Quantum Mechanics and Atomic Physics

Lecture 6:

Potential Wells: Part II

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

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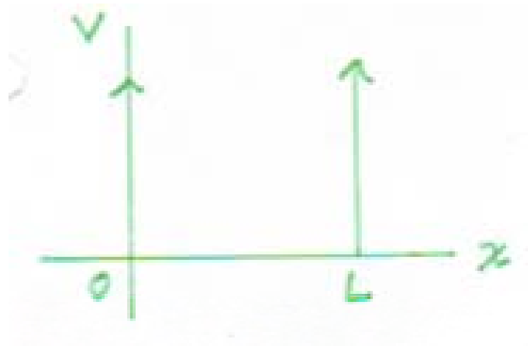
Last Time

- We solved S.E. for the Infinite Potential Well



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

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

Next: we consider the Finite Potential Well

The Finite Square Well

- Mass m in a potential well of finite depth
  - This is a more realistic case than infinite square well: e.g. electron trapped in surface of metal which needs a few eV to escape (as in photoelectric effect)
- $V=0$ for $-L \leq x \leq L$
  - Inside the well
- $V= V_0$ for $|x|>L$
  - Outside the well

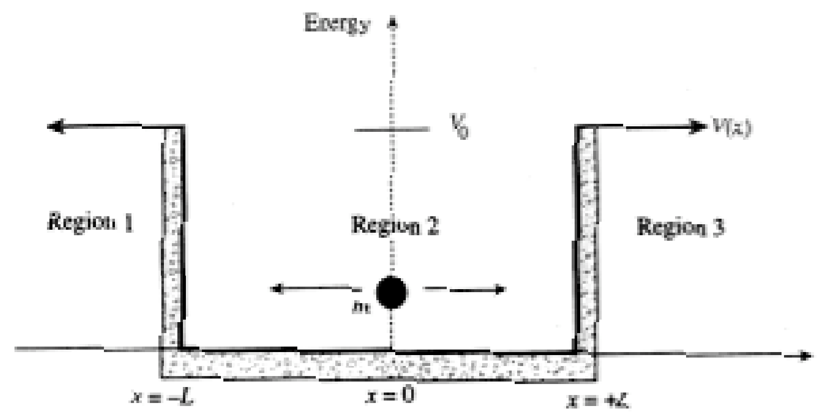


FIGURE 2.7 Finite rectangular well.

Reed: Chapter 3

- For $E< V_0$ we are seeking *bound energy states* (bottom of the well is at $V=0$)

Solutions inside and outside the well

- In regions ① and ③ : $V(x) = V_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{out}}{dx^2} = (E - V_0)\,\psi_{out}$$

- In region ② : $V(x) = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{in}}{dx^2} = E\,\psi_{in}$$ (like infinite square well)

Let's rewrite:

$$\frac{d^2\psi_{out}}{dx^2} = k_1^2\,\psi_{out} \qquad k_1^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

(used $k_1 = k_3$)

indices label the regions

$$\frac{d^2\psi_{in}}{dx^2} = -k_2^2\,\psi_{in} \qquad k_2^2 = \frac{2mE}{\hbar^2}$$

k_1 & k_2 are positive and real.

Inside and outside the well

In region 2 (in):

$$\psi_2 = A e^{ik_2 x} + B e^{-ik_2 x} \qquad (-L \le x \le L)$$

In regions 1 & 3:

$$\psi_1 = C e^{\kappa_1 x} + D e^{-\kappa_1 x} \qquad (x \le -L)$$

$$\psi_3 = G e^{\kappa_1 x} + F e^{-\kappa_1 x} \qquad (x \ge L)$$

Boundary Conditions

- $\psi_1 = \psi_2$ at $x = -L$

  $\psi_2 = \psi_3$ at $x = +L$

- $\left.\frac{d\psi_1}{dx}\right|_{-L} = \left.\frac{d\psi_2}{dx}\right|_{-L}$ and $\left.\frac{d\psi_2}{dx}\right|_{+L} = \left.\frac{d\psi_3}{dx}\right|_{+L}$

and

- $\int_{-\infty}^{-L} \psi_1^* \psi_1 \, dx + \int_{-L}^{L} \psi_2^* \psi_2 \, dx + \int_{L}^{\infty} \psi_3^* \psi_3 \, dx = 1$

