# PH 101: Physics I

Module 3: Introduction to Quantum Mechanics

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# Contents covered in QM

Necessity to have Quantum Mechanics: Photoelectric effect, Black body radiation, Compton effect, Line spectra, etc.

Old quantum mechanics: Bohr’s model.

Wave-particle duality: De Broglie hypothesis, Representation of the quantum particle as a wave packet, uncertainty relation.

Introduction and interpretation of the Schrödinger wave equation for quantum-mechanical (matter) waves.

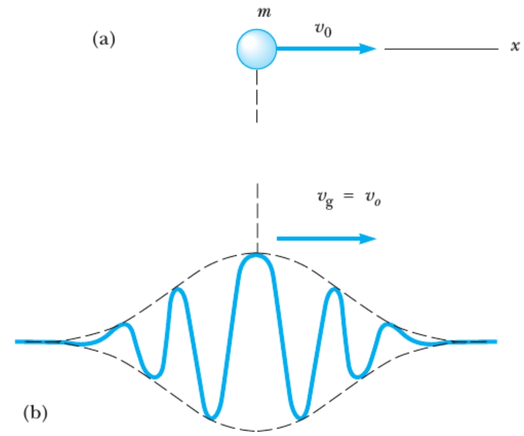
Solution of  the Schrödinger equation for a one-dimensional “particle in a box”.

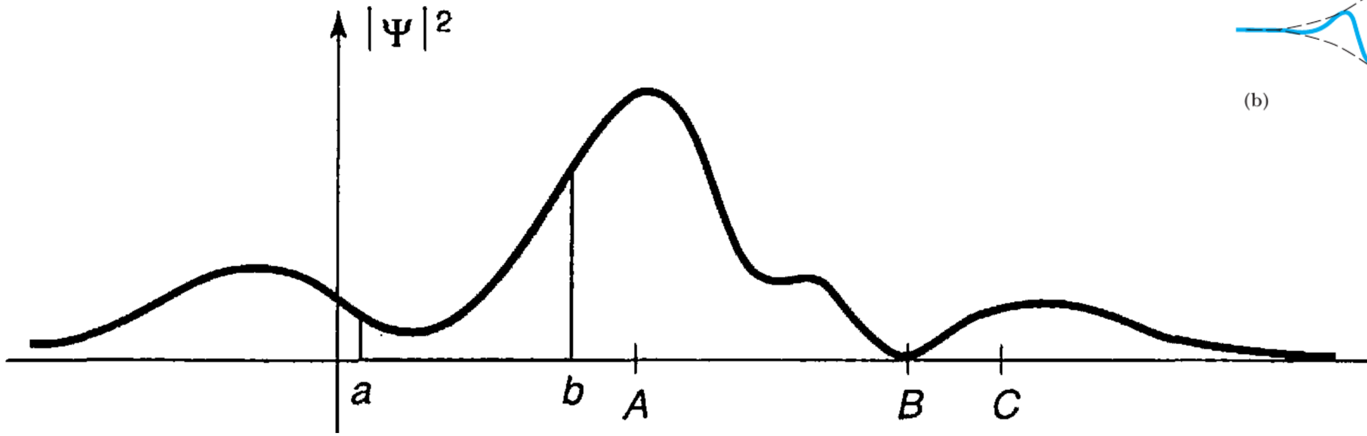
Behvaiour behavior of a quantum-mechanical particle in a finite potential well.

Identification of tunneling, in which quantum mechanics allows a particle to travel through a region that would be forbidden by Newtonian physics

