

# PHYS 2210 Quantum Physics 1

## Class 08

- Determining the expansion coefficients for mixed states
- Time evolution of mixed states
- Piecewise Potentials and some rules for predicting wavefunction behavior.
- The Finite Quantum Well

# Orthogonality of eigenfunctions $\psi_n(x)$

When  $n \neq n'$

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} \cos \frac{n\pi x}{a} \cos \frac{n'\pi x}{a} dx = 0$$

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} \sin \frac{n\pi x}{a} \cos \frac{n'\pi x}{a} dx = 0$$

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} \sin \frac{n\pi x}{a} \sin \frac{n'\pi x}{a} dx = 0$$

# Completeness

Any physically admissible wavefunction can be expanded in the complete set of eigenfunctions, provided that the wavefunction obeys the same boundary conditions as the eigenfunctions.

$$\psi(x) = \sum_i c_i \psi_i$$

We find the coefficients using orthogonality!

$$\int \psi(x) \psi_n(x) dx = \int \sum_i c_i \psi_i \psi_n dx = c_i$$

# Mixed States

- A wavefunction that satisfies the Schrodinger Equation and obeys the same boundary conditions as the eigenfunctions can be expressed as the sum of eigenstates (called an expansion in eigenfunctions)

$$\Psi(x, t) = c_1\psi_1(x, t) + c_2\psi_2(x, t) \dots$$

- We can find the expansion coefficients  $c_1, c_2 \dots$  by using the orthogonality of eigenfunctions.

$$c_n = \int \Psi(x, 0)\psi_n(x, 0)dx$$

(Integrated over the range of the eigenfunctions.)

# Understanding expansion coefficients

- The expansion coefficient is the amplitude of a specific eigenfunction that is needed to construct the wavefunction.
- We can sometimes guess/estimate the coefficient just by looking at a wavefunction.
  - If the wavefunction is an even function, then the expansion coefficients for odd eigenfunctions will be zero.
  - If the wavefunction looks like an eigenfunction then the coefficient is probably a significant fraction of one.

# Time evolution

- Once the expansion coefficients are known, we can calculate the time evolution of the wavefunction.

$$\psi_i(x, t) = \psi_i(x, 0)e^{i\omega_i t}$$

$$\Psi(x, t) = \sum_i c_i \psi_i(x, t)$$

- Finding the coefficients:

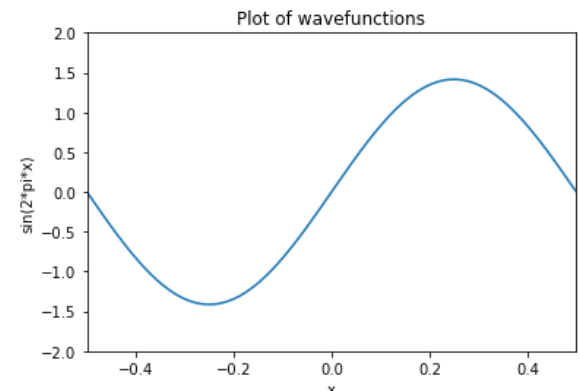
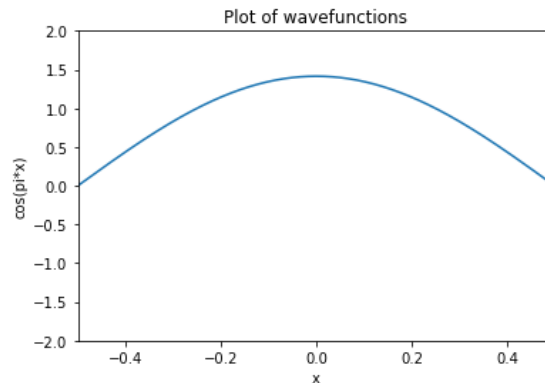
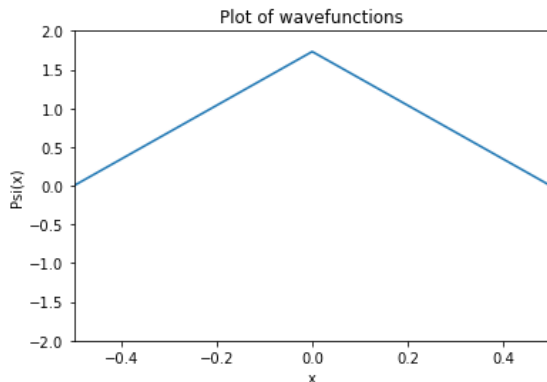
[PHYS2210Spring2022\\_Class08\\_1DWavefunctionCoefficients.ipynb](#)

