)}, \quad \kappa = \sqrt{(2m(V_0 - E))}/\hbar$$

WHAT IT MEANS

There is a small chance the particle appears on the far side. T falls very quickly as the barrier gets wider or taller.

WHERE IT MATTERS

- Scanning tunnelling microscope: current depends on tip gap
- Alpha decay of nuclei
- Tunnel diodes and flash memory
- Nuclear fusion in the Sun

$V = \frac{1}{2}kx^2$

Application 4: Harmonic oscillator

SET-UP

A particle in a parabolic potential $V = \frac{1}{2}m\omega^2x^2$, a model for any small vibration around equilibrium, such as atoms in a molecule.

$$E_n = (n + \tfrac{1}{2})\,\hbar\omega, \quad n = 0, 1, 2\ldots$$

TWO SURPRISES

Evenly spaced levels (spacing $\hbar\omega$). The lowest energy is $\frac{1}{2}\hbar\omega$, not zero: the zero-point energy.

APPLICATIONS

- Molecular vibrations and infrared spectra
- Atoms vibrating in a crystal (phonons)
- Quantized light modes (photons)
- Ground state $\psi_0 \propto e^{\wedge}(-m\omega x^2/2\hbar)$ is a Gaussian

Summary: four systems compared

System	Potential	Energy levels	Key idea
Free particle	$V = 0$	$E = \hbar^2k^2/2m$ (continuous)	Plane waves, no quantization
Infinite box	0 inside, ∞ outside	$E_n = n^2h^2/8mL^2$	Standing waves, $E_1 > 0$
Barrier	V_0 over width a	Any E; T ≈ e^(−2κa)	Tunnelling through classically forbidden region
Harmonic oscillator	$\frac{1}{2}m\omega^2x^2$	$(n + \frac{1}{2})\hbar\omega$	Equal spacing, zero-point energy

Same recipe each time: write V, solve the equation, apply boundary conditions, normalize.

Test yourself

TRY THESE (answers on the next slide)

1. Find the ground-state energy of an electron in a 0.5 nm box (use $E_1 = 0.376$ eV for 1 nm).
2. Why can the particle in a box not have $E = 0$?
3. For ψ_1 in a box, find the probability of finding the particle in the left third (0 to L/3).
4. A harmonic oscillator has $\hbar\omega = 0.20$ eV. Find E_0 and E_1.
5. If a barrier is made twice as wide, what happens to T?

Answers and key takeaways

ANSWERS

1. $E_1 \propto 1/L^2$, so $E_1 = 0.376 \times 4 = 1.50$ eV
2. $E = 0$ would give $\psi = 0$ everywhere (no particle). It also violates the uncertainty principle.
3. $P = 1/3 - \sin(2\pi/3)/2\pi \approx 0.196$, about 19.6%
4. $E_0 = 0.10$ eV, $E_1 = 0.30$ eV
5. T becomes roughly T^2: much smaller, since the exponent doubles

REMEMBER

- Schrödinger equation: how Ψ evolves
- Time-independent form: eigenvalue problem for energy
- Bound states: quantized energies from boundary conditions
- Box: $E_n \propto n^2$
- Oscillator: $E_n = (n + ½)\hbar\omega$
- Tunnelling: $T \approx e^{(-2\kappa a)}$
- Further reading: Griffiths, Introduction to Quantum Mechanics (Ch. 2)