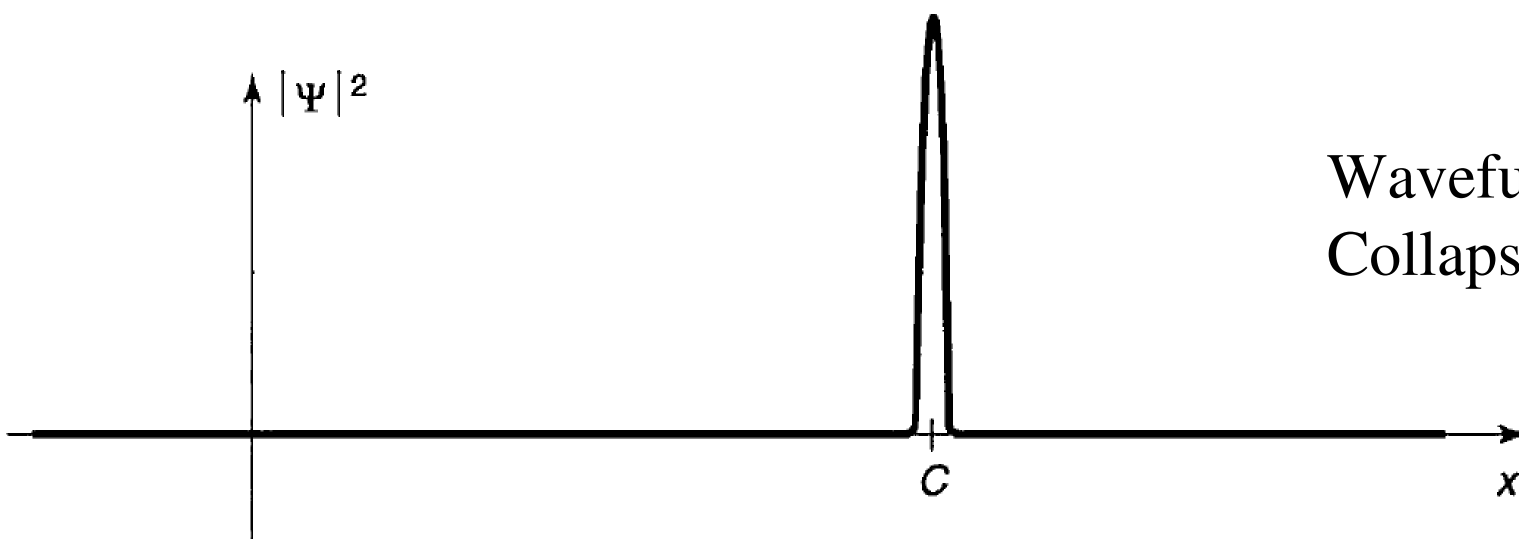
The quantum-mechanical harmonic oscillator, a model for molecular vibrations.

# Measurement in QM




Wavefunction




Wavefunction Collapse

# Uncertainty Principle

$$\Delta x \Delta k \geq 1/2$$

where $\Delta x$ and $\Delta k$ is the standard deviation in the $x$ and $k$ respectively and given by $\Delta x = \sqrt{< x^2 > - < x >^2}$ and $\Delta k = \sqrt{< k^2 > - < k >^2}$ where, $< . >$ represents the average (or expectation) value.

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} \qquad p = \frac{hk}{2\pi}$$

Hence an uncertainty $\Delta k$ in the wave number of the de Broglie waves associated with the particle results in an uncertainty $\Delta p$ in the particle's momentum according to the formula

$$\Delta p = \frac{h\,\Delta k}{2\pi}$$

Since $\Delta x\,\Delta k \geq \frac{1}{2}$, $\Delta k \geq 1/(2\Delta x)$ and

**Uncertainty principle**

$$\Delta x\,\Delta p \geq \frac{h}{4\pi}$$

It states that the product of the uncertainty $\Delta x$ in the position of an object at some instant and the uncertainty $\Delta p$ in its momentum component in the $x$ direction at the same instant is equal to or greater than $h/4\pi$.

Werner Heisenberg
German
1901-1976

It was in Copenhagen, in 1927, that Heisenberg developed his uncertainty principle, while working on the mathematical foundations of quantum mechanics.

## *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**

For Stationary state:

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

## *Time-Independent Schrodinger Wave Equation*

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

# Probability Current

Let $P_{ab}(t)$ be the probability of finding a particle in the range $(a < x < b)$, at time $t$

Then

$$\frac{dP_{ab}}{dt} = J(a, t) - J(b, t),$$

where

$$J(x, t) \equiv \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right).$$

$J$ is called the **probability current**.

# Measurement in QM

$$\langle j \rangle = \frac{\sum jN(j)}{N} = \sum_{j=0}^{\infty} jP(j)$$

$$\langle j^2 \rangle = \sum_{j=0}^{\infty} j^2 P(j)$$

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j)P(j)$$

$$\Delta j = j - \langle j \rangle$$

$$\begin{aligned}\langle \Delta j \rangle &= \sum (j - \langle j \rangle) P(j) = \sum jP(j) - \langle j \rangle \sum P(j) \\ &= \langle j \rangle - \langle j \rangle = 0.\end{aligned}$$

Define $\sigma^2 \equiv \langle (\Delta j)^2 \rangle$

$$\begin{aligned}\sigma^2 = \langle (\Delta j)^2 \rangle &= \sum (\Delta j)^2 P(j) = \sum (j - \langle j \rangle)^2 P(j) \\ &= \sum (j^2 - 2j\langle j \rangle + \langle j \rangle^2) P(j) \\ &= \sum j^2 P(j) - 2\langle j \rangle \sum jP(j) + \langle j \rangle^2 \sum P(j) \\ &= \langle j^2 \rangle - 2\langle j \rangle \langle j \rangle + \langle j \rangle^2 = \langle j^2 \rangle - \langle j \rangle^2.\end{aligned}$$

$$\boxed{\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}}$$

# Expectation value

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2\, dx.$$

$$\frac{d\langle x \rangle}{dt} = \int x \frac{\partial}{\partial t}|\Psi|^2\, dx = \frac{i\hbar}{2m}\int x \frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) dx$$