Finiteness of Wavefunctions

- But, are the wavefunctions finite?
  - $\Psi_1 \rightarrow \infty$ as $x \rightarrow -\infty$ and $\Psi_3 \rightarrow \infty$ as $x \rightarrow \infty$
- Therefore finiteness requires that D=0 and G=0
- That leaves <u>four</u> constants: A, B, C and F
- But we have <u>five</u> constraints!
  - The four boundary conditions plus normalization
    - Are we over-determined?
    - How about k_1 and k_2 ?
    - k_1 and k_2 are determined by energy and so energy cannot take any arbitrary values ➔ energy quantization!!

Boundary Conditions, con't

In region 2:

$$\psi_2 = A e^{ik_2 x} + B e^{-ik_2 x}$$

but more convenient to write as:

$$\psi_2 = A \sin k_2 x + B \cos k_2 x$$

- ψ at $x = -L$: $\quad C e^{-\kappa_1 L} = -A \sin k_2 L + B \cos k_2 L$
- $\frac{d\psi}{dx}$ at $x = -L$: $\quad \kappa_1 C e^{-\kappa_1 L} = k_2 A \cos k_2 L + k_2 B \sin k_2 L$

- ψ at $x = +L$: $\quad F e^{-\kappa_1 L} = A \sin k_2 L + B \cos k_2 L$
- $\frac{d\psi}{dx}$ at $x = +L$: $\quad -\kappa_1 F e^{-\kappa_1 L} = k_2 A \cos k_2 L - k_2 B \sin k_2 L$

Let's define two new constants:

$$\eta = k_1 L = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\,L \quad , \quad \xi = k_2 L = \sqrt{\frac{2mE}{\hbar^2}}\,L$$

$$\left.\begin{aligned}
C e^{-\eta} &= -A\sin\xi + B\cos\xi && (1)\\
\left(\frac{\eta}{\xi}\right) C e^{-\eta} &= A\cos\xi + B\sin\xi && (2)\\
F e^{-\eta} &= A\sin\xi + B\cos\xi && (3)\\
-\left(\frac{\eta}{\xi}\right) F e^{-\eta} &= A\cos\xi - B\sin\xi && (4)
\end{aligned}\right\} \begin{array}{l}\text{Four}\\ \text{equations}\\ \quad \&\\ \text{Four}\\ \text{unknowns.}\end{array}$$

Divide:

$$\frac{(3)}{(1)} \Rightarrow \frac{F}{C} = \frac{(A\sin\xi + B\cos\xi)}{(-A\sin\xi + B\cos\xi)}$$

$$\frac{(4)}{(2)} \Rightarrow \frac{F}{C} = -\frac{(A\cos\xi - B\sin\xi)}{A\cos\xi + B\sin\xi}$$

Set equal & cross multiply:

$$A^2\sin\xi\cos\xi + B^2\sin\xi\cos\xi + AB = A^2\sin\xi\cos\xi + B^2\sin\xi\cos\xi - AB$$

$$\Rightarrow AB = -AB \Rightarrow 2AB = 0 \Rightarrow \boxed{AB = 0}$$

Square eqn (1):

$$(Ce^{-\kappa})^2 = A^2\sin^2\xi + B^2\cos^2\xi - 2AB\sin\xi\cos\xi$$

Square eqn (3)

$$(Fe^{-\kappa})^2 = A^2\sin^2\xi + B^2\cos^2\xi + 2AB\sin\xi\cos\xi$$

use $AB = -AB$ or $AB = 0$

$$\Rightarrow \boxed{F^2 = C^2}$$

So, F=±C

Two classes of solutions!

