Particle in a Box

Outline

- Review: Schrödinger Equation
- Particle in a 1-D Box
    - . Eigenenergies
    - . Eigenstates
    - . Probability densities

TRUE / FALSE

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

The Schrodinger equation is given above.

1. The wavefunction Ψ can be complex, so we should remember to take the Real part of Ψ. _____

2. Time-harmonic solutions to Schrodinger equation are of the form: $\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$ _____

3. Ψ(x,t) is a measurable quantity and represents the probability distribution of finding the particle. _____

Schrodinger: A Wave Equation for Electrons

$$E = \hbar\omega \qquad\qquad p = \hbar k$$

Schrodinger *guessed* that there was some wave-like quantity that could be related to energy and momentum …

$$\psi \approx e^{j(\omega t - k_x x)}$$ wavefunction

$$\frac{\partial}{\partial t}\psi = j\omega\psi \quad \Rightarrow \quad E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi$$

$$\frac{\partial}{\partial x}\psi = -jk_x\psi \quad \Rightarrow \quad p_x\psi = \hbar k_x\psi = j\hbar\frac{\partial}{\partial x}\psi$$

Schrodinger: A Wave Equation for Electrons

$$E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi \qquad p_x\psi = \hbar k\psi = j\hbar\frac{\partial}{\partial x}\psi$$

$$E = \frac{p^2}{2m} \quad \text{(free-particle)}$$

$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad \text{(free-particle)}$$

..The Free-Particle Schrodinger Wave Equation !

Erwin Schrödinger (1887–1961)
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Schrodinger Equation and Energy Conservation

... The Schrodinger Wave Equation !

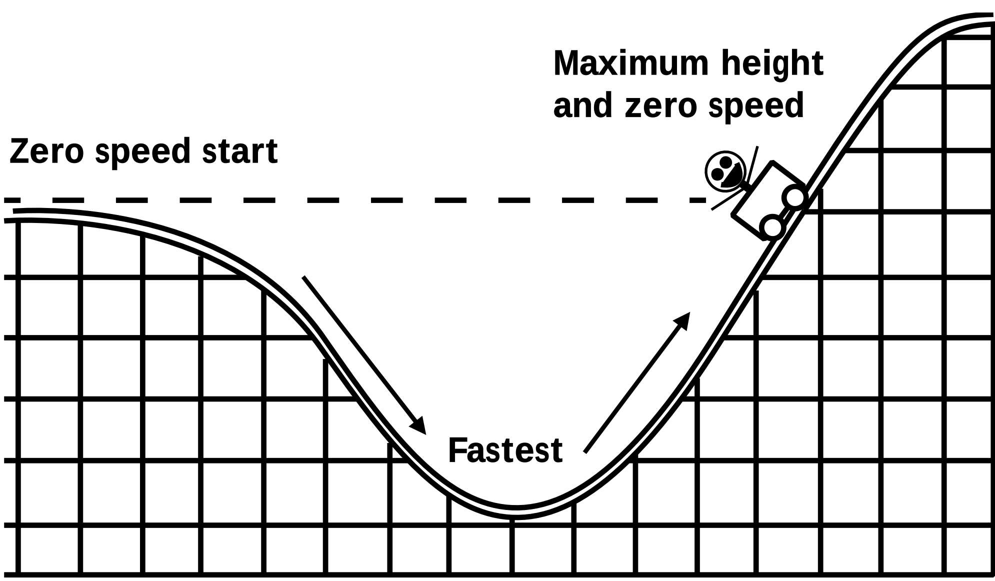
$$E = K + V$$

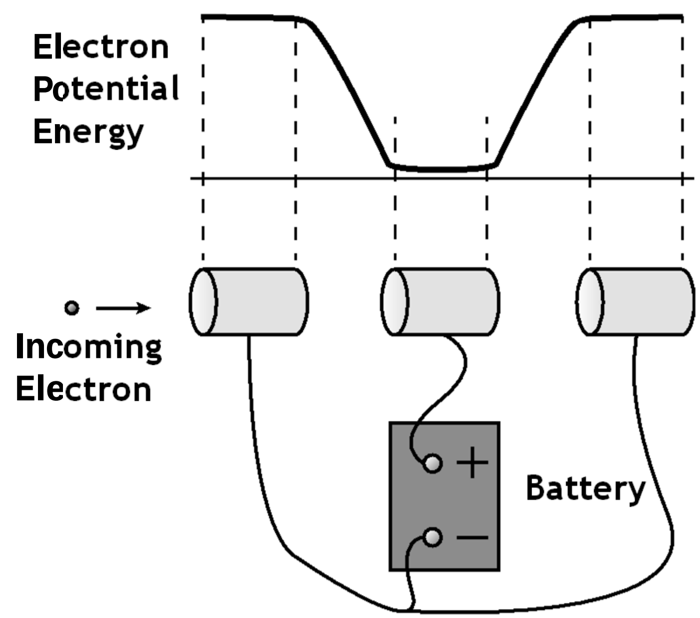
$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

Total E term **K.E. term** **P.E. term**

... In physics notation and in 3-D this is how it looks:

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





*Time-**Dependent** Schrodinger Wave Equation*

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

PHYSICS NOTATION

Total E term

K.E. term

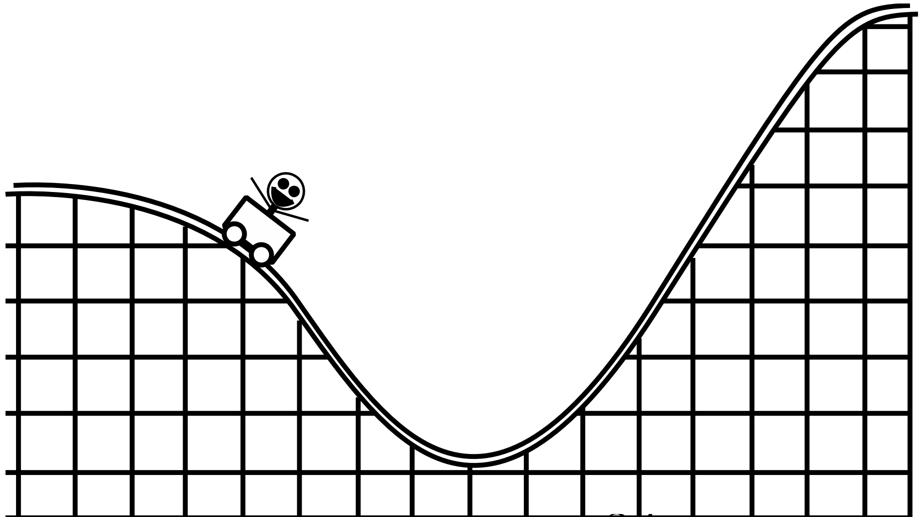
P.E. term

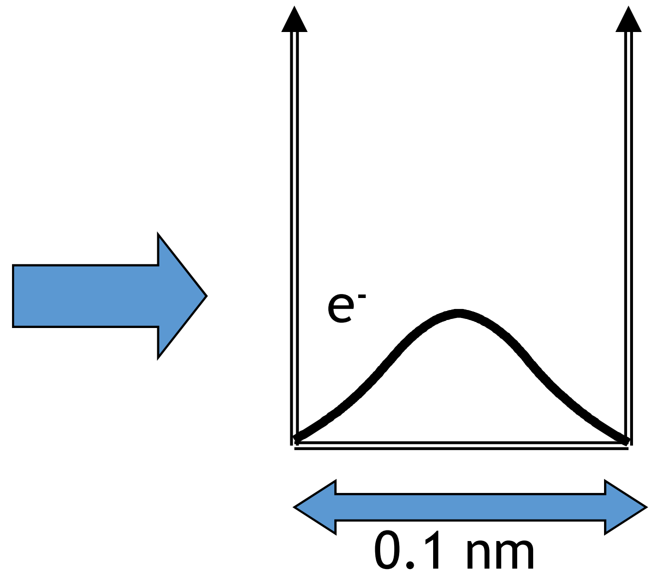
$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$$

*Time-**Independent** Schrodinger Wave Equation*

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

Particle in a Box





$$\hbar = 1.054 \times 10^{-34}\,[\mathrm{J \cdot s}]$$

The particle the box is bound within certain regions of space.
If bound, can the particle still be described as a wave ?
→ YES … as a standing wave
(wave that does not change its $P(x) = |\Psi(x,t)|^2\,dx$ with time)

$$\Psi(x,t) \approx e^{j(\omega t - k_x x)} = \psi(x) e^{j\omega t} \quad \Rightarrow \quad \boxed{P(x) = |\psi|^2\,dx}$$

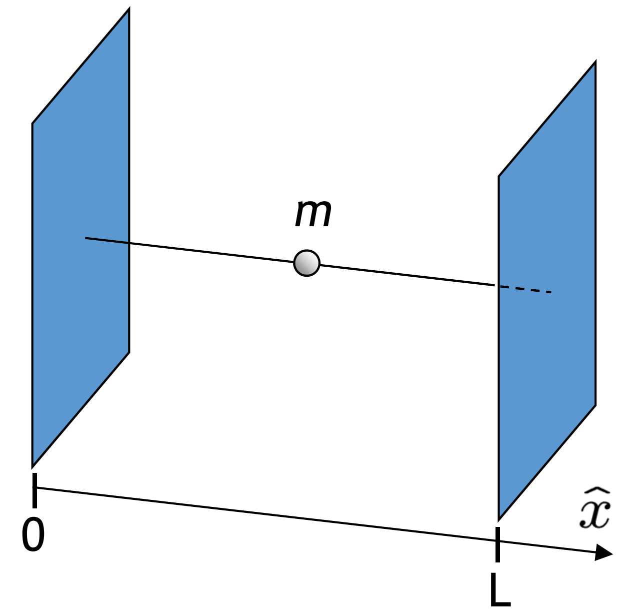
A point mass *m* constrained to move on an infinitely-thin, frictionless wire which is strung tightly between two impenetrable walls a distance *L* apart

for $(x \leq 0, x \geq L)$

$$V(x) = \infty$$

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

→ $\psi = 0$



for $(0 < x < L)$

$$V(x) = 0$$

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

WE WILL HAVE MULTIPLE SOLUTIONS FOR ψ, SO WE INTRODUCE LABEL n

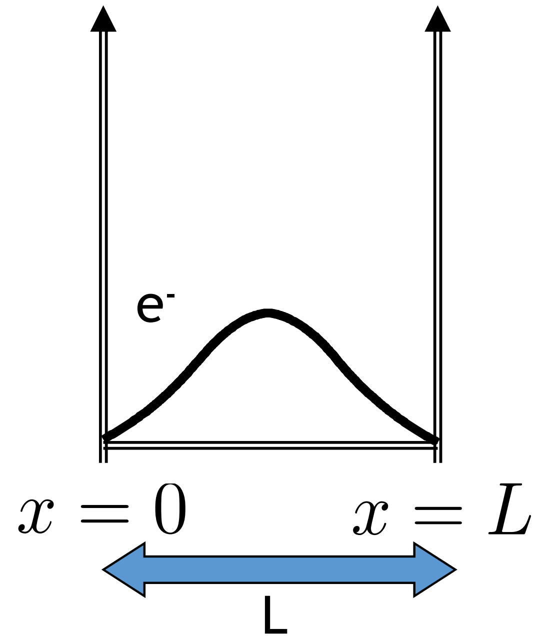
→ $\psi(0) = \psi(L) = 0$

ψ IS CONTINUOUS

$$\text{for } (0 < x < L): \ V(x) = 0$$

$$E_n \psi_n = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n}{\partial x^2}$$

WE WILL HAVE MULTIPLE SOLUTIONS FOR ψ, SO WE INTRODUCE LABEL *n*



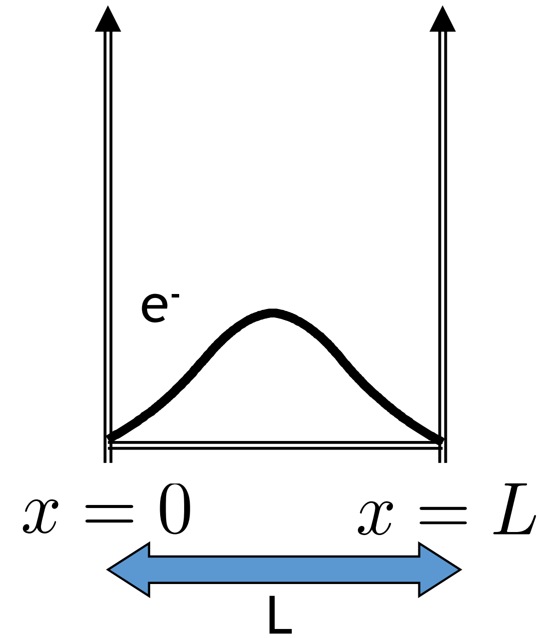
REWRITE AS:

$$\frac{\partial^2 \psi_n}{\partial x^2} + k_n^2 \psi_n = 0 \qquad \text{WHERE} \qquad k_n^2 = \frac{2mE_n}{\hbar^2}$$