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi$$

Now the Schrödinger equation says that

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

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

so

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

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{2m}\int\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) dx$$

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m}\int \Psi^*\frac{\partial \Psi}{\partial x}\, dx.$$

# Expectation value

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = -i\hbar \int \left( \Psi^* \frac{\partial \Psi}{\partial x} \right) dx.$$

$$\boxed{\begin{gathered} \langle x \rangle = \int \Psi^*(x) \Psi \, dx, \\ \langle p \rangle = \int \Psi^* \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx \end{gathered}}$$

$$\boxed{\langle Q(x, p) \rangle = \int \Psi^* Q\left( x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx.}$$

Problem:

Calculate $d\langle p \rangle / dt$. *Answer*:

$$\frac{d\langle p \rangle}{dt} = \left\langle -\frac{\partial V}{\partial x} \right\rangle$$

This is called the Ehrenfest's theorem

# Measurement in QM

$$\int_a^b |\Psi(x,t)|^2\,dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between } a \text{ and } b\text{, at time } t. \end{array} \right\}$$

$$1 = \int_{-\infty}^{+\infty} \rho(x)\,dx,$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\rho(x)\,dx,$$

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\rho(x)\,dx$$

$$\sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

Example:

Consider the **gaussian** distribution

$$\rho(x) = Ae^{-\lambda(x-a)^2}$$

where $A$, $a$, and $\lambda$ are positive real constants.

(a) determine $A$.

(b) Find $\langle x \rangle$, $\langle x^2 \rangle$, and $\sigma$.

(c) Sketch the graph of $\rho(x)$.

# Solution

**(a)**

$$1 = \int_{-\infty}^{\infty} A e^{-\lambda(x-a)^2} dx. \qquad \text{Let } u \equiv x - a,\ du = dx,\ u : -\infty \to \infty.$$

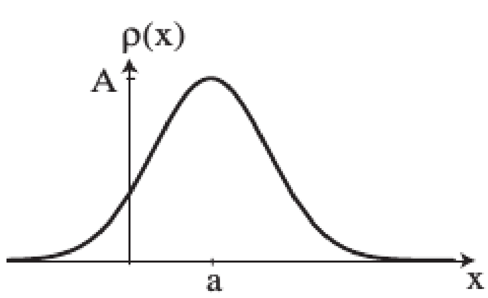
$$1 = A \int_{-\infty}^{\infty} e^{-\lambda u^2} du = A\sqrt{\frac{\pi}{\lambda}} \quad \Rightarrow \quad \boxed{A = \sqrt{\frac{\lambda}{\pi}}.}$$

**(b)**

$$\langle x \rangle = A \int_{-\infty}^{\infty} x e^{-\lambda(x-a)^2} dx = A \int_{-\infty}^{\infty} (u+a) e^{-\lambda u^2} du$$
$$= A\left[\int_{-\infty}^{\infty} u e^{-\lambda u^2} du + a \int_{-\infty}^{\infty} e^{-\lambda u^2} du\right] = A\left(0 + a\sqrt{\frac{\pi}{\lambda}}\right) = \boxed{a.}$$

$$\langle x^2 \rangle = A \int_{-\infty}^{\infty} x^2 e^{-\lambda(x-a)^2} dx$$
$$= A\left\{\int_{-\infty}^{\infty} u^2 e^{-\lambda u^2} du + 2a \int_{-\infty}^{\infty} u e^{-\lambda u^2} du + a^2 \int_{-\infty}^{\infty} e^{-\lambda u^2} du\right\}$$
$$= A\left[\frac{1}{2\lambda}\sqrt{\frac{\pi}{\lambda}} + 0 + a^2\sqrt{\frac{\pi}{\lambda}}\right] = \boxed{a^2 + \frac{1}{2\lambda}.}$$

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2 + \frac{1}{2\lambda} - a^2 = \frac{1}{2\lambda}; \qquad \boxed{\sigma = \frac{1}{\sqrt{2\lambda}}.}$$



# Normalization

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 \, dx = 1.$$

If a wave function is normalised at t=$t_0$, then it remains normalised at a later time.

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

# Example

Show that

$$\frac{d}{dt}\int_{-\infty}^{\infty} \Psi_1^* \Psi_2 \, dx = 0$$

for any two (normalizable) solutions to the Schrödinger equation, $\Psi_1$ and $\Psi_2$.

