PHYS-3301

Lecture 10

Sep. 26, 2024

Chapter. 5
Bound States: Simple Case

Outline:

- The Schrödinger Equation (for interacting particles)
- Stationary States
- Physics Conditions: Well-Behaved Functions
- A Review of Classical Bound States
- Case 1: Particles in a Box – The Infinite Well
- Case 2: The Finite Well
- Case 3: The Simple Harmonic Oscillator
- Expectation Values, Uncertainties, and Operators

Chapter. 5
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- Case 1: Particles in a Box – The Infinite Well
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5.5 Case. I
Particle in a Box: The Infinite Well

The situation in which the particle-confining U(x) allows the simplest solution of the time-independent Schrödinger equation is called "particle in a box", or "infinite well"

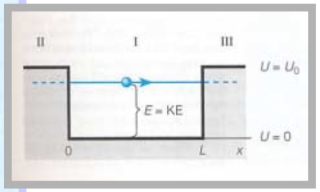
CM: simply bounce back & forth

QM: standing waves ← Schrödinger Eq.

Finite Potential Well:

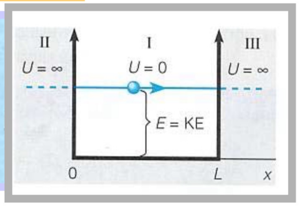
$$\psi(x) = \begin{cases} Ce^{+\alpha x} & x < 0 \\ A \sin kx + B \cos kx & 0 < x < L \\ Ge^{-\alpha x} & x > L \end{cases}$$

where $k \sqrt{\frac{2mE}{\hbar^2}}$ and $\alpha \equiv \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$



Infinite Potential Well:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & 0 < x < L \\ 0 & x < 0,\ x > L \end{cases}$$



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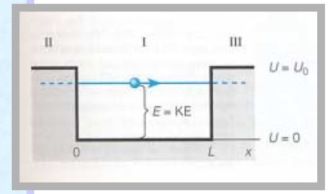
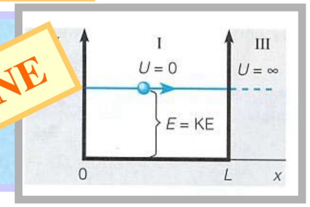
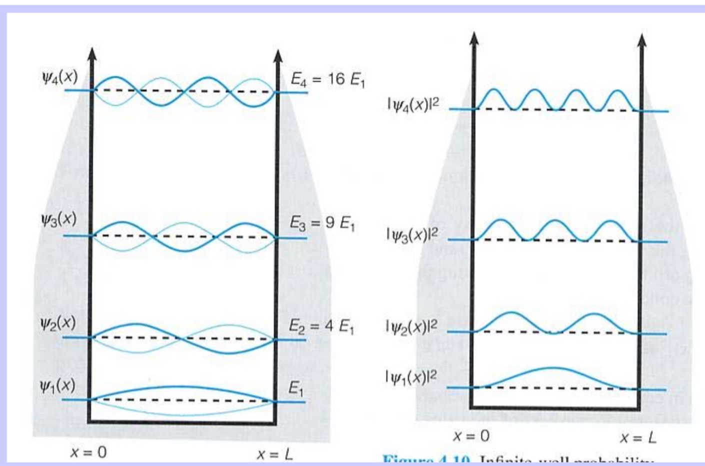


Infinite Potential Well:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & 0 < x < L \\ 0 & x < 0,\ x > L \end{cases}$$

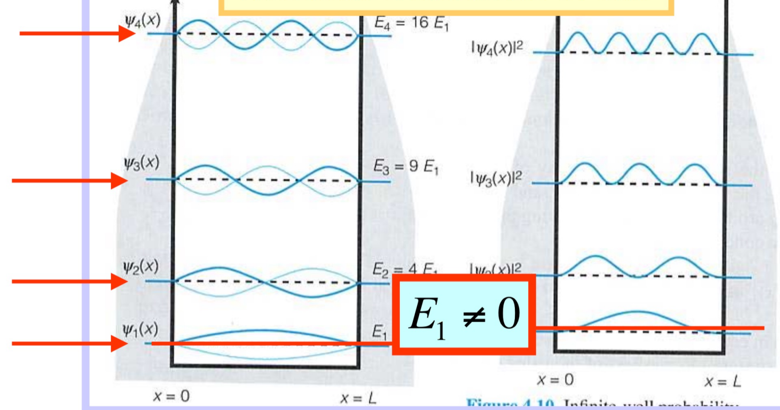
DONE





$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & 0 < x < L \\ 0 & x < 0,\ x > L \end{cases} \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