GENERAL SOLUTION:

$$\psi_n(x) = A \sin k_n x + B \cos k_n x \quad \text{OR} \quad \psi_n = C_1 e^{jk_n x} + C_2 e^{-jk_n x}$$

USE BOUNDARY CONDITIONS TO DETERMINE COEFFICIENTS A and B



$$k_n L = n\pi$$

$B = 0$ since $\psi(0) = 0$

NORMALIZE THE INTEGRAL OF PROBABILITY TO 1

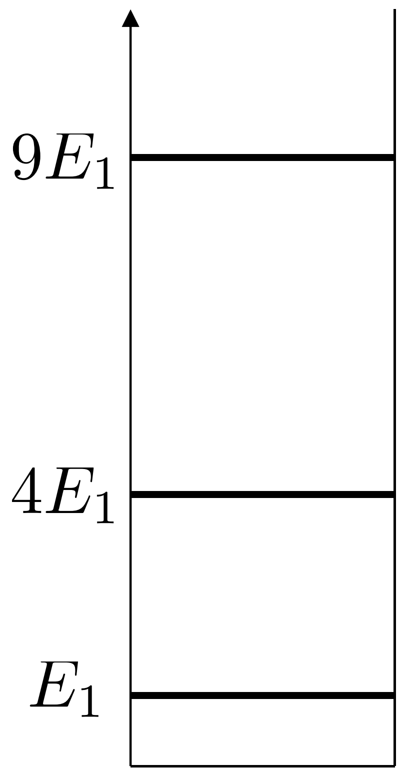
$$\psi(x) = \sqrt{9}\frac{2}{L} \sin \frac{n\pi x}{L}$$

$$k_n^2 = \frac{2mE_n}{\hbar^2}$$

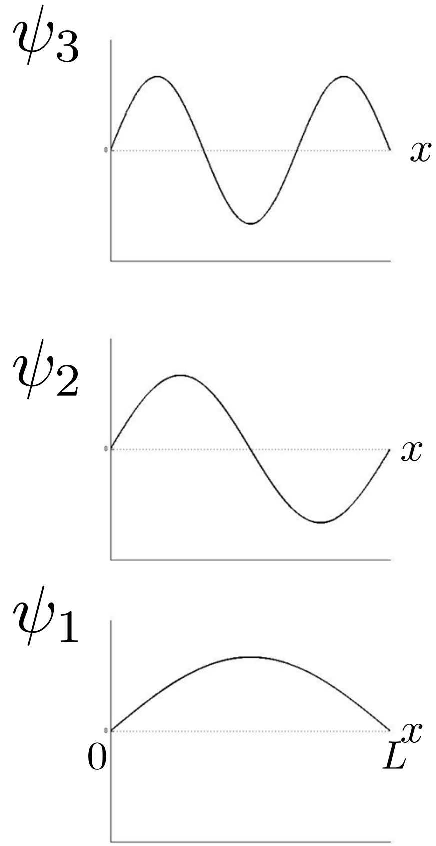
$$E_n = n^2 E_1$$

$$E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}$$

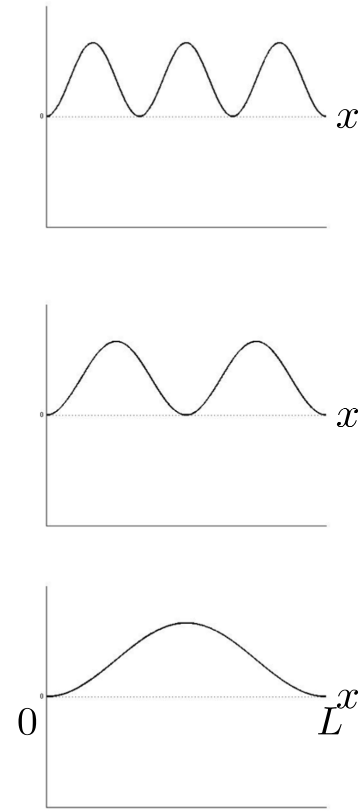
EIGENENERGIES for 1-D BOX



EIGENSTATES for 1-D BOX



PROBABILITY DENSITIES



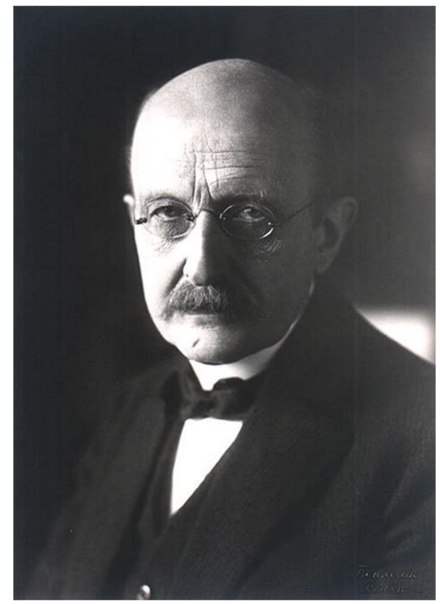
$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$P(x) = |\psi(x)|^2 \, dx = \frac{2}{L} \sin^2 \frac{n\pi x}{L} dx$$

Today’s Culture Moment

Max Planck

- Planck was a gifted musician. He played piano, organ and cello, and composed songs and operas.
- The Munich physics professor Jolly advised Planck against going into physics, saying, “in this field, almost everything is already discovered, and all that remains is to fill a few holes.”
- In 1877 he went to Berlin for a year of study with physicists Helmholtz and Kirchhoff. He wrote that Kirchhoff spoke in carefully prepared lectures which were dry and monotonous. He eventually became Kirchhoff’s successor in Berlin.
- The concept of the photon was initially rejected by Planck. He wrote "The theory of light would be thrown back not by decades, but by centuries, into the age when Christian Huygens dared to fight against the mighty emission theory of Isaac Newton.“
- In his *Scientific Autobiography and Other Papers,* he stated Planck's Principle, which holds that "A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die and a new generation grows up that is familiar with it."