Solutions:

$$\begin{aligned}
\frac{d}{dt}\int_{-\infty}^{\infty} \Psi_1^*\Psi_2 \, dx &= \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\Psi_1^*\Psi_2\right) dx = \int_{-\infty}^{\infty} \left(\frac{\partial \Psi_1^*}{\partial t}\Psi_2 + \Psi_1^*\frac{\partial \Psi_2}{\partial t}\right) dx \\
&= \int_{-\infty}^{\infty} \left[\left(\frac{-i\hbar}{2m}\frac{\partial^2 \Psi_1^*}{\partial x^2} + \frac{i}{\hbar}V\Psi_1^*\right)\Psi_2 + \Psi_1^*\left(\frac{i\hbar}{2m}\frac{\partial^2 \Psi_2}{\partial x^2} - \frac{i}{\hbar}V\Psi_2\right)\right] dx \\
&= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty} \left(\frac{\partial^2 \Psi_1^*}{\partial x^2}\Psi_2 - \Psi_1^*\frac{\partial^2 \Psi_2}{\partial x^2}\right) dx \\
&= -\frac{i\hbar}{2m}\left[\frac{\partial \Psi_1^*}{\partial x}\Psi_2\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi_1^*}{\partial x}\frac{\partial \Psi_2}{\partial x}\, dx - \Psi_1^*\frac{\partial \Psi_2}{\partial x}\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial \Psi_1^*}{\partial x}\frac{\partial \Psi_2}{\partial x}\, dx\right] = 0.
\end{aligned}$$

# Example

At time $t = 0$ a particle is represented by the wave function

$$\Psi(x, 0) = \begin{cases} A\dfrac{x}{a}, & \text{if } 0 \le x \le a, \\ A\dfrac{(b-x)}{(b-a)}, & \text{if } a \le x \le b, \\ 0, & \text{otherwise,} \end{cases}$$

where $A$, $a$, and $b$ are constants.

(a) Normalize $\Psi$ (that is, find $A$, in terms of $a$ and $b$).

(b) Sketch $\Psi(x, 0)$, as a function of $x$.

(c) Where is the particle most likely to be found, at $t = 0$?

(d) What is the probability of finding the particle to the left of $a$? Check your result in the limiting cases $b = a$ and $b = 2a$.

(e) What is the expectation value of $x$?

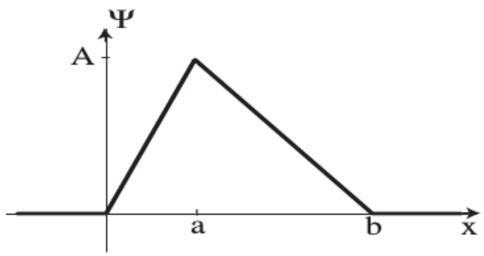
# Solution

**(a)**

$$1 = \frac{|A|^2}{a^2}\int_0^a x^2 dx + \frac{|A|^2}{(b-a)^2}\int_a^b (b-x)^2 dx = |A|^2\left\{\frac{1}{a^2}\left(\frac{x^3}{3}\right)\Big|_0^a + \frac{1}{(b-a)^2}\left(-\frac{(b-x)^3}{3}\right)\Big|_a^b\right\}$$

$$= |A|^2\left[\frac{a}{3}+\frac{b-a}{3}\right] = |A|^2\frac{b}{3} \;\Rightarrow\; \boxed{A = \sqrt{\frac{3}{b}}.}$$

**(b)**




**(c)** At $\boxed{x = a.}$

**(d)**

$$P = \int_0^a |\Psi|^2 dx = \frac{|A|^2}{a^2}\int_0^a x^2 dx = |A|^2\frac{a}{3} = \boxed{\frac{a}{b}.}\begin{cases} P = 1 & \text{if } b = a, \checkmark \\ P = 1/2 & \text{if } b = 2a. \checkmark \end{cases}$$

**(e)**

$$\langle x\rangle = \int x|\Psi|^2 dx = |A|^2\left\{\frac{1}{a^2}\int_0^a x^3 dx + \frac{1}{(b-a)^2}\int_a^b x(b-x)^2 dx\right\}$$

$$= \frac{3}{b}\left\{\frac{1}{a^2}\left(\frac{x^4}{4}\right)\Big|_0^a + \frac{1}{(b-a)^2}\left(b^2\frac{x^2}{2} - 2b\frac{x^3}{3} + \frac{x^4}{4}\right)\Big|_a^b\right\}$$

$$= \frac{3}{4b(b-a)^2}\left[a^2(b-a)^2 + 2b^4 - 8b^4/3 + b^4 - 2a^2b^2 + 8a^3b/3 - a^4\right]$$

$$= \frac{3}{4b(b-a)^2}\left(\frac{b^4}{3} - a^2b^2 + \frac{2}{3}a^3b\right) = \frac{1}{4(b-a)^2}(b^3 - 3a^2b + 2a^3) = \boxed{\frac{2a+b}{4}.}$$