- Even Parity solutions:

• If $A=0$: $C e^{-\kappa_1 L} = B \cos k_2 L$

$F e^{-\kappa_1 L} = B \cos k_2 L$

$\Rightarrow C = F$

And $\psi_2 = B \cos k_2 x$

Even parity: $\psi_2(x) = \psi_2(-x)$

- Odd Parity solutions:

• If $B=0$: $C e^{-\kappa_1 L} = -A \sin k_2 L$

$F e^{-\kappa_1 L} = A \sin k_2 L$

$\Rightarrow C = -F$

And $\psi_2 = A \sin k_2 x$

Odd Parity: $\psi_2(x) = -\psi_2(-x)$

The Strength Parameter

$$\xi^2 + \eta^2 = \frac{2mV_0L^2}{\hbar^2} = K^2 = \text{constant}$$

- For a given K, only certain values of ξ will satisfy the boundary conditions
- From our definitions of η and ξ, these will correspond to particular values of the energy of the particle.
- The energy levels are given by:

$$E_n = \xi_n^2 \frac{\hbar^2}{2mL^2}$$

Finite Square Well: Even Solutions

$A = 0$; $C = F$

$$\psi_1 = Ce^{k_1 x} \qquad (x < -L)$$

$$\psi_2 = B\cos k_2 x \qquad (-L \le x \le L)$$

$$\psi_3 = Ce^{-k_1 x} \qquad (x > L)$$

$$C = B\cos k_2 L \, e^{k_1 L}$$
$$= B\cos\xi \, e^{\eta}$$

so,

$$\psi_1 = B\cos\xi \, e^{\eta} e^{k_1 x} \qquad (x < -L)$$

$$\psi_2 = B\cos k_2 x \qquad (-L \le x \le L)$$

$$\psi_3 = B\cos\xi \, e^{\eta} e^{-k_1 x} \qquad (x > L)$$

Dividing eqns $\frac{(2)}{(1)}$:

$$\left(\frac{\kappa}{\xi}\right) = \frac{A\cos\xi + B\sin\xi}{-A\sin\xi + B\cos\xi}$$ and w/ $A=0$

$$\left(\frac{\kappa}{\xi}\right) = \frac{\sin\xi}{\cos\xi} = \tan\xi$$ This gives us the energy equation!

$$\tan\xi = \frac{\kappa}{\xi} = \sqrt{\frac{V_0 - E}{E}} \Rightarrow \tan k_2 L = \sqrt{\frac{V_0 - E}{E}}$$

$$\Rightarrow \boxed{\tan\left(L\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{V_0 - E}{E}}} \Leftrightarrow \tan(\xi) = \frac{\sqrt{K^2 - \xi^2}}{\xi}$$

$$\xi^2 + \eta^2 = K^2$$

$$K^2 \equiv \frac{2mV_0 L^2}{\hbar^2}$$

This is what gives us energy quantization!