1858 - 1947

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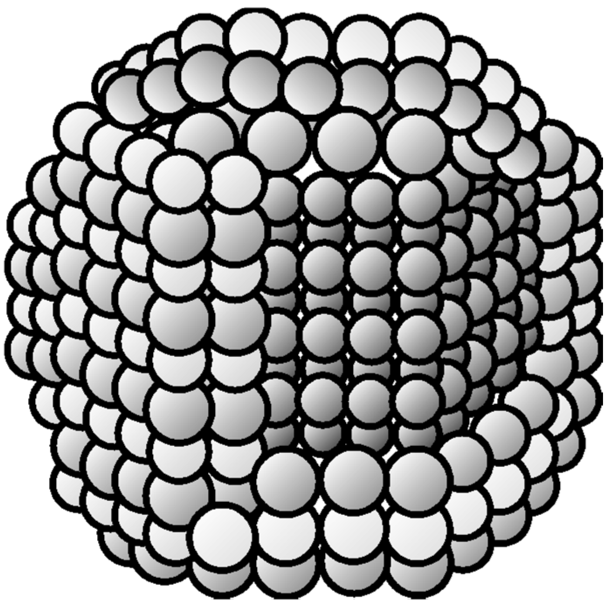
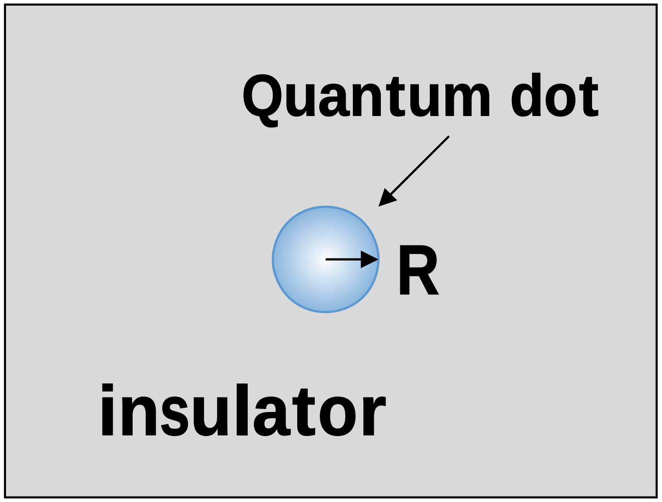
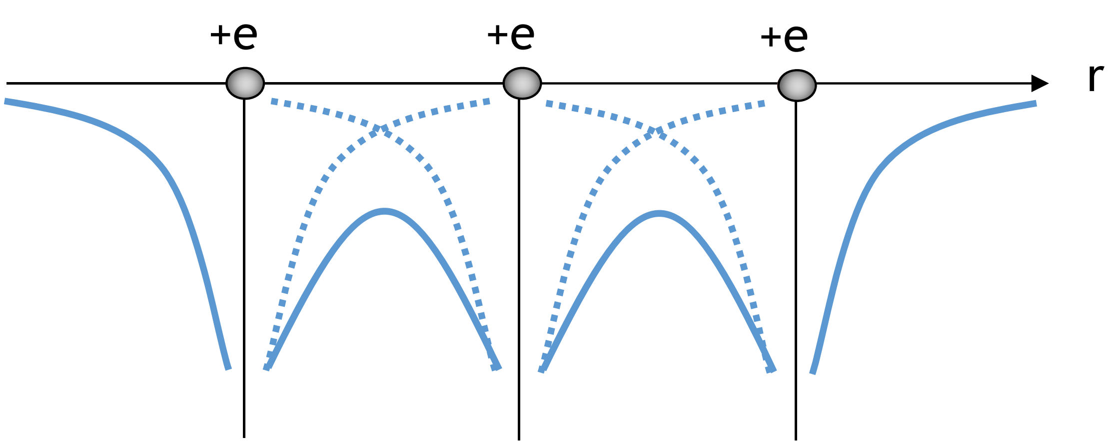
Quantum Confinement

another way to know Δx





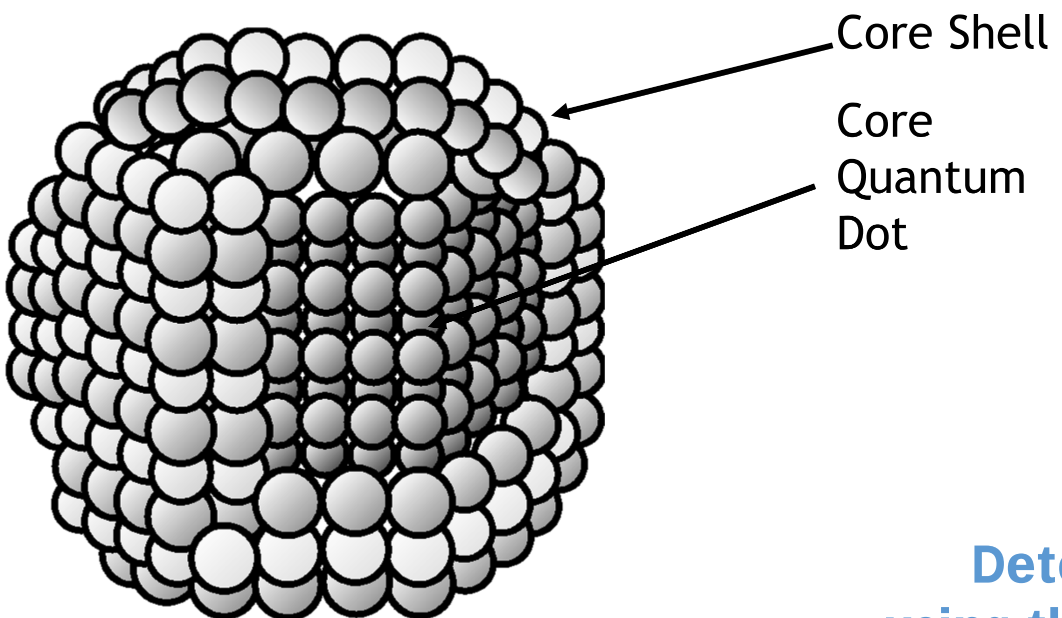


electron can be anywhere in the dot

$$< \Delta x^2 > \sim R^2$$

Semiconductor Nanoparticles

(aka: Quantum Dots)



Red: bigger dots!

Blue: smaller dots!