## *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**

For Stationary state:

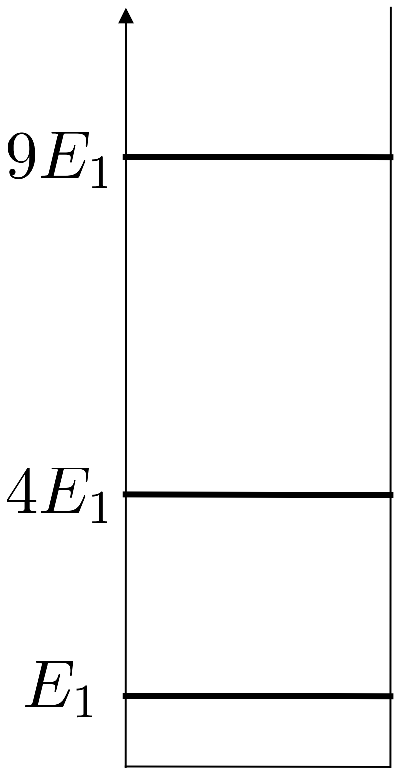
$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$$

## *Time-Independent Schrodinger Wave Equation*

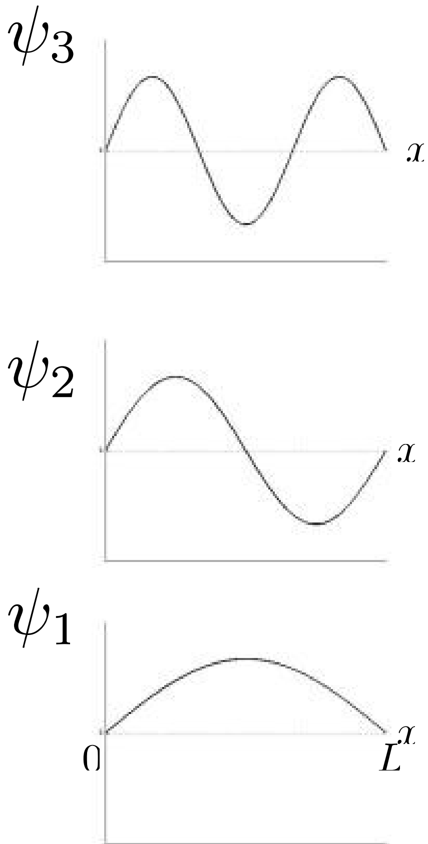
$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)$$

# Particle in a box

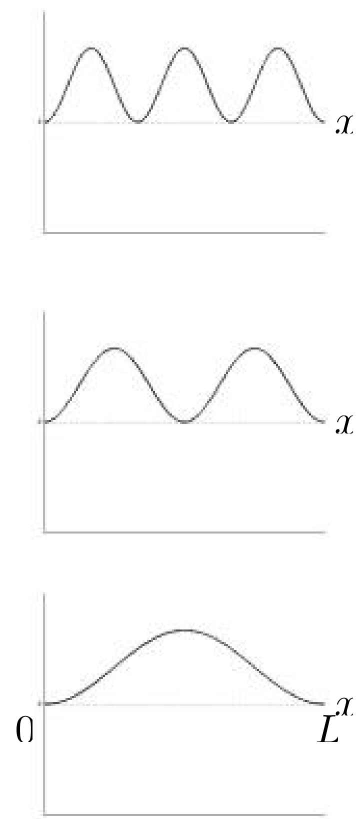
EIGENENERGIES for 1-D BOX




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.

# Orthonormality

Orthonormality Condtion:

$$\int \psi_m(x)^* \psi_n(x)\, dx = \delta_{mn}.$$

$$\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n; \\ 1, & \text{if } m = n. \end{cases}$$

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

$$1 = \int |\Psi(x,0)|^2\, dx = \int \left( \sum_{m=1}^{\infty} c_m \psi_m(x) \right)^* \left( \sum_{n=1}^{\infty} c_n \psi_n(x) \right) dx$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n \int \psi_m(x)^* \psi_n(x)\, dx$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_m^* c_n \delta_{mn} = \sum_{n=1}^{\infty} |c_n|^2.$$

