Quantum Mechanics and Atomic Physics

Lecture 5:

Potential Wells: Part I

http://www.physics.rutgers.edu/ugrad/361

Prof. Sean Oh

Announcement

- Next HW is due Monday 26th.
- There will be a quiz, next class (Wed, Sept. 21st): Closed book, Closed note, no calculator needed; Will cover topics up to today: If you understand the concept and the standard math, it will take less than 5 minutes.

Last time

- Boundary Conditions
  1. Ψ must be square integrable: $\int \Psi^*(x,t)\,\Psi(x,t)dx = 1$
  2. The wavefunction Ψ must be a continuous function!
     - This means forcing two solutions at the boundary to agree:

     $\Psi^<$(boundary) = $\Psi^>$(boundary)
  3. If V(x) is continuous or finitely discontinuous across a boundary, then the first derivative of Ψ, $d\Psi/dx$, must be made continuous across the boundary. But if V(x) is infinitely discontinuous across the boundary, then $d\Psi/dx$ can be discontinuous across the boundary.
- Introduced a "particle-in-a-box"

Solutions to S.E. in 1-dimension: Overview

- Examples of applications of solutions to the S.E. for a 1-dimensional potential function, V(x)
  - Modeling of real electronic devices (e.g. CCD chips)
  - Understanding nuclear phenomena (beyond the energy levels of the H-atom) such as alpha-decay
- In the next few lectures we will:
  - Examine potential wells
  - Solve the S.E. for the first time for an infinite well
  - Consider the finite well
    - Quantum tunneling
  - Consider potential barriers
    - A potential well turned inside-out
    - Important for understanding nuclear structure/scattering

Concept of a Potential Well: Classical Newtonian Example

- Let's consider a car of mass m on a roller coaster track

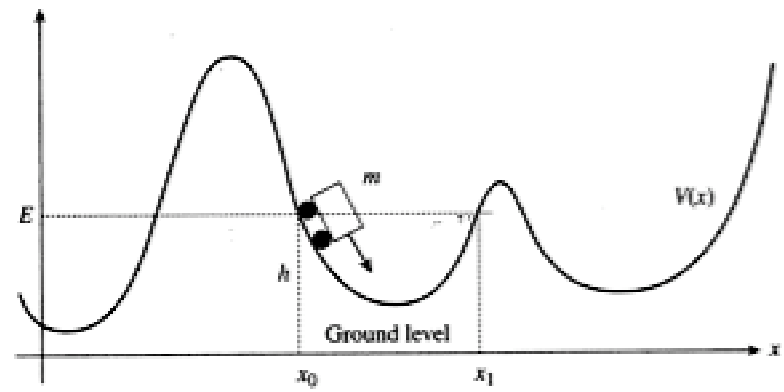

FIGURE 3.1 Car on a roller-coaster track.

Reed: Chapter 3

- $V(x)=mgh(x)$
- If released from rest, total energy $E=mgh(x_0)$
- If no friction/air resistance, it will remain in valley (or well) between x_0 an x_1.
  - **Constrained in potential well**
  - **In a bound energy state**
    - Total energy is less than $V(x)$ as $x \rightarrow \infty$

Newtonian example, con't

- What if car is released from x_0 with some non-zero speed?
- Total energy $E=mv_0^2/2 + mgh(x_0)$
- Now car is in a new bound energy state

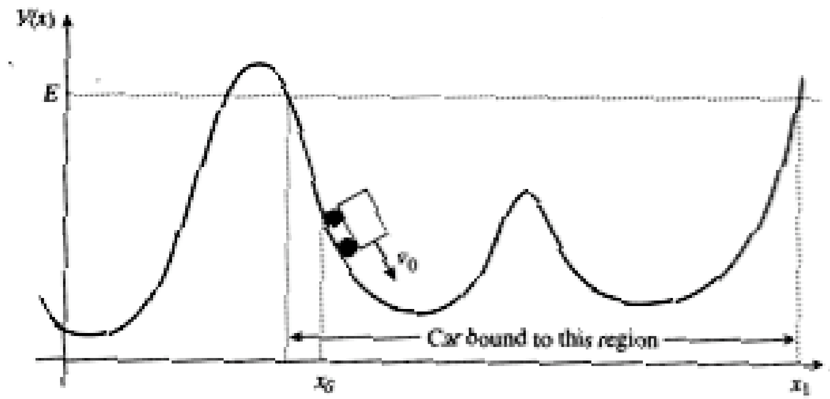

FIGURE 3.2 Car in a bound energy state.