- Viewing time evolution:

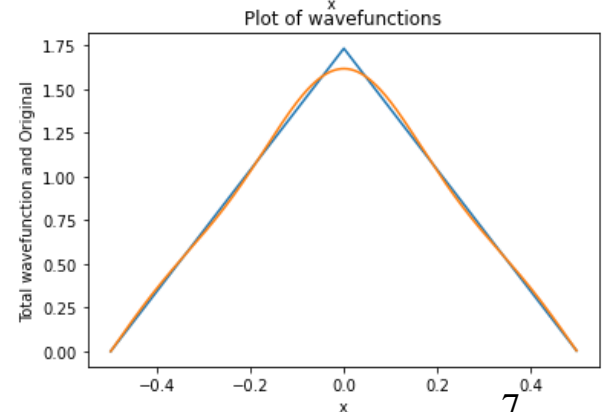
[Falstad.com/qm1d](http://Falstad.com/qm1d)

# Composing a wavefunction from eigenfunctions

$$\Psi(x) = \sqrt{\frac{12}{a^2}} \left( \frac{a}{2} - |x| \right) = c_1 \sqrt{\frac{2}{a}} \cos \frac{\pi x}{a} + c_2 \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}$$



Here is the sum for  $c_1=0.99$ ,  
 $c_3=0.11$ ,  $c_5=0.04$  and  
 $c_2, c_4, c_6...=0$



# Calculating Energy for Mixed States

- $\langle E \rangle = \int \Psi^* \hat{H} \Psi dx$
- $\int (c_1 \psi_1 + c_2 \psi_2)^* H (c_1 \psi_1 + c_2 \psi_2) dx$
- $\int (c_1 \psi_1 + c_2 \psi_2)^* (E_1 c_1 \psi_1 + E_2 c_2 \psi_2) dx$
- $\langle E \rangle = c_1^2 E_1 + c_2^2 E_2$



# Solving the Schrodinger Equation for Piecewise Constant Potentials

# The Schrodinger Equation

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

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x, t)\psi = i\hbar \frac{\partial \psi}{\partial t}$$

and if  $V(x)$  is constant in time,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + (E - V)\psi(x) = 0$$

# Piecewise potentials 1

- Many quantum physics problems can be solved by using the solutions for constant potential in each region and then matching up the solutions and derivatives at the boundaries.
  - Wavefunctions must always be matched.
  - Derivatives must be matched if there are no infinite potential steps in the problem.

## Piecewise potentials 2

Solution to the TISE in a region where  $V$  is a constant and  $E > V$ :

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + (E - V)\psi(x) = 0$$

Guess:  $\psi = e^{ikx}$

$$-\frac{\hbar^2 k^2}{2m} = (E - V) \Rightarrow k = \pm \sqrt{\frac{2m(E - V)}{\hbar^2}}$$

$$\psi = Ae^{ikx} + Be^{-ikx}$$

# Piecewise potentials 3

Solution to the TISE in a region where  $V$  is a constant and  $E < V$ :

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} - |E - V| \psi(x) = 0$$

Guess:  $\psi = e^{ikx}$

$$\frac{\hbar^2 k^2}{2m} = -|E - V| \quad \Rightarrow \quad k = \pm i \sqrt{\frac{2m|E - V|}{\hbar^2}}$$

$$\text{Let } K = ik = \pm \sqrt{\frac{2m|E - V|}{\hbar^2}} \quad (\because K \text{ is a real number})$$