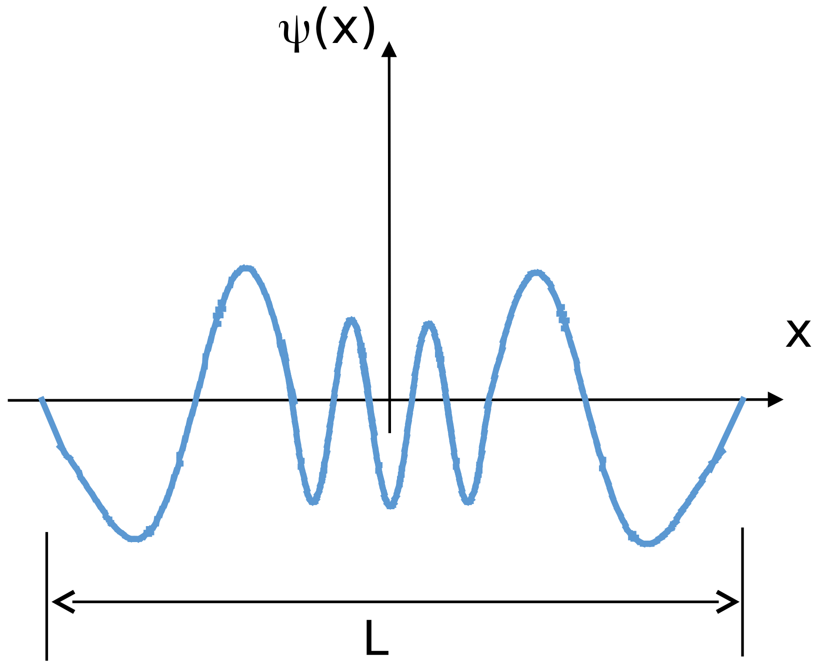
# *Solutions to Schrodinger's Equation*

In what energy level is the particle?  n = …

(a)  7

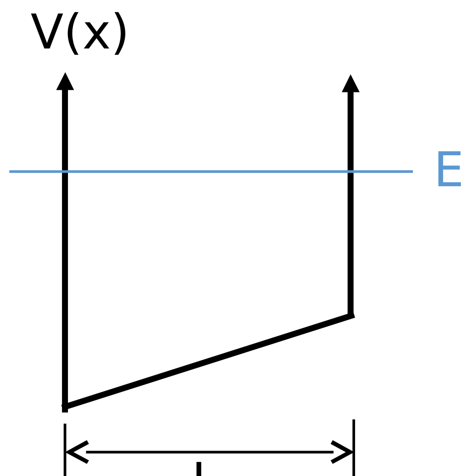
(b)  8

(c)  9

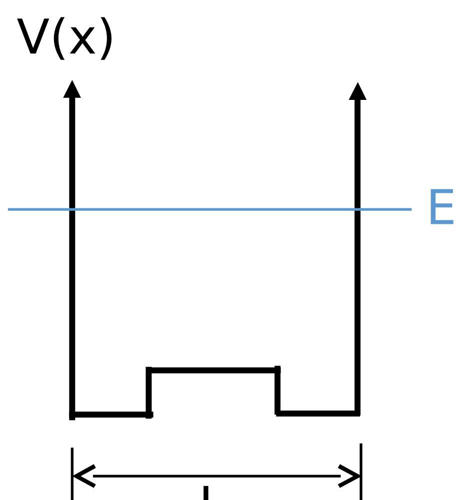



What is the approximate shape of the potential V(x) in which this particle is confined?

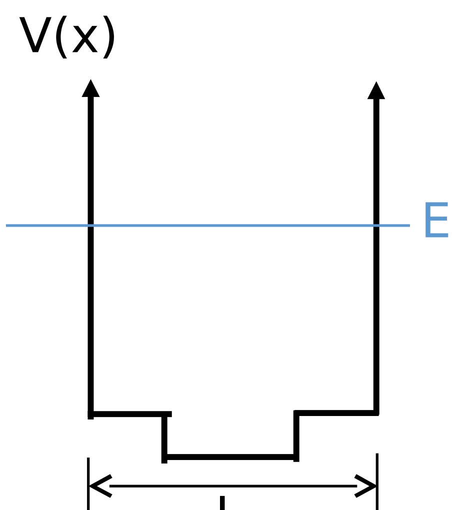
(a)




(b)




(c)