Reed: Chapter 3

Newtonian example, con't

- Now, what if the track to the right of the release point is always lower than the vertical level of the release point?

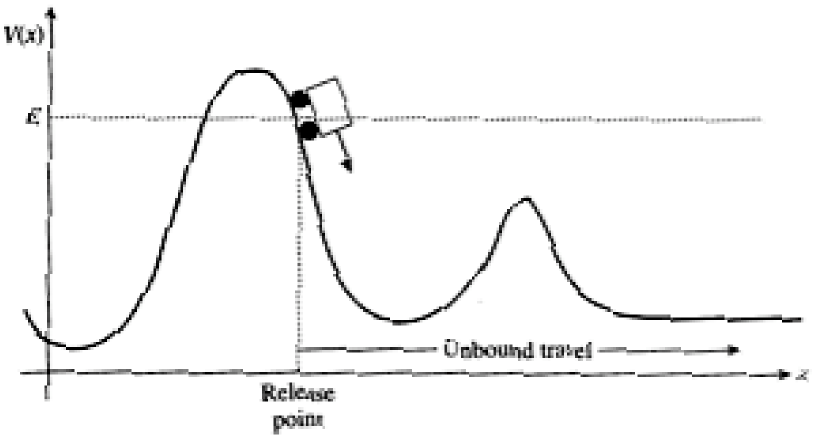

FIGURE 3.3 Car in an unbound energy state.

Reed: Chapter 3

- The car will eventually reach x= ∞
- This is an illustration of an **unbound energy state**

In classical mechanics the energy E is unrestricted - E does not appear in Newton's second law.

In QM, it does enter explicitly in S.E. and for a given potential energy, the total energy E is a parameter of the solutions to S.E.

Time-Independent Potentials

- Let's revisit S.E. for a time-independent potential V(x,t)=V(x):

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

Assume $\Psi(x,t)=\psi(x)\,\phi(t)$

$$-\frac{\hbar^2}{2m}\phi(t)\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)\phi(t)=i\hbar\psi(x)\frac{d\phi(t)}{dt}$$

Divide by $\psi(x)\,\phi(t)$:

$$\underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2}+V(x)}_{\text{Depends only on } x}=\underbrace{i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt}}_{\text{Depends only on } t.}$$

Time-Independent Potentials, con't

- "Separation of variables"
- Left hand side = Right hand side
  - Each must be a constant, and the same constant

$$i\hbar \frac{1}{\varphi(t)} \frac{d\varphi(t)}{dt} = E \qquad (1)$$

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

Solve (1):

$$\frac{d\varphi}{\varphi} = \frac{E}{i\hbar}\,dt = -i\frac{E}{\hbar}\,dt$$

$$\int \frac{d\phi}{\phi} = -\frac{iE}{\hbar}\int dt$$

$$\ln\phi = \frac{-iE}{\hbar}\,t$$

We can ignore the constant of integration since it gets absorbed into the normalization anyway.

$$\Rightarrow \boxed{\varphi(t) = e^{-iEt/\hbar}}$$

This equation has now been solved once and forever. For any time-independent V(x). We can pretty much ignore it from now on.

Multiply (2) by $\psi(x)$:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)}$$

Does this look familiar? It's the time-independent S.E.

Example

- Is $\Psi(x,t) = A\sin(kx - \omega t)$ a valid wavefunction for a region where V(x)=0?

the Schrödinger equation becomes

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

Left side: $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(A\sin(kx-\omega t))$

$$= +\frac{\hbar^2}{2m}k^2(A\sin(kx-\omega t))$$

Example Cont'd

Right side: $i\hbar \frac{\partial}{\partial t} \Psi(x,t) = i\hbar \frac{\partial}{\partial t}\left(A\sin(kx-\omega t)\right)$