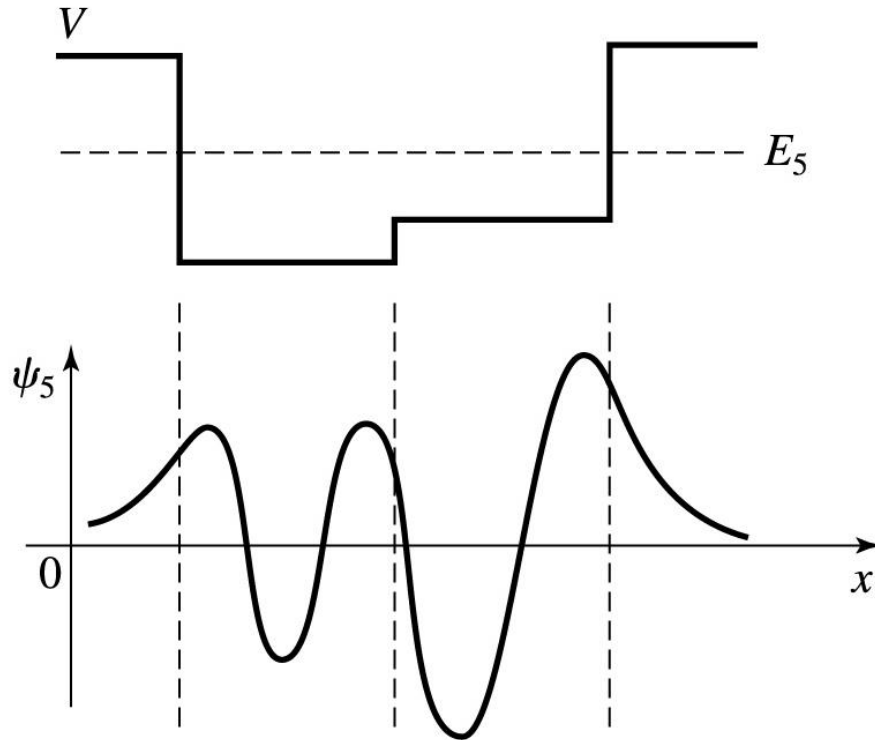
$$\psi = Ae^{Kx} + Be^{-Kx} \quad (\text{exponential growth or decay})$$

# Some “intuitive” rules for sketching wavefunctions\*

1. Solutions for the Schrodinger equation curve toward the x-axis in classically allowed ( $E > V$ ) regions and away from the axis in classically forbidden regions.
2. For bound states, the wavefunction must go to zero for large distances outside the well. (must be normalizable)
3. Curvature increases for larger  $|E - V(x)|$ .
4. Solutions are continuous and smooth if the potential has no infinite steps.
5. Energy eigenfunctions have an integer number of antinodes on classically allowed regions.
6. The wavefunction amplitude is usually larger in regions with small  $E > V$ .

\* From <https://www.asc.ohio-state.edu/physics/ntg/H133/handouts/wavefunctions.pdf>