# Finite potential well Solutions to Schrodinger's Equation

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

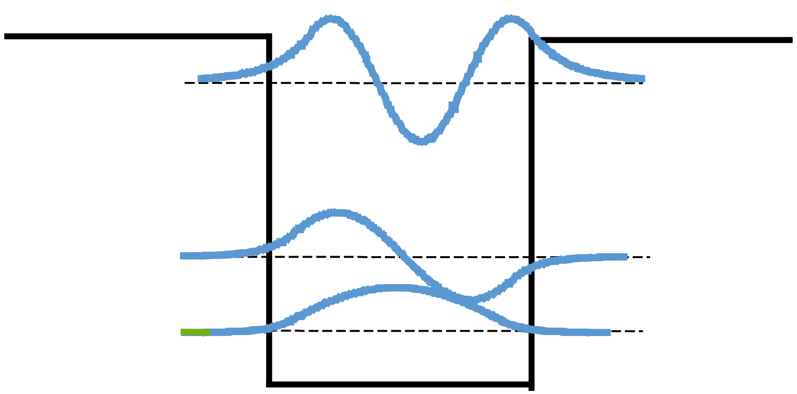
The kinetic energy of the electron is related to the curvature of the wavefunction

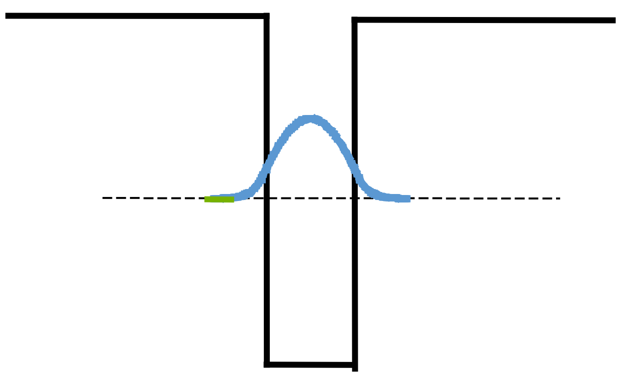
Tighter confinement $\Rightarrow$ Higher energy

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

Nodes in wavefunction $\Rightarrow$ Higher energy

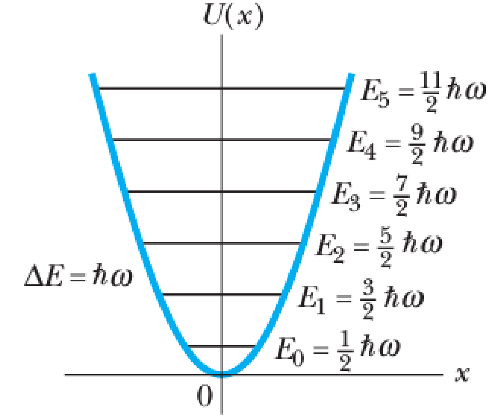
*The n-th wavefunction (eigenstate) has (n-1) zero-crossings*





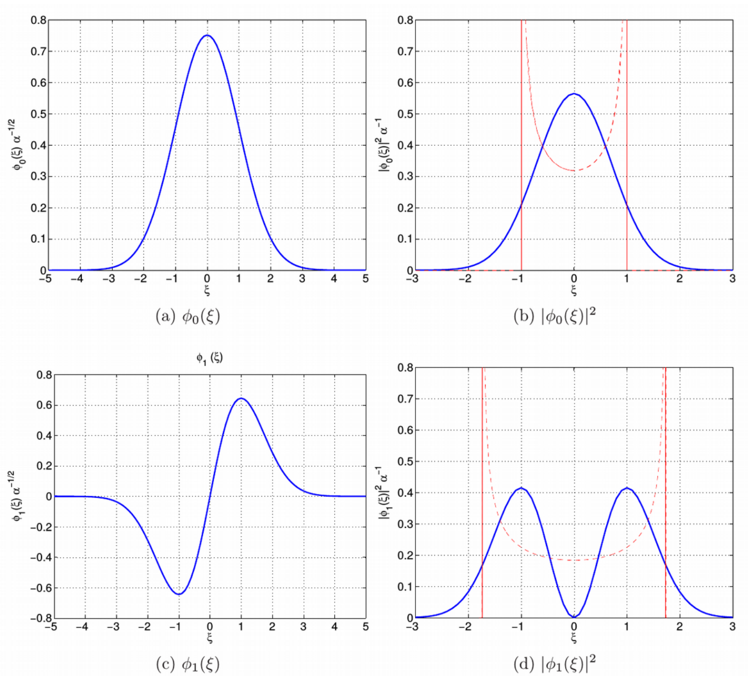
# Harmonic Oscillator

| $n$ | $\frac{2E_n}{\hbar\omega}$ | $\phi(x;n)e^{+\frac{x^2}{2a^2}}$ |
|---|---|---|
| 0 | 1 | $N_0$ |
| 1 | 3 | $N_1 \cdot \left(\frac{2x}{a}\right)$ |
| 2 | 5 | $N_2 \cdot \left(\frac{4x^2}{a^2} - 2\right)$ |
| $\vdots$ | $\vdots$ | $\vdots$ |
| $n$ | $2n+1$ | $N_n \mathcal{H}_n\left(\frac{x}{a}\right)$ |