$= -i\hbar\,\omega\left(A\cos(kx-\omega t)\right)$

No matter what, $\sin(kx-\omega t) \neq \text{const}\cdot\cos(kx-\omega t)$

$\therefore$ $\Psi(x,t)=A\sin(kx-\omega t)$ is not a valid wavefcn

Example Cont'd

- How about $\Psi(x,t) = A\sin(kx)e^{-iwt}$?
- If valid, evaluate the total energy.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(A\sin(kx)e^{-i\omega t}\right)$$

$$= \frac{\hbar^2}{2m}k^2\left(A\sin(kx)e^{-i\omega t}\right)$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\left(A\sin(kx)e^{-i\omega t}\right)$$

$$= \hbar\omega\left(A\sin(kx)e^{-i\omega t}\right)$$

$\therefore$ O.K. if $\quad \hbar\omega = \frac{\hbar^2}{2m}k^2 \; (\equiv E)$

The Infinite Potential Well

- A particle is trapped between walls so energetically high it would require an infinite amount of energy to get over them.
- Also called *infinite square well* or *infinite rectangular well*
- $V=0$ for $0 \leq x \leq L$
  - Inside the well
- $V=\infty$ for $x<0$, $x>L$
  - Outside the well

- Look for bound-state solutions with $E>0$

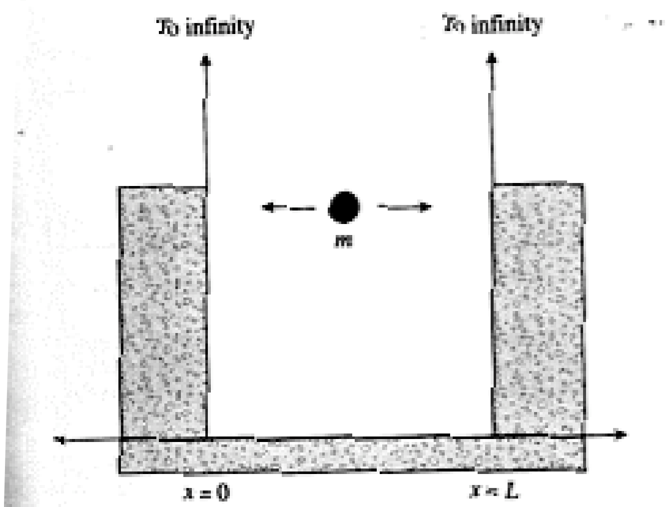

FIGURE 3.4 Infinite square well.

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Real Example: Electron trapped in a "box"

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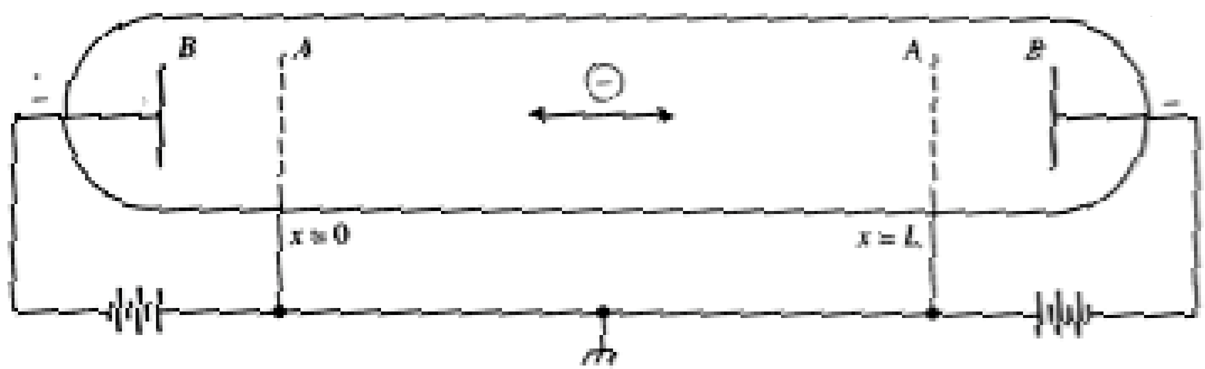


FIGURE 3.5 Schematic diagram of an electron trapped in a one-dimensional "box" made of electrodes and grids in an evacuated tube. From *An Introduction to Quantum Physics* by A. P. French and Edwin F. Taylor. Copyright © 1978 by the Massachusetts Institute of Technology. Used by permission of W. W. Norton & Company, Inc.