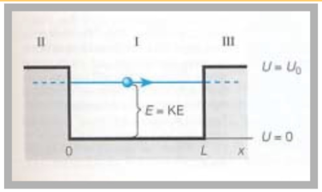
Infinite Potential Well:



$E_1 \neq 0$

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} & 0 < x < L \\ 0 & x < 0,\ x > L \end{cases} \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Case 2: The Finite Potential Well

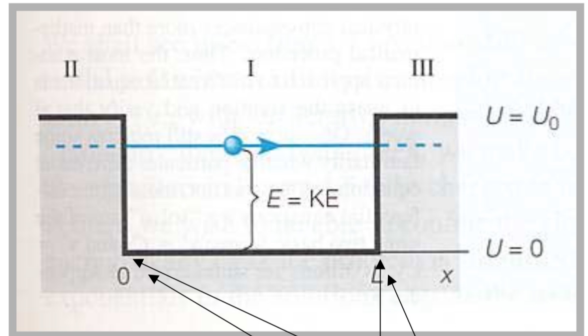


$$\psi(x) = \begin{cases} Ce^{+\alpha x} & x < 0 \\ A \sin kx + B \cos kx & 0 < x < L \\ Ge^{-\alpha x} & x > L \end{cases}$$

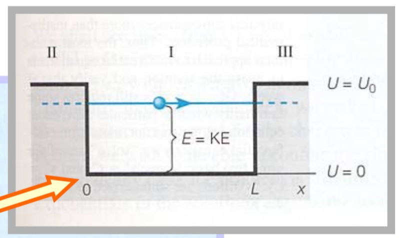
where $k \sqrt{\frac{2mE}{\hbar^2}}$ and $\alpha \equiv \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$

$$A, B, C, G, E_n = ?$$

Requirement:



1. Continuity of $\psi(x,t)$
2. Continuity of $(d\psi(x)/dx)$



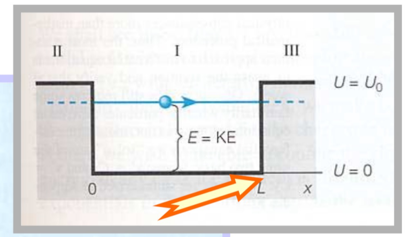
$$\psi(x) = \begin{cases} Ce^{+\alpha x} \\ A \sin kx + B \cos kx \\ Ge^{-\alpha x} \end{cases}$$

$\psi(x)$ continuous at $x = 0$: $\psi_{II}(0) = \psi_I(0)$

$$Ce^{+\alpha 0} = A \sin k0 + B \cos k0 \quad \Rightarrow \quad C = B$$

$\frac{\partial \psi(x)}{\partial x}$ continuous at $x = 0$: $\left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_I}{\partial x}\right|_{x=0}$

$$\alpha Ce^{+\alpha 0} = kA \cos k0 - kB \sin k0 \quad \Rightarrow \quad \alpha C = kA$$



$$\psi(x) = \begin{cases} Ce^{+\alpha x} \\ A \sin kx + B \cos kx \\ Ge^{-\alpha x} \end{cases}$$

$\psi(x)$ continuous at $x = L$: $\psi_I(L) = \psi_{III}(L)$

$$A \sin kL + B \cos kL = Ge^{-\alpha L}$$

$\frac{\partial \psi(x)}{\partial x}$ continuous at $x = L$: $\left.\frac{\partial \psi_I}{\partial x}\right|_{x=L} = \left.\frac{\partial \psi_{III}}{\partial x}\right|_{x=L}$

$$kA \cos kL - kB \sin kL = -\alpha Ge^{-\alpha L}$$

$\psi(x)$ **continuous at** $x = 0$: $\psi_{II}(0) = \psi_I(0)$

$$Ce^{+\alpha 0} = A \sin k0 + B \cos k0 \quad \Rightarrow \quad C = B$$

$\dfrac{\partial \psi(x)}{\partial x}$ **continuous at** $x = 0$: $\left.\dfrac{\partial \psi_{II}}{\partial x}\right|_{x=0} = \left.\dfrac{\partial \psi_I}{\partial x}\right|_{x=0}$