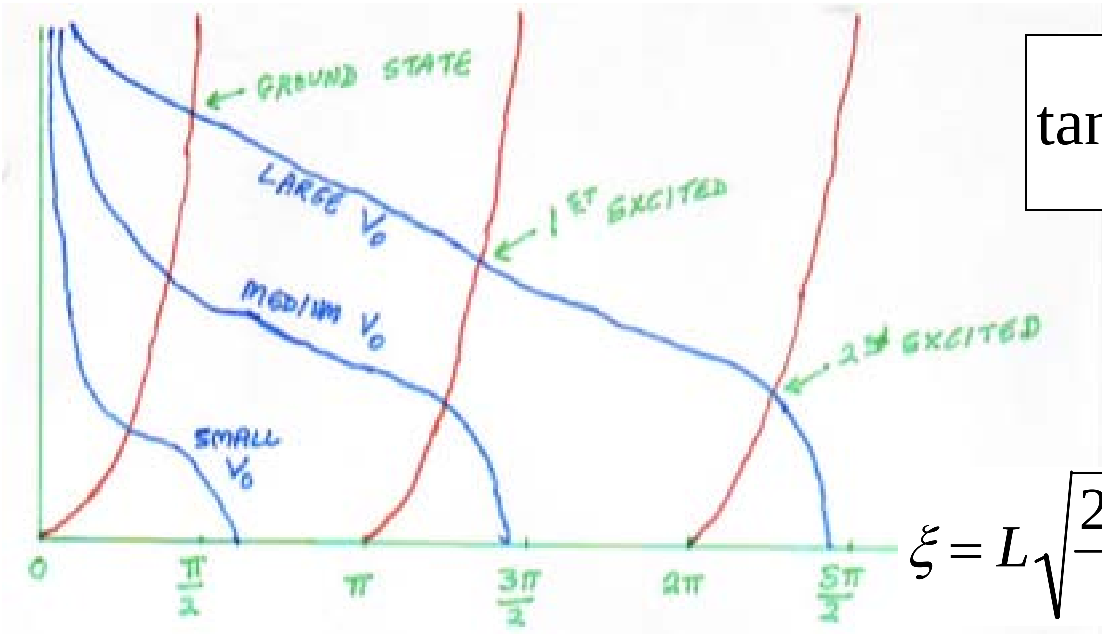
Energy Quantization

$$\boxed{\tan\left(L\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{V_0 - E}{E}}}$$

- This expression cannot be solved analytically.
- Let's plot both the left hand side and right hand side on the same graph
- Note:
  - the right hand side = ∞ for $E=0$
  - The left hand side = 0 for $E=V_0$

Graphical Solution

$$\tan\left(L\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{V_0 - E}{E}}$$

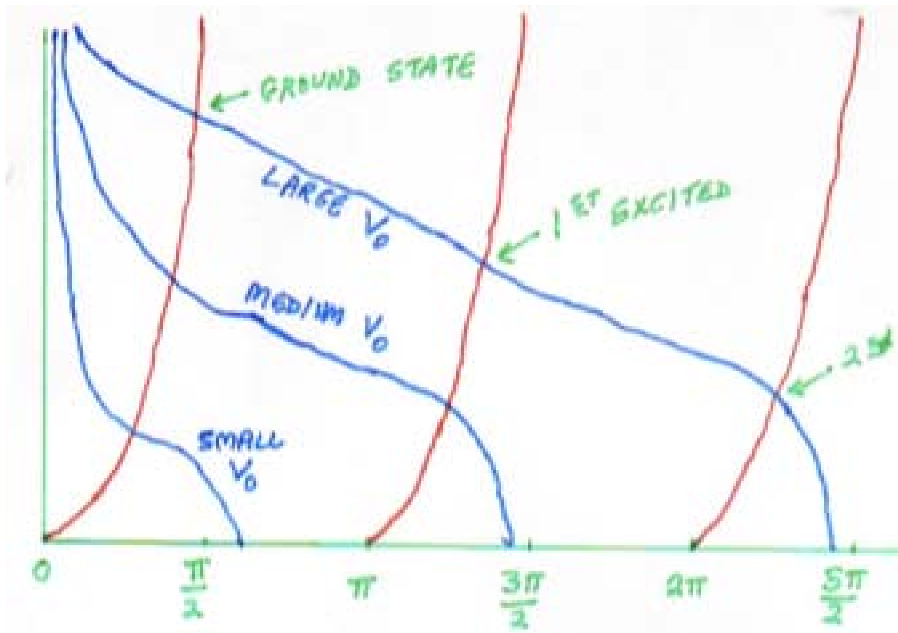


$$\xi = L\sqrt{\frac{2mE}{\hbar^2}}$$

- Red: Left hand side
- Blue: Right hand side
  - expressed as functions of $\xi = L\sqrt{\frac{2mE}{\hbar^2}}$