Determining QD energy using the Uncertainty Principle

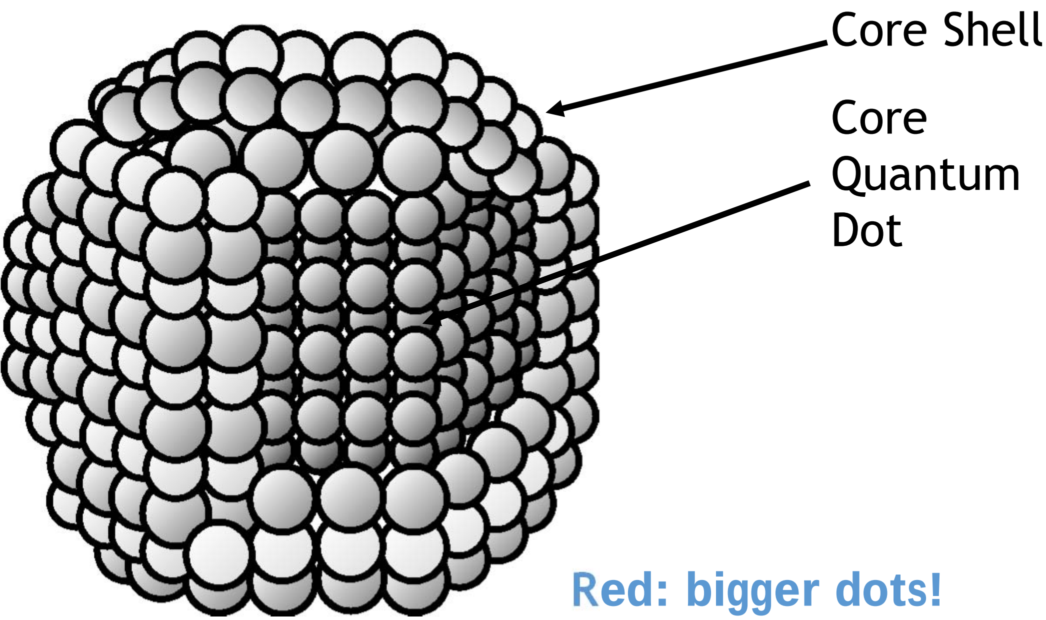
$$< \Delta x^2 > \sim R^2$$

$$< \Delta p^2 > \sim \left(\frac{\hbar^2}{2R}\right)^2$$

$$< E > = \frac{< \Delta p^2 >}{2m} \sim \frac{1}{R^2}$$

Semiconductor Nanoparticles

(aka: Quantum Dots)



Determining QD energy using the Schrödinger Equation

$$E_1 = n^2 E_1 \qquad E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}$$

Red: bigger dots!
Blue: smaller dots!

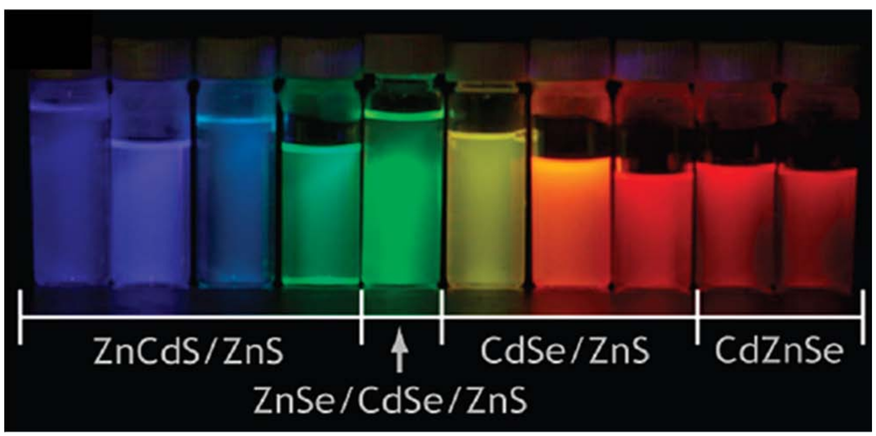
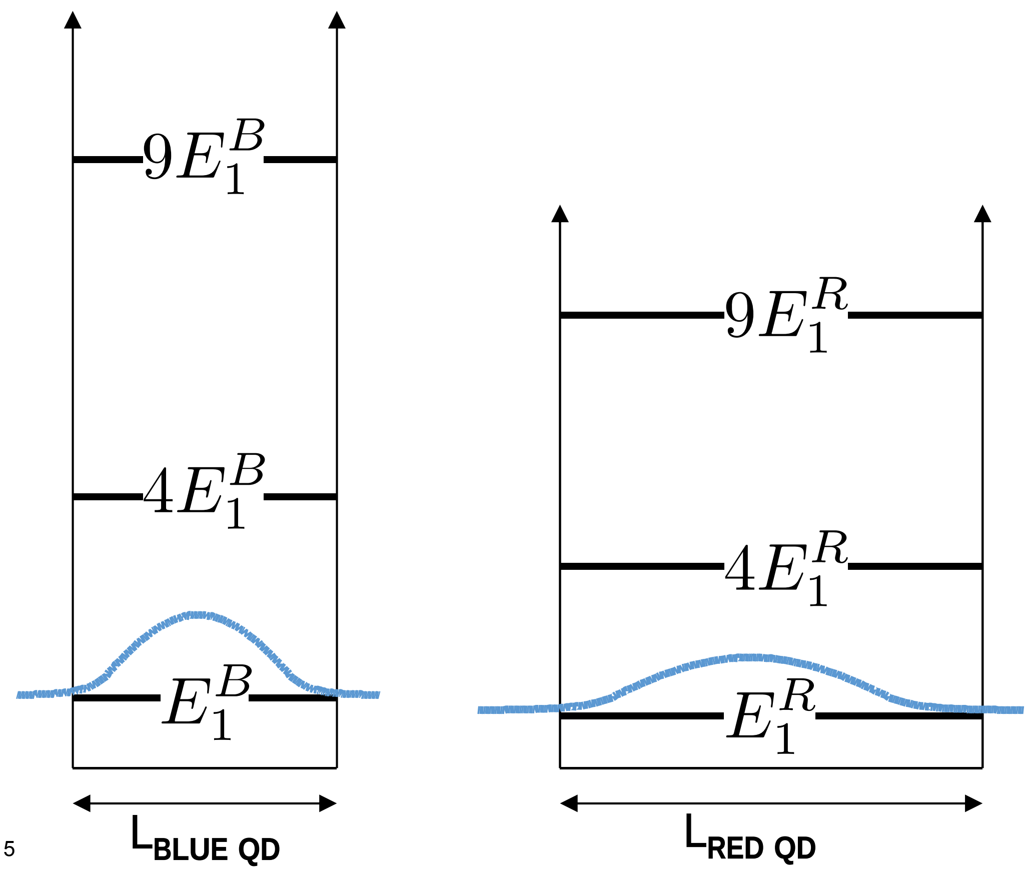


Photo by J. Halpert, Courtesy of M. Bawendi Group, EECS, MIT.