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continuity at x = 0

$\psi(x)$ **continuous at** $x = L$: $\psi_I(L) = \psi_{III}(L)$

$$A \sin kL + B \cos kL = Ge^{-\alpha L}$$

$\dfrac{\partial \psi(x)}{\partial x}$ **continuous at** $x = L$: $\left.\dfrac{\partial \psi_I}{\partial x}\right|_{x=L} = \left.\dfrac{\partial \psi_{III}}{\partial x}\right|_{x=L}$

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continuity at x = L

$\psi(x)$ **continuous at** $x = 0$: $\psi_{II}(0) = \psi_I(0)$

$$Ce^{+\alpha 0} = A \sin k0 + B \cos k0 \quad \Rightarrow \quad C = B$$

$\dfrac{\partial \psi(x)}{\partial x}$ **continuous at** $x = 0$: $\left.\dfrac{\partial \psi_{II}}{\partial x}\right|_{x=0} = \left.\dfrac{\partial \psi_I}{\partial x}\right|_{x=0}$

$$\alpha Ce^{+\alpha 0} = kA \cos k0 - kB \sin k0 \quad \Rightarrow \quad \alpha C = kA$$

continuity at x = 0

$$A = \frac{\alpha C}{k}, B = C$$

$\psi(x)$ **continuous at** $x = L$: $\psi_I(L) = \psi_{III}(L)$

$$A \sin kL + B \cos kL = Ge^{-\alpha L}$$

$\dfrac{\partial \psi(x)}{\partial x}$ **continuous at** $x = L$: $\left.\dfrac{\partial \psi_I}{\partial x}\right|_{x=L} = \left.\dfrac{\partial \psi_{III}}{\partial x}\right|_{x=L}$

$$kA \cos kL - kB \sin kL = -\alpha Ge^{-\alpha L}$$

continuity at x = L

$$\frac{\alpha}{k} C \sin kL + C \cos kL = Ge^{-\alpha L}$$

$$k\frac{\alpha}{k} C \cos kL - kC \sin kL = -\alpha Ge^{-\alpha L} \qquad /(-\alpha)$$

$$\frac{\alpha}{k} \cancel{C} \sin kL + \cancel{C} \cos kL = -\cancel{C} \cos kL + \frac{k}{\alpha} \cancel{C} \sin kL$$

$$2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k}$$

$$\frac{\alpha}{k} C \sin kL + C \cos kL = Ge^{-\alpha L}$$

$$k\frac{\alpha}{k} C \cos kL - kC \sin kL = -\alpha Ge^{-\alpha L} \qquad /(-\alpha)$$

$$\frac{\alpha}{k} \cancel{C} \sin kL + \cancel{C} \cos kL = -\cancel{C} \cos kL + \frac{k}{\alpha} \cancel{C} \sin kL$$

$$2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k}$$

Transcendental Equation –

impossible to solve *analytically*

Transcendental Equation –

impossible to solve analytically, but "NUMERICAL" Solution is possible

(e.g. "graphing solution")

$$2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k}$$

Graphing solution

$$2 \cot kL = \frac{k}{\alpha} - \frac{\alpha}{k}$$

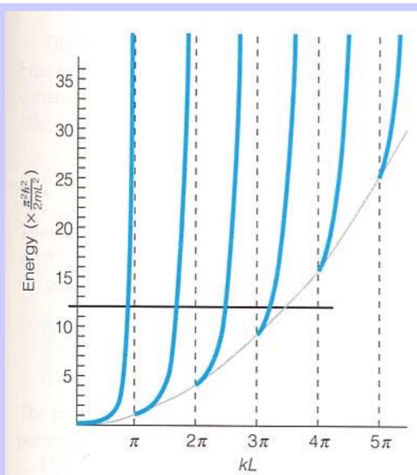
$$\alpha = \begin{cases} k \tan \frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ -k \cot \frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$