- For three different values of V_0

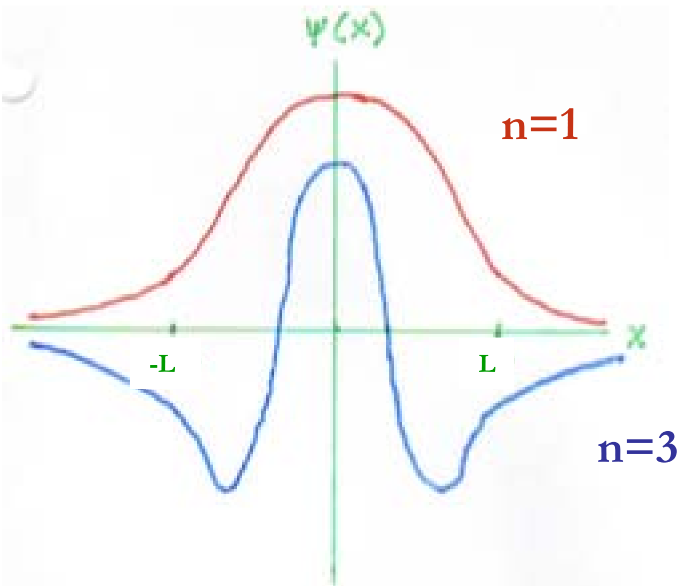
Graphical Solution, con't



$$\xi = L\sqrt{\frac{2mE}{\hbar^2}}$$

- Features:
  - We get quantized energy eigenvalues
  - At least one solution must exist, no matter how small V_0 is (remember that $E<V_0$)
  - Total number of solutions is finite, no matter how large V_0 is.

Even Solution Eigenfunctions



$$\psi_1 = B\cos\xi\, e^{\eta}\, e^{\kappa_1 x} \quad (x < -L)$$

$$\psi_2 = B\cos\kappa_2 x \quad (-L \le x \le L)$$

$$\psi_3 = B\cos\xi\, e^{\eta}\, e^{-\kappa_1 x} \quad (x > L)$$

- Two possible eigenfunctions are shown (n=1 and n=3)
- Ψ is symmetric in x: $\Psi(-x) = \Psi(x)$
  - Since cosine is symmetric
  - We have even parity
- **Note: we get penetration into the classically forbidden regions (1) and (3)**
- For the case $E>V_0$ we get oscillatory solutions in all three regions. No bound states: continuum of energies is possible.

Normalization

- We can get B from the normalization condition

Normalization:

$$\underbrace{\int_{-\infty}^{-L} \psi_1^* \psi_1 \, dx}_{} + \int_{-L}^{L} \psi_2^* \psi_2 \, dx + \underbrace{\int_{L}^{\infty} \psi_3^* \psi_3 \, dx}_{} = 1$$

equal

$$\int_{-\infty}^{-L} \psi_1^* \psi_1 \, dx = \int_{L}^{\infty} \psi_3^* \psi_3 \, dx = C^2 \int_{L}^{\infty} e^{-2\kappa_1 x} \, dx$$

$$= \frac{C^2}{-2\kappa_1} \left[0 - e^{-2\kappa L} \right] = \frac{C^2}{2\kappa_1} e^{-2\kappa L}$$

So this term enters
twice in the normalization

$$\int_{-L}^{L} \psi_2^* \psi_2 \, dx = B^2 \int_{-L}^{L} \cos^2 \varkappa_2 x \, dx$$

$$= B^2 \left[\frac{x}{2} + \frac{\sin(2\varkappa_2 x)}{4\varkappa_2} \right]_{-L}^{L}$$

$$= B^2 \left[\frac{\sin 2\xi}{2\varkappa_2} + L \right]$$

$$2 \times \frac{C^2}{2\varkappa_1} e^{-2\eta} + B^2 \left[\frac{\sin 2\xi}{2\varkappa_2} + L \right] = 1$$

Substitute $C = B\cos\xi \, e^{\eta}$

$$2 \frac{B^2 \cos^2 \xi}{2\varkappa_1} + B^2 \left[\frac{\sin 2\xi}{2\varkappa_2} + L \right] = 1$$ Multiply by $\frac{1}{L}$

$$2 \frac{B^2 \cos^2 \xi}{2\eta} + \frac{B^2 \sin 2\xi}{2\xi} + B^2 = \frac{1}{L}$$

$$B^2\left[\frac{\cos^2\xi}{\cancel{\xi}\, n} + \frac{\sin 2\xi}{2\xi} + 1\right] = \frac{1}{L}$$

$$B^2 = \frac{1}{L\left[\frac{\cos^2\xi}{n} + \frac{\sin 2\xi}{2\xi} + 1\right]}$$

Multiply by $n\xi$ & use $\sin 2\xi = 2\sin\xi\cos\xi$

$$B^2 = \frac{n\xi}{L\left[\xi\cos^2\xi + n\sin\xi\cos\xi + n\xi\right]}$$

- Once a given energy state ξ_n is specified, the B (and therefore C) can be computed
- Unlike the infinite well, here the normalization constants depend on the energy eigenvalue involved!
- <u>Exercise you can try on your own</u>: determine the probability of finding the particle outside the well (cross check with eqn. 3.4.11 in your book). It depends on the energy eigenvalue.

