# Finite-well bound states and hydrogenic quantum numbers

GRE undergraduate preparation · local supported objectives

# Finite-well bound states and hydrogenic quantum numbers

- Match wavefunctions at the walls of a finite well.
- Solve for **bound state 束缚态** energies, at least graphically.
- Tell bound states from **scattering states 散射态**.
- Use hydrogen's quantum numbers, degeneracy and **radial probability 径向概率**.

# The finite square well

- Inside: $k = \sqrt{2m(E + V_0)}/\hbar$, and the wavefunction oscillates.
- Outside: the **decay constant 衰减常数** $\kappa = \sqrt{-2mE}/\hbar$, and the wavefunction falls as $e^{-\kappa|x|}$.
- Match both $\psi$ and $d\psi/dx$ at each wall. Even states need $k\tan ka = \kappa$; odd states need $-k\cot ka = \kappa$.

# Solving for the energies

- Solve graphically or numerically.
- In one dimension every attractive well has at least one bound state; when $\rho < \pi/2$ there is only that one, and no odd state.

$$z \tan z = \sqrt{\rho^2 - z^2}, \qquad \frac{E}{V_0} = \frac{z^2}{\rho^2} - 1$$

# Bound and scattering states

- Bound states: discrete energies, normalisable wavefunctions, decaying tails.
- **Scattering states** ($E > 0$): any energy, travelling waves outside.
- The decaying tail is what makes **tunnelling** through a finite barrier possible. Find the probability in the tail by integrating $|\psi|^2$ after normalising; the raw amplitude is not a probability.

# Hydrogen-like quantum numbers

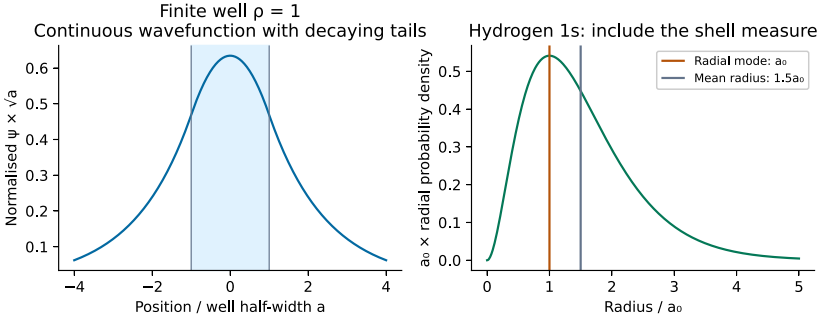
- $E_n = -13.6\,Z^2/n^2$ eV; $l = 0, \dots, n-1$; $L^2 = l(l+1)\hbar^2$.
- Each $n$ has $n^2$ spatial states, and $2n^2$ with spin.
- $m_l$ runs from $-l$ to $+l$, and $L_z = m_l\hbar$.

# Radial probability

- For 1s, $|\psi|^2$ is largest at the nucleus, but $P(r)$ peaks at the Bohr radius $a_0$.
- The mean radius of 1s is $\frac{3}{2}a_0$.

$$P(r) = r^2|R(r)|^2 \quad \text{(normalised)}$$

# Figure: Radial probability




- Identify the axes, units, directions and the stated model.

## Worked example: a shallow well

- The even condition becomes $z\tan z = \sqrt{1 - z^2}$, which simplifies to $z = \cos z$. So $z = 0.739$.
- $E/V_0 = 0.739^2 - 1 = -0.454$.
- Since $\rho < \pi/2$, this is the only bound state.

# Worked example: hydrogen 1s and n = 3

- For 1s, $P(r) = \dfrac{4r^2}{a_0^3} e^{-2r/a_0}$. Setting $dP/dr = 0$ gives $r = a_0$.
- The $n = 3$ level has $l = 0, 1, 2$ and $1 + 3 + 5 = 9$ spatial states, or 18 with spin.
- A $3d$ electron ($l = 2$) has $L^2 = 6\hbar^2$, so $|L| = \sqrt{6}\,\hbar$, never $2\hbar$.

# Common errors

- Matching $\psi$ but not $d\psi/dx$ at a finite wall.
- Saying a shallow one-dimensional well may have no bound state.
- Reading the tail amplitude as a probability.

# Common errors (2)

- Putting the most probable 1s radius at the nucleus; the $r^2$ factor moves it to $a_0$.
- Writing $|L| = l\hbar$ instead of $\sqrt{l(l+1)}\,\hbar$.

# Key terms

- **finite square well**: A potential well with walls of finite height.
- **tunnelling**: Passing through a region where the energy is below the potential.
- **bound state**: A state confined to a region, with discrete energy.
- **scattering state**: An unbound state with any energy above the potential outside.

# Check yourself

- A one-dimensional well has $\rho < \pi/2$. How many bound states does it have?
- What is the most probable radius of a hydrogen 1s electron?
- How many spatial states does hydrogen's $n = 4$ level have?