Reed: Chapter 3

In the outside regions: x<0, x>L

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

For $x<0$, $x>L$ $V=\infty$

So,

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} + \infty\,\psi = E\psi$$

E is assumed to be finite.

Equation is satisfied only if

$\underline{\psi=0}$

In the inside region: 0≤ x ≤ L

In $0 \le x \le L$, $V = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

define $k^2 = \frac{2mE}{\hbar^2}$

$$\Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi$$

General solution:

$$\psi = A\sin kx + B\cos kx$$

- Let's apply boundary conditions
  - 3rd condition cannot be applied since we have infinite potential discontinuities
  - We can apply conditions 1 and 2

Continuous Wavefunction

* Requirement of continuity:

$\psi(0) = \psi(L) = 0$

- $\psi(0) = 0 \Rightarrow \psi = A \cdot 0 + B = 0 \Rightarrow B = 0$

So, $\psi = A \sin kx$

- $\psi(L) = 0 \Rightarrow kL = n\pi \Rightarrow \sqrt{\frac{2mE}{\hbar^2}} \cdot L = n\pi$

For $n = 1, 2, 3, \ldots \Rightarrow \boxed{E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}}$

$\Rightarrow \boxed{\psi_n(x) = A \sin \frac{n\pi x}{L}}$

Energy Eigenvalues E_n

n is principle quantum number

Ground state energy corresponds to n=1

(n=0 leads to a null solution)

- We just <u>derived</u> the quantization of energy!

Normalized Wavefunction

$*$ Requirement of normalization:

$$\int \psi^* \psi \, dx = 1 = \int_0^L A^2 \sin^2 \frac{n\pi x}{L} \, dx$$

$$= A^2 \int_0^L \frac{1}{2}\left(1 - \cos \frac{2n\pi x}{L}\right) dx$$

$$= \frac{1}{2} A^2 \left[x - \frac{L}{2n\pi} \sin \frac{2n\pi x}{L} \right]_0^L$$

$$= \frac{1}{2} A^2 L$$

$$\Rightarrow \quad A = \sqrt{\frac{2}{L}}$$

$$\Rightarrow \quad \boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}} \qquad 0 \le x \le L$$

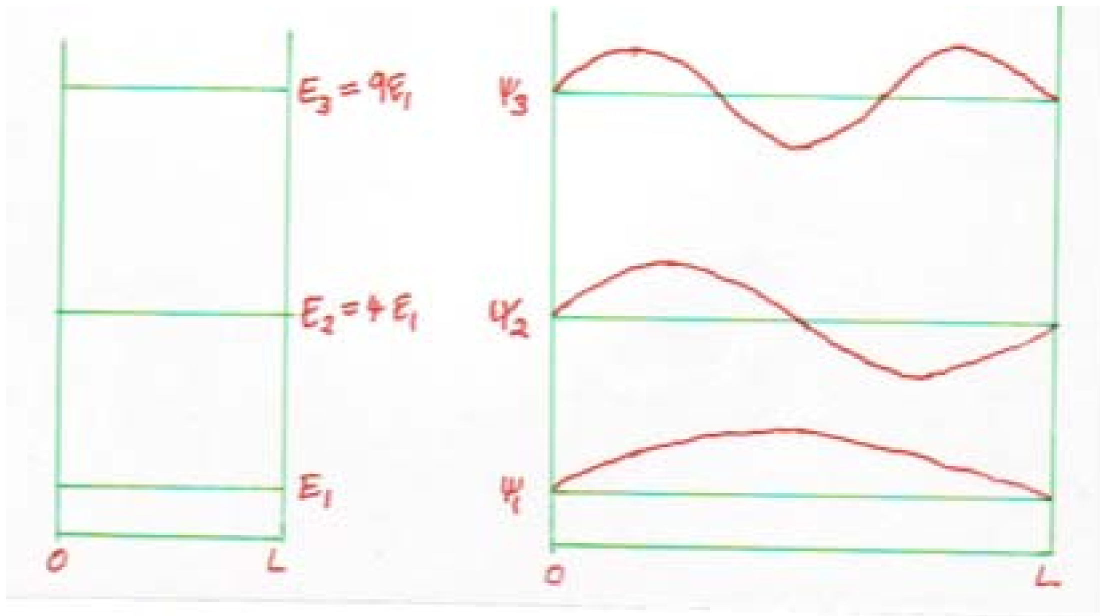
$$n = 1, 2, 3, \ldots$$

Eigenfunction: solution to the time-independent S.E.