The Wavefunction

- $|\psi|^2\,dx$ corresponds to a physically meaningful quantity –
  - the probability of finding the particle near x
- $\left|\psi^* \frac{d\psi}{dx}\right| dx$ is related to the momentum probability density -
  - the probability of finding a particle with a particular momentum

PHYSICALLY MEANINGFUL STATES MUST HAVE THE FOLLOWING PROPERTIES:

ψ(x) must be single-valued, and finite
(finite to avoid infinite probability density)

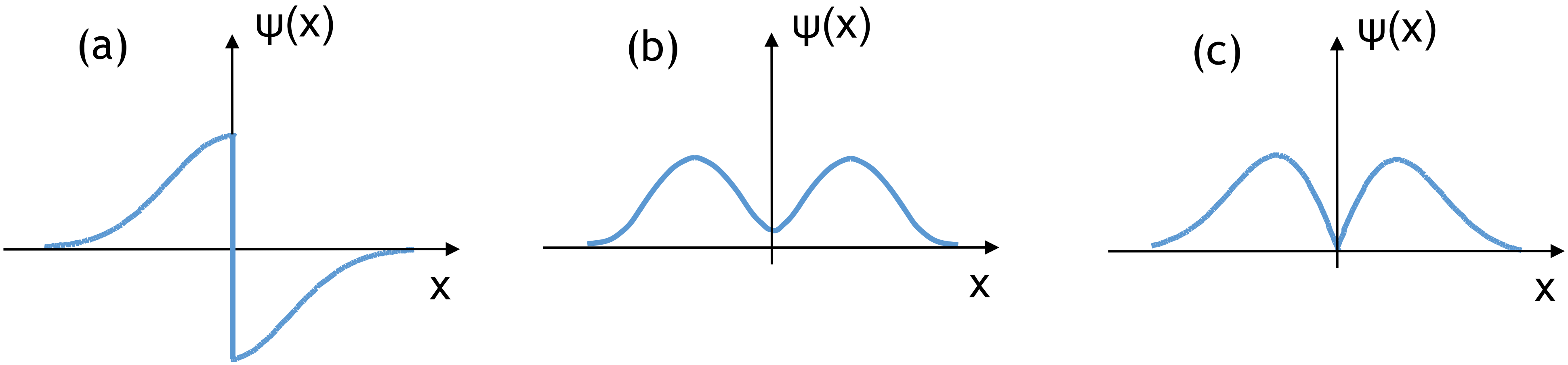
ψ(x) must be continuous, with finite dψ/dx
(because dψ/dx is related to the momentum density)

In regions with finite potential, dψ/dx must be continuous
(with finite $d^2\psi/dx^2$, to avoid infinite energies)

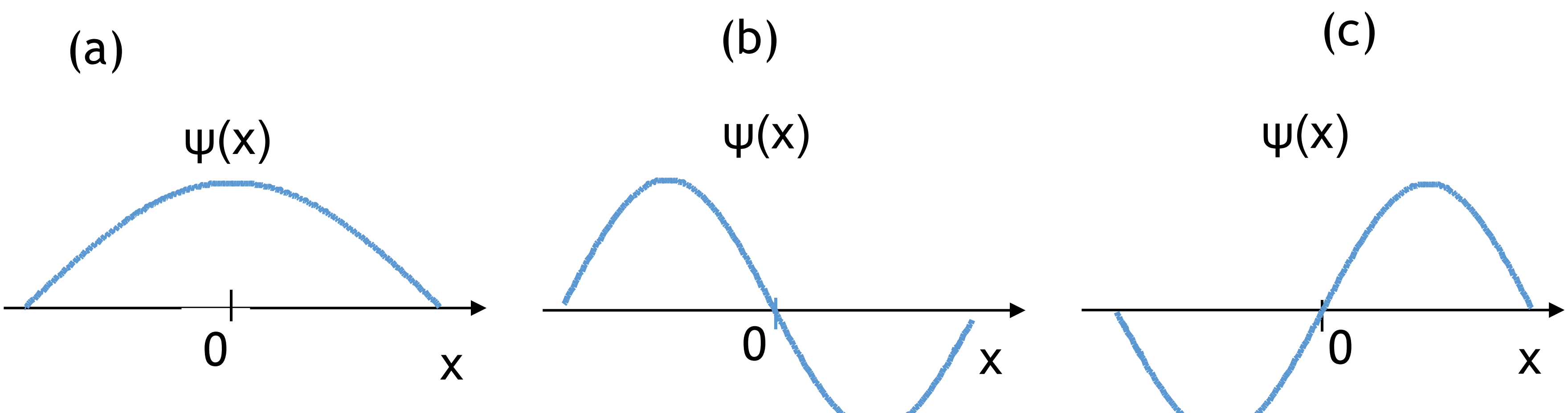
There is usually no significance to the overall *sign* of ψ(x)
(it goes away when we take the absolute square)
(In fact, ψ(x,t) is usually complex !)

Physically Meaningful Wavefunctions

1. Which of the following hypothetical wavefunctions is acceptable for a particle in some realistic potential V(x)?



2. Which of the following wavefunctions corresponds to a particle more likely to be found on the left side?



Schrodinger Equation and Energy Conservation

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

- Notice that if V(x) = constant, this equation has the simple form:

$$\frac{\partial^2\psi}{\partial x^2} = C\psi$$

where $C = \frac{2m}{\hbar^2}(V - E)$ is a constant that might be positive or negative.