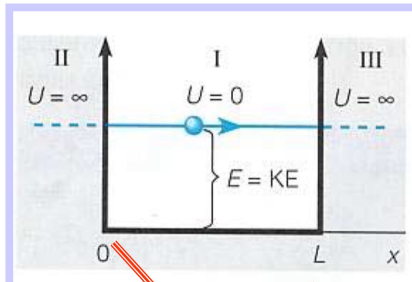
$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m} \sec^2 \frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ \frac{\hbar^2 k^2}{2m} \csc^2 \frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$

Graphing solution

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m} \sec^2 \frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ \frac{\hbar^2 k^2}{2m} \csc^2 \frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$





$$\psi(x) = \begin{cases} A \sin kx + B \cos kx & 0 < x < L \\ 0 & x < 0,\ x > L \end{cases}$$

$\psi_{I}(L) = \psi_{III}(L)$

or

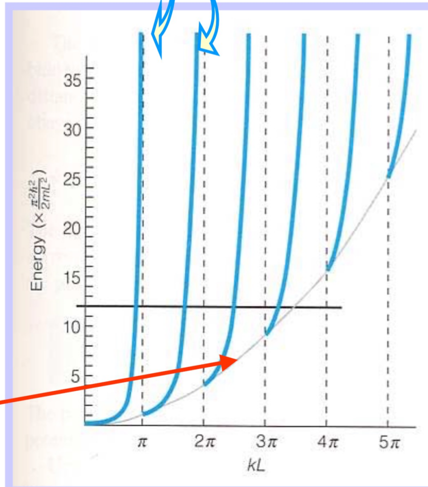
$A \sin kL = 0$

$$kL = n\pi$$

Graphing solution

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m}\sec^2\frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ \frac{\hbar^2 k^2}{2m}\csc^2\frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$

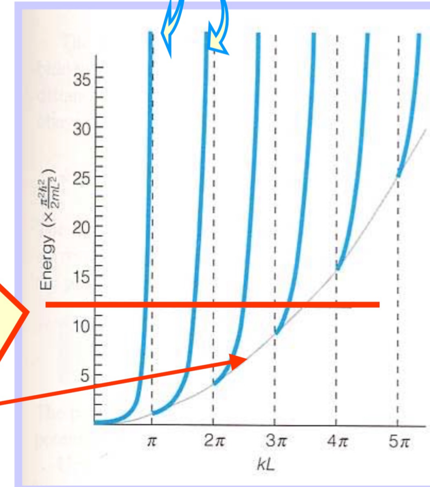


$kL = n\pi$

Parabola ~ k^2

Graphing solution

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m}\sec^2\frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ \frac{\hbar^2 k^2}{2m}\csc^2\frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$



Parabola ~ k^2

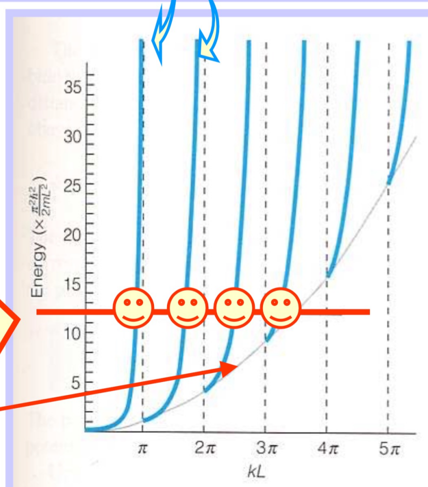
Graphing solution

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m}\sec^2\frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ \frac{\hbar^2 k^2}{2m}\csc^2\frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$