Two key lessons

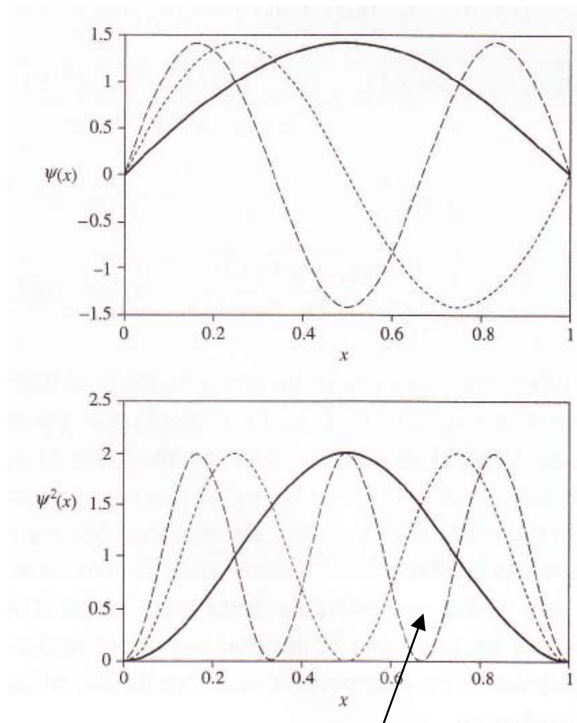
- The quantized energy levels E_n(**energy eigenvalues**) resulted naturally by imposing the boundary conditions to the S.E.
  - Lead to the quantum numbers, n, allowing us to label the energy eignevalues
- There is a wavefunction Ψ (**eigenfunction**) corresponding to each eigenvalue
  - Gives the probability distribution of the system for a total energy E_n

Energy levels and Wavefunctions



- n=1 is ground state
- Number of extrema in wavefunction is equal to n
- Nodes are where Ψ=0
  - where we never expect to find the particle
  - Number of nodes for state n is n-1 excluding the boudaries

Wavefunctions and Probablility Distributions



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- Probability distributions $|\Psi_n|^2$
  - Peaks correspond to where there is a high probability to find the particle
  - Valleys correspond to low probability

Why do we not detect a wavy nature in everyday life?

- **For a microscopic object**
  - Let's evaluate the quantum number for an electron with energy E=20eV trapped in a potential well of L=1Angstrom

$$E = 20\,eV = 3.20 \times 10^{-18}\,J$$

$$L = 1\,\text{Å} = 10^{-10}\,m$$

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

$$\Rightarrow n = \sqrt{\frac{2mL^2E}{\pi^2\hbar^2}} = \sqrt{\frac{2 \cdot (9.11\times10^{-31}\,kg)(1\times10^{-10}\,m)^2(3.20\times10^{-18}\,J)}{(3.14159)^2(1.055\times10^{-34}\,J\cdot s)^2}}$$

$$\approx 0.73 \approx 1$$

Now for a macroscopic object

- Let's evaluate the quantum number for an object of mass m=1kg, energy E=1J trapped in a potential well of width L=1m.

$m = 1\,kg \quad , \quad E = 1\,J \quad , \quad L = 1\,m$

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

$$= \sqrt{\frac{2(1\,kg)(1\,m)^2\,(1\,J)}{\pi^2\,(1.055\times10^{-34}\,J\cdot s)^2}}$$

$$\underline{n \simeq 4.3\times10^{33} \quad !}$$

This value of n is so large that we would never be able to distinguish the quantized nature of energy levels.

For example, the difference in energy between two consecutive states, $n_1=4.3\mathrm{x}10^{33}$ and $n_2=4.3\mathrm{x}10^{33}+1$ is around 10^{-34}J! This is much too small to be detected.