For positive C, what is the form of the solution?

a) sin kx b) cos kx c) e^{ax} d) e^{-ax}

For negative C, what is the form of the solution?

a) sin kx b) cos kx c) e^{ax} d) e^{-ax}

Solutions to Schrodinger's Equation

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

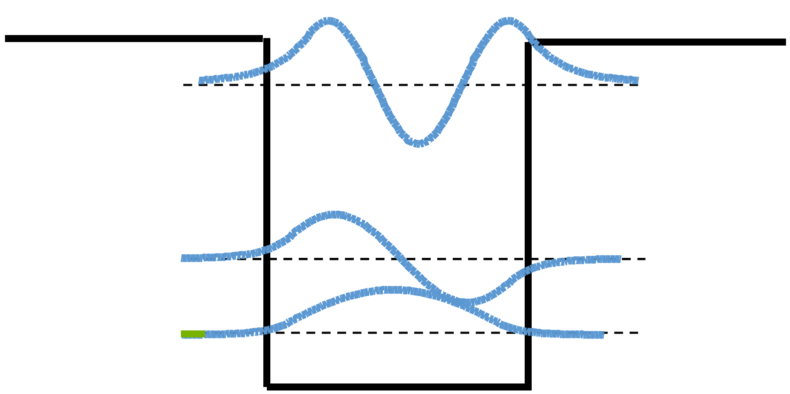
The kinetic energy of the electron is related to the curvature of the wavefunction

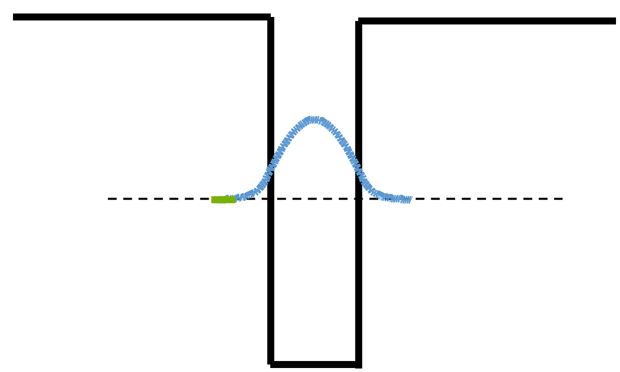
Tighter confinement → Higher energy

Even the lowest energy bound state requires some wavefunction curvature (kinetic energy) to satisfy boundary conditions..

Nodes in wavefunction → Higher energy

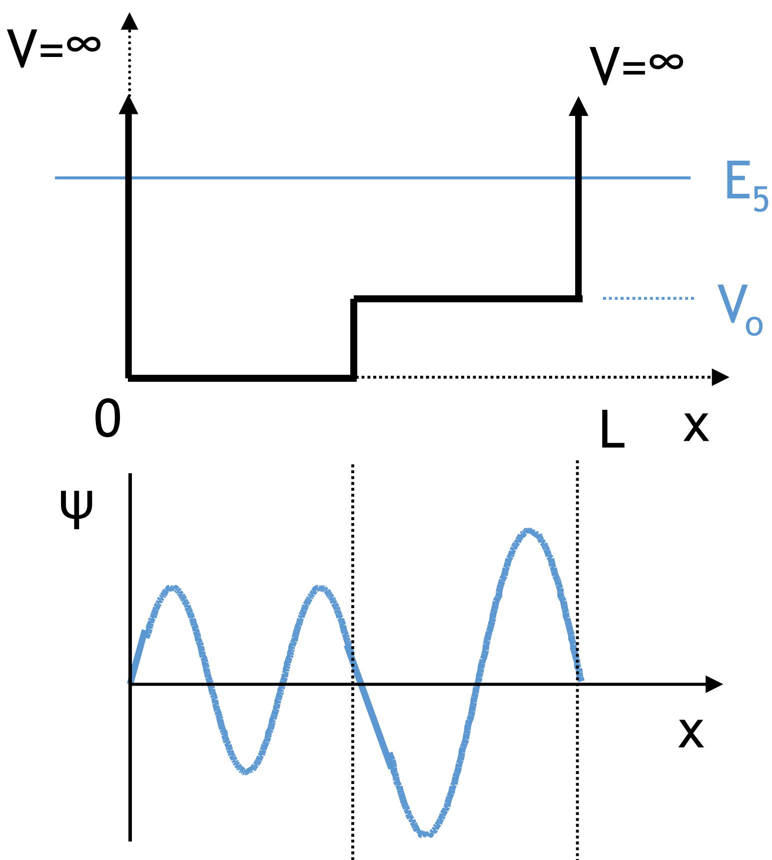
The n-th wavefunction (eigenstate) has (n-1) zero-crossings





Sketching Solutions to Schrodinger's Equation

- Estimate the wavefunction for an electron in the 5th energy level of this potential, without solving the Schrodinger Eq. Qualitatively sketch the 5th wavefunction:



Things to consider:

(1) 5th wavefunction has __ zero-crossings.

(2) Wavefunction must go to zero at <u>x = 0</u> and <u>x = L.</u>

(3) Kinetic energy is ______ on right side of well, so the curvature of ψ is _____ there (wavelength is longer).

(4) Because kinetic energy is ______ on right side of the well, the amplitude is _______ .