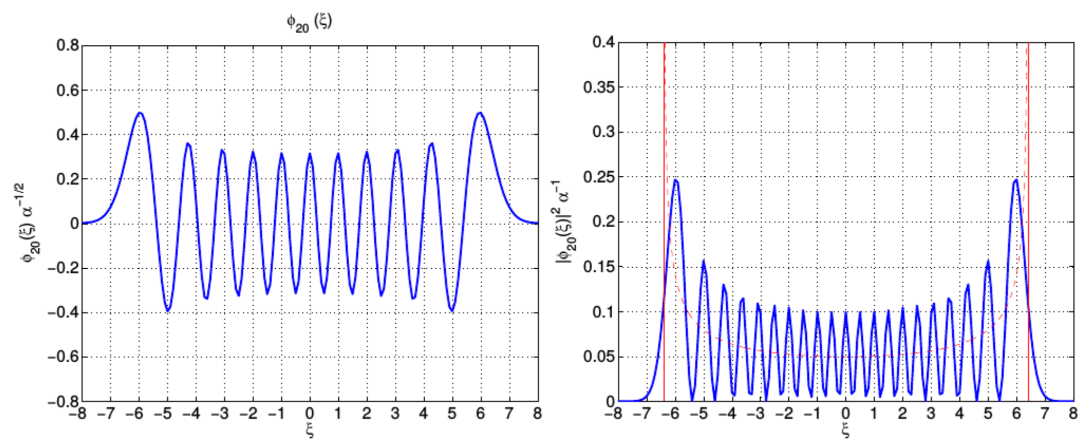

$$E_n = \hbar\left(n + \frac{1}{2}\right)\omega.$$

$$N_n = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} (2^n n!)^{-\frac{1}{2}}$$




(a) $\phi_0(\xi)$ (b) $|\phi_0(\xi)|^2$

(c) $\phi_1(\xi)$ (d) $|\phi_1(\xi)|^2$




(e) $\phi_{20}(\xi)$ (f) $|\phi_{20}(\xi)|^2$

# Expectation value of H

In Hilbert space a general function has the expansion in terms of the basis functions,

$$\psi(x) = c_1\,\varphi_1(x) + c_2\,\varphi_2(x) + \ldots\ldots \qquad [1]$$

and the coefficients are similarly given as,

$$c_j \equiv <\varphi_j|\psi> = \int_{-\infty}^{\infty} \varphi_j^*(x)\psi(x)\, dx$$

$$\langle H \rangle = \sum_{n=1} |c_n|^2 E_n$$

$$\langle H \rangle = \int \Psi^* H \Psi\, dx = \int \left(\sum c_m \psi_m\right)^* H \left(\sum c_n \psi_n\right) dx$$

$$= \sum\sum c_m^* c_n E_n \int \psi_m^* \psi_n\, dx = \sum |c_n|^2 E_n.$$

# Example

A particle in the harmonic oscillator potential starts out in the state

$$\Psi(x, 0) = A[3\psi_0(x) + 4\psi_1(x)].$$

(a) Find $A$.

(b) Construct $\Psi(x, t)$ and $|\Psi(x, t)|^2$.

## Solution

(a)

$$\begin{aligned} 1 &= \int |\Psi(x,0)|^2 dx = |A|^2 \int \left(9|\psi_0|^2 + 12\psi_0^*\psi_1 + 12\psi_1^*\psi_0 + 16|\psi_1|^2\right) dx \\ &= |A|^2(9+0+0+16) = 25|A|^2 \Rightarrow \boxed{A = 1/5.} \end{aligned}$$

$$\Psi(x,t) = \frac{1}{5}\left[3\psi_0(x)e^{-iE_0t/\hbar} + 4\psi_1(x)e^{-iE_1t/\hbar}\right] = \boxed{\frac{1}{5}\left[3\psi_0(x)e^{-i\omega t/2} + 4\psi_1(x)e^{-3i\omega t/2}\right].}$$

$$\begin{aligned} |\Psi(x,t)|^2 &= \frac{1}{25}\left[9\psi_0^2 + 12\psi_0\psi_1 e^{i\omega t/2}e^{-3i\omega t/2} + 12\psi_0\psi_1 e^{-i\omega t/2}e^{3i\omega t/2} + 16\psi_1^2\right] \\ &= \boxed{\frac{1}{25}\left[9\psi_0^2 + 16\psi_1^2 + 24\psi_0\psi_1\cos(\omega t)\right].} \end{aligned}$$