This also shows that quantum predictions must agree with classical results in the limit of large quantum numbers: Bohr's correspondence principle

Bohr's correspondence principle

$$\lim_{n\to\infty} \text{Quantum Physics} = \text{Classical Physics}$$

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

$$\Rightarrow \Delta E = E_{n+1} - E_n$$

$$\Delta E = \frac{\pi^2 \hbar^2}{2mL^2}\left[(n+1)^2 - n^2 \right]$$

$$= \frac{\pi^2 \hbar^2}{2mL^2} (2n+1)$$

$$\frac{\Delta E}{E} = \frac{2n+1}{n^2} \Rightarrow \lim_{n\to\infty} \frac{\Delta E}{E} = \frac{2}{n} \to 0$$

Classically: continuum of energies so $\Delta E/E=0$

Bohr's correspondence principle, con't

- Let's evaluate the probability to find a particle in $x_1 \leq x \leq x_2$

$$P = \int_{x_1}^{x_2} \psi^* \psi \, dx = \frac{2}{L} \int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{L} \, dx$$

$$= \frac{2}{L} \int_{x_1}^{x_2} \frac{1}{2}\left(1 - \cos \frac{2n\pi x}{L}\right) dx = \frac{1}{L} \left[x - \frac{L}{2n\pi} \sin \frac{2n\pi x}{L} \right]_{x_1}^{x_2}$$

$$= \frac{x_2 - x_1}{L} - \underbrace{\frac{1}{2n\pi} \Bigg(\underbrace{\sin \frac{2n\pi x_2}{L} - \sin \frac{2n\pi x_1}{L}}_{\text{Bounded } -2 \leq \cdots \leq 2} \Bigg)}_{\propto \frac{1}{n} \text{ so goes to zero as } n \to \infty}$$

So,

$$\lim_{n \to \infty} P = \frac{x_2 - x_1}{L}$$

Indeed this is the classical expectation!

Example

- Probabilities for a particle in a box:
  - A particle is known to be in the ground state of a infinite square well with length L. Calculate the probability that this particle will be found in the middle half of the well, between x=L/4 and x=3L/4.
    - Classically: we expect 1/2 - a classical particle spends equal time in all parts of the well

Ground state $n=1$: $\psi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$

$$P = \int_{L/4}^{3L/4} \psi_1^* \psi_1 \, dx = \frac{2}{L} \int_{L/4}^{3L/4} \sin^2 \frac{\pi x}{L} \, dx$$

$$= \frac{2}{L} \int_{L/4}^{3L/4} \frac{1}{2}\left(1 - \cos \frac{2\pi x}{L}\right) dx$$

$$= \frac{1}{L} \left[x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{L/4}^{3L/4}$$

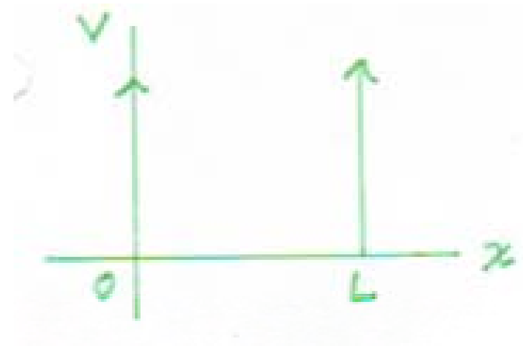
$$= \frac{1}{L} \left[\frac{3L}{4} - \frac{L}{4} - \frac{L}{2\pi}\left(\sin \frac{3\pi}{2} - \sin \frac{\pi}{2} \right) \right]$$

$$= \frac{1}{L} \left[\frac{L}{2} - \frac{L}{2\pi}(-1-1) \right] = \frac{1}{2} + \frac{1}{\pi} \approx 0.82$$

$$= \underline{82\%}$$

Full Wavefunction for Infinite Potential Well

- In summary,



$$\Psi(x,t) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \cdot e^{-iE_n t/\hbar}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \ldots.$$

Summary/Announcements

- Introduction to concept of Potential Wells
- The Infinite Square Well

- Next time:
  - More on Potential Wells
- Next homework due on Monday Sept 26!
- There will be a quiz, next class (Wed, Sept. 21^{st}): Closed book, Closed note, no calculator needed.