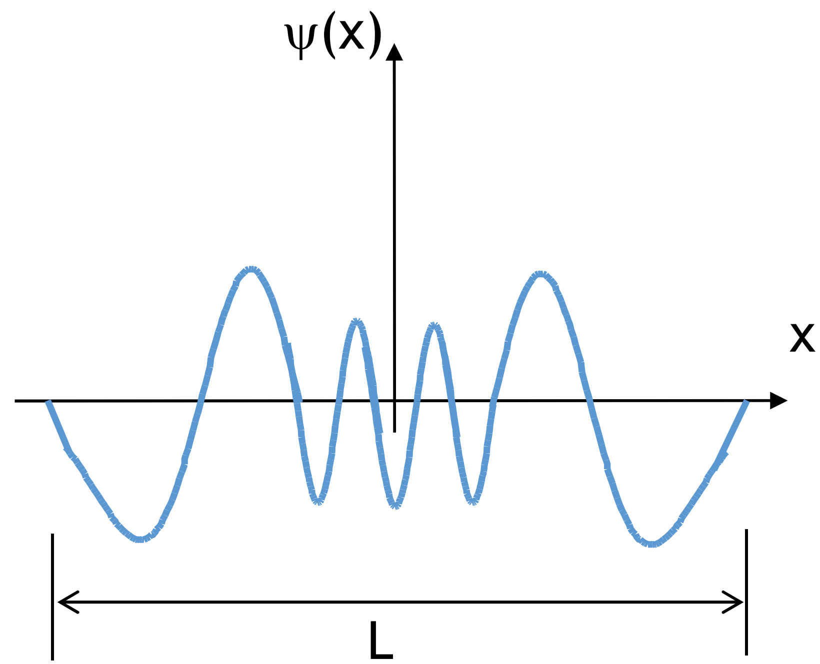
Solutions to Schrodinger's Equation

In what energy level is the particle? n = …

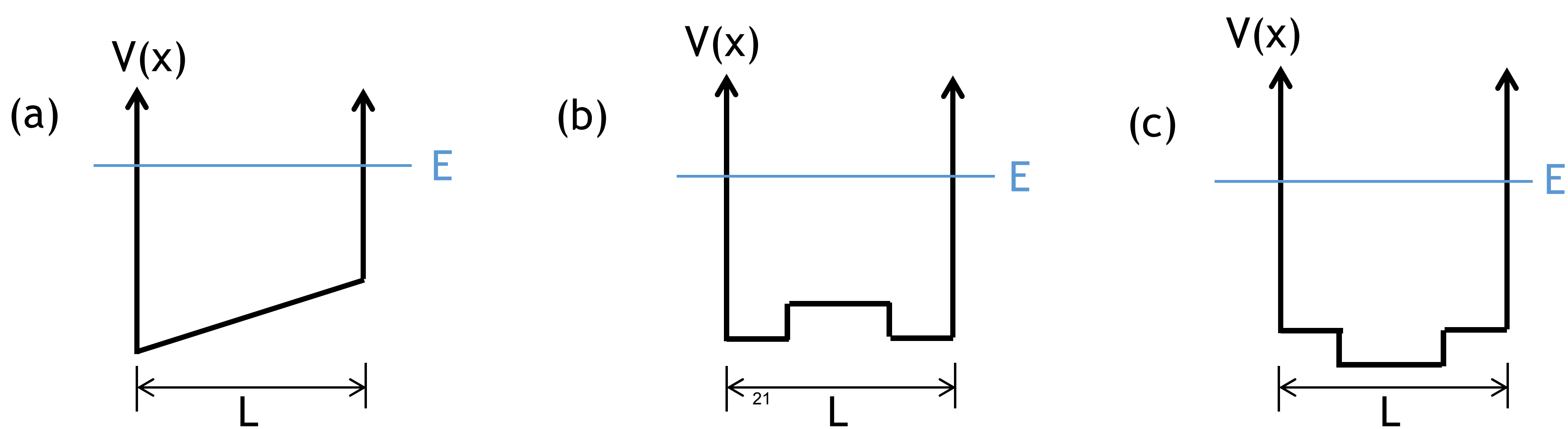
(a) 7

(b) 8

(c) 9

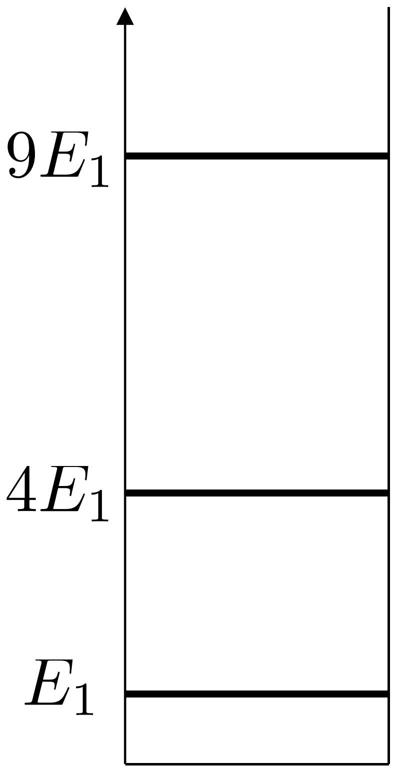


What is the approximate shape of the potential V(x) in which this particle is confined?

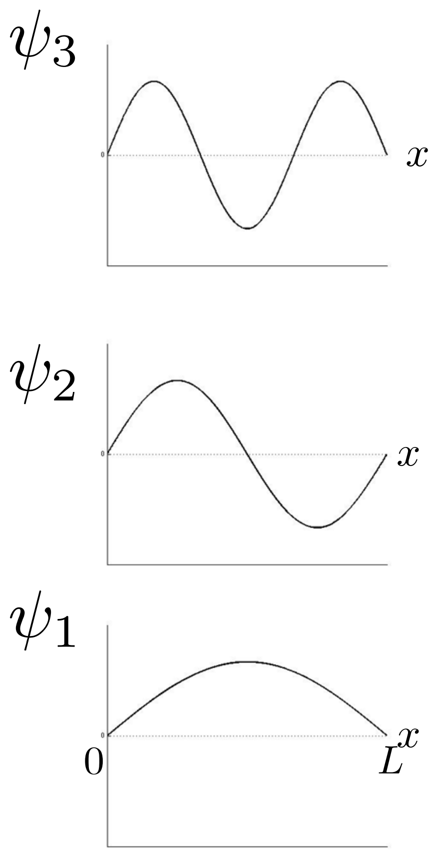


Key Takeaways

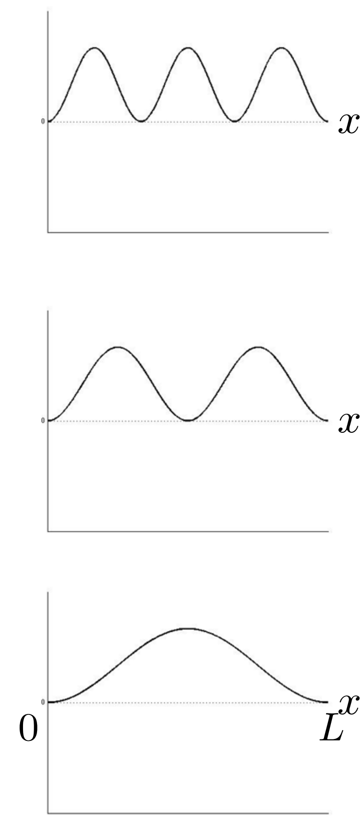
EIGENENERGIES for 1-D BOX



EIGENSTATES for 1-D BOX



PROBABILITY DENSITIES



$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

When drawing a wavefunction by inspection:

1. The wavefunction of the **n**th Energy level has **n**-1 zero crossings
2. Higher kinetic energy means higher curvature and lower amplitude.
3. Exponential decay occurs when the Kinetic energy is “smaller” than the Potential energy.

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