Solutions

☺

left=right



Parabola ~ k^2

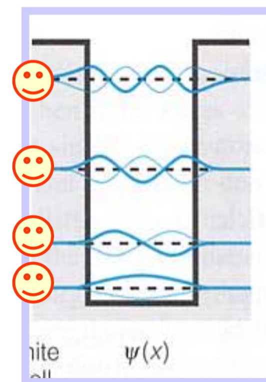
Graphing solution

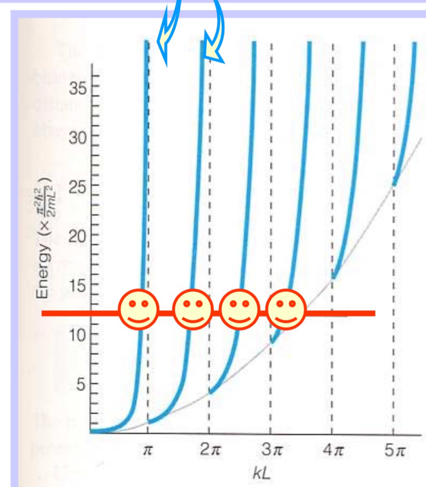
Solutions

☺

left=right

$$U_0 = \begin{cases} \frac{\hbar^2 k^2}{2m}\sec^2\frac{1}{2}kL & 2n\pi < kL < 2n\pi + \pi \\ \frac{\hbar^2 k^2}{2m}\csc^2\frac{1}{2}kL & 2n\pi - \pi < kL < 2n\pi \end{cases}$$





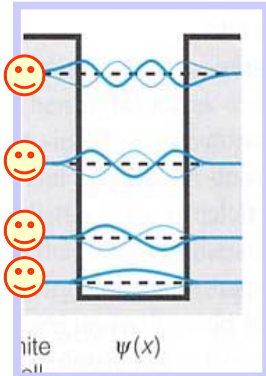
Graphing solution

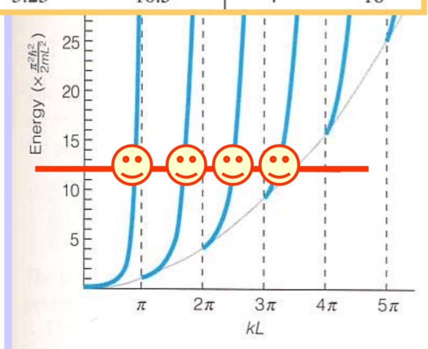
Solutions

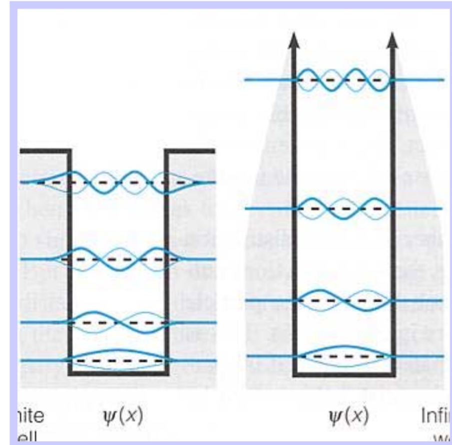
☺

left=right

n	Finite Well $U_0 = 12\frac{\pi^2\hbar^2}{2mL^2}$ k^*	$E^\dagger$	Infinite Well $U_0 = \infty$ k^*	$E^\dagger$
1	0.84	0.71	1	1
2	1.68	2.82	2	4
3	2.49	6.20	3	9
4	3.23	10.5	4	16