# Illustrated “intuitive” rules

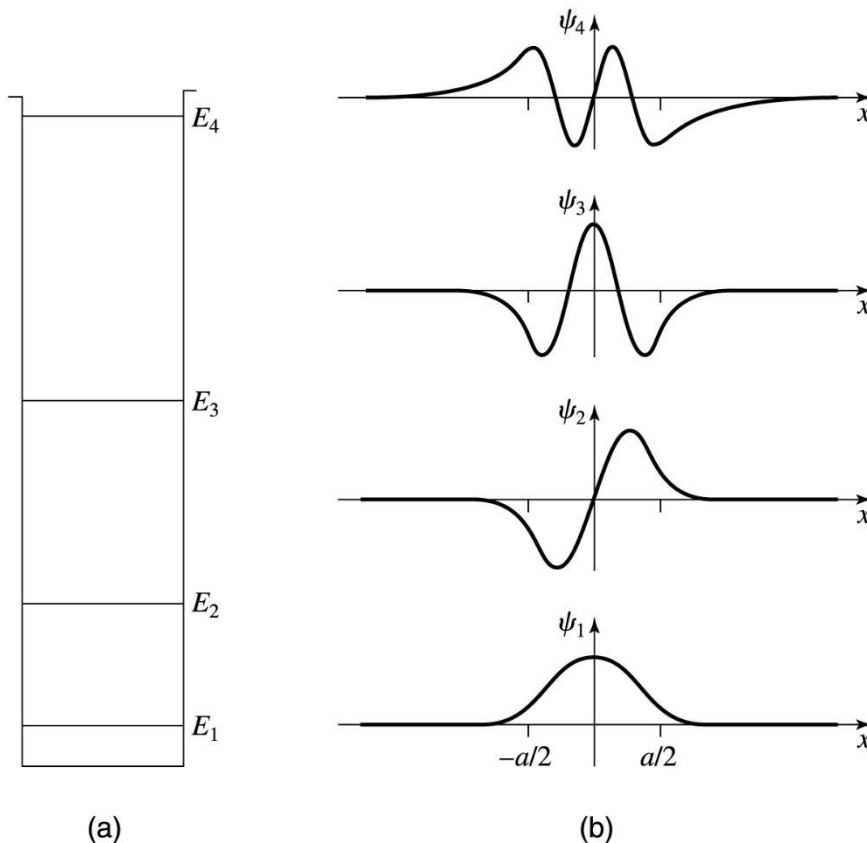


1. Curvature direction.
2. Goes to zero outside well.
3. Curvature magnitude.
4. Continuity/smoothity.
5. Integer antinodes.
6. Wavefunction amplitude

Figure 4.10 copyright 2009 University Science Books

\* from Townsend Ch 4

# Bound state wavefunctions for symmetric potentials

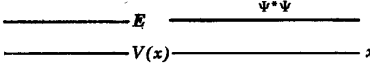
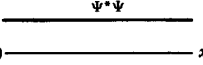
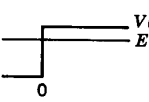
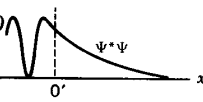
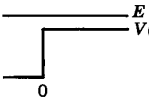
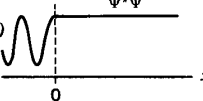
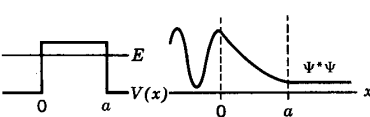
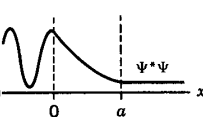
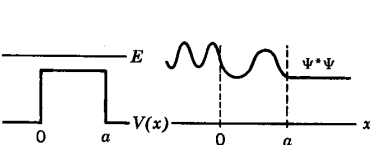
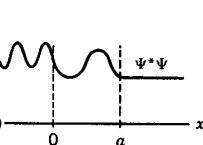
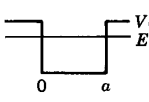
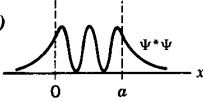
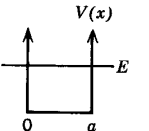
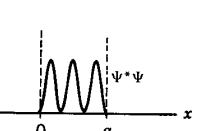
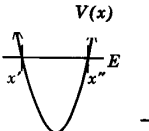
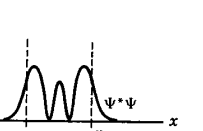


Same rules: +

- Ground state has one antinode, centered
- Alternating odd and even functions.

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Name of System	Physical Example	Potential and Total Energies	Probability Density	Significant Feature
Zero potential	Proton in beam from cyclotron			Results used for other systems
Step potential (energy below top)	Conduction electron near surface of metal			Penetration of excluded region
Step potential (energy above top)	Neutron trying to escape nucleus			Partial reflection at potential discontinuity
Barrier potential (energy below top)	$\alpha$ particle trying to escape Coloumb barrier			Tunneling
Barrier potential (energy above top)	Electron scattering from negatively ionized atom			No reflection at certain energies
Finite square well potential	Neutron bound in nucleus			Energy quantization
Infinite square well potential	Molecule strictly confined to box			Approximation to finite square well
Simple harmonic oscillator potential	Atom of vibrating diatomic molecule			Zero-point energy

from Eisberg and Resnick