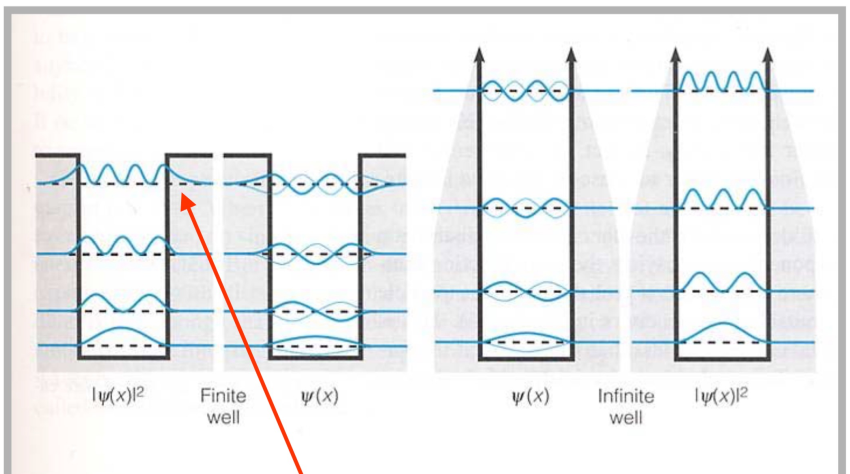






Finite Potential Well

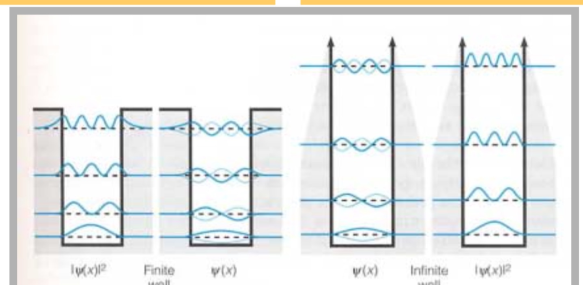
Infinite Potential Well:



Finite probability - *penetration*

Finite Potential Well

Infinite Potential Well:



n	Finite Well $U_0 = 12\frac{\pi^2\hbar^2}{2mL^2}$ k^*	$E^\dagger$	Infinite Well $U_0 = \infty$ k^*	$E^\dagger$
1	0.84	0.71	1	1
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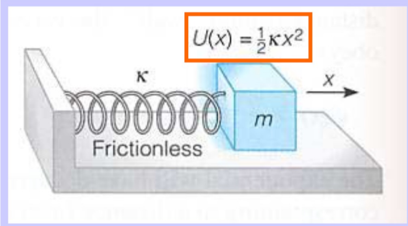
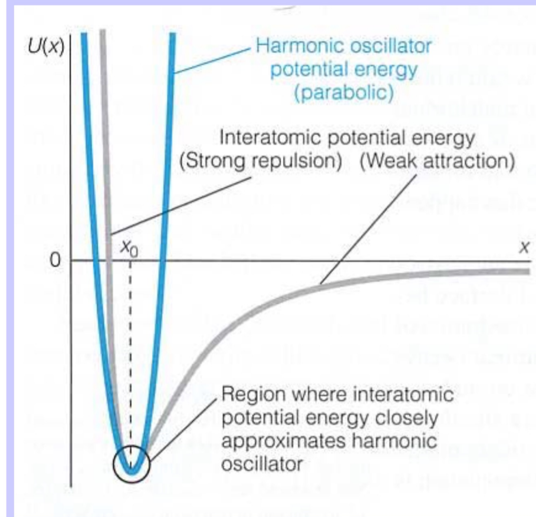
Case 3: The Simple Harmonic Oscillator



$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}\kappa x^2\psi(x) = E\psi(x)$$

The Importance of the Harmonic Oscillator



$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}\kappa x^2\psi(x) = E\psi(x)$$

Solutions

$[b \equiv (m\kappa/\hbar^2)^{1/4}]$

n	$\psi_n(x)$
0	$\left(\frac{b}{\sqrt{\pi}}\right)^{1/2} e^{-(1/2)b^2x^2}$
1	$\left(\frac{b}{2\sqrt{\pi}}\right)^{1/2} (2bx)e^{-(1/2)b^2x^2}$
2	$\left(\frac{b}{8\sqrt{\pi}}\right)^{1/2} (4b^2x^2 - 2)e^{-(1/2)b^2x^2}$
3	$\left(\frac{b}{48\sqrt{\pi}}\right)^{1/2} (8b^3x^3 - 12bx)e^{-(1/2)b^2x^2}$
n	$\left(\frac{b}{2^n n!\sqrt{\pi}}\right)^{1/2} H_n(bx)e^{-(1/2)b^2x^2}$

$$E = (n + \tfrac{1}{2})\hbar\omega_0 \quad (n = 0, 1, 2, 3, \ldots)$$

$$\text{where } \omega_0 \equiv \sqrt{\frac{\kappa}{m}}$$

$$E = (n + \tfrac{1}{2})\hbar\omega_0 \quad (n = 0, 1, 2, 3, \ldots)$$