Finite Square Well: Odd Solutions

$B = 0, \quad C = -F$

$$\psi_1 = C e^{\kappa_1 x} \qquad (x < -L)$$
$$\psi_2 = A \sin \kappa_2 x \qquad (-L \le x \le L)$$
$$\psi_3 = -C e^{-\kappa_1 x} \qquad (x > L)$$

$$C = -A \sin k_2 L \, e^{\kappa_1 L} = -A \sin \xi \, e^{\eta}$$

So,

$$\psi_1 = -A \sin \xi \, e^{\eta} e^{\kappa_1 x} \qquad (x < -L)$$
$$\psi_2 = A \sin \kappa_2 x \qquad (-L \le x \le L)$$
$$\psi_3 = A \sin \xi \, e^{\eta} e^{-\kappa_1 x} \qquad (x > L)$$

Dividing $\frac{(2)}{(1)}$:

$$\left(\frac{\kappa}{\xi}\right) = \frac{A\cos\xi + B\sin\xi}{-A\sin\xi + B\cos\xi}$$

and w/ $B=0$

$$\left(\frac{\kappa}{\xi}\right) = -\frac{\cos\xi}{\sin\xi} = -\cot\xi$$

$$-\cot\xi = \frac{\kappa}{\xi} = \sqrt{\frac{V_0-E}{E}}$$

But $-\cot\xi = \tan\left(\xi \pm \frac{\pi}{2}\right)$

Odd Solution Eigenfunctions

- Again, two possible eigenfunctions are shown (n=2 and n=4)
- This time Ψ is anti-symmetric in x: Ψ(-x) = -Ψ(x)
  - Since sine is anti-symmetric
  - We have odd parity

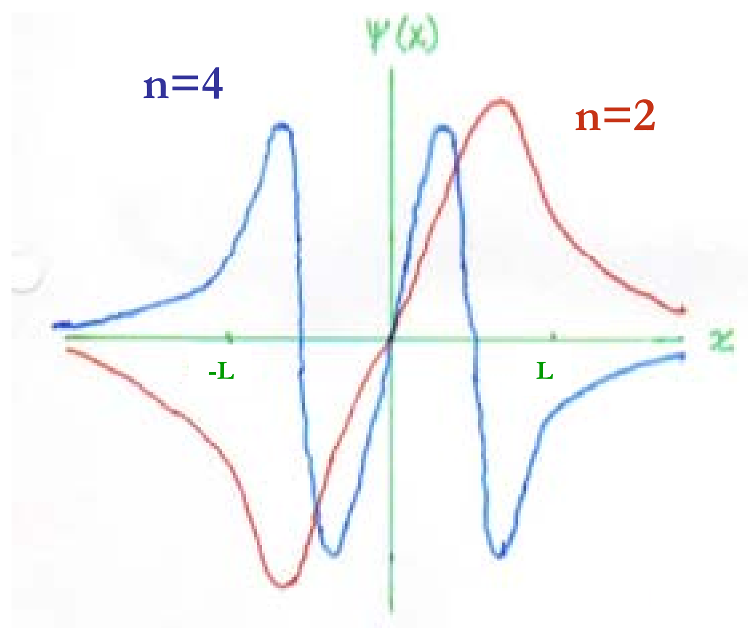
$$\psi_1 = -A \sin\xi \, e^{\eta} e^{\kappa_1 x} \qquad (x < -L)$$

$$\psi_2 = A \sin \kappa_2 x \qquad (-L \le x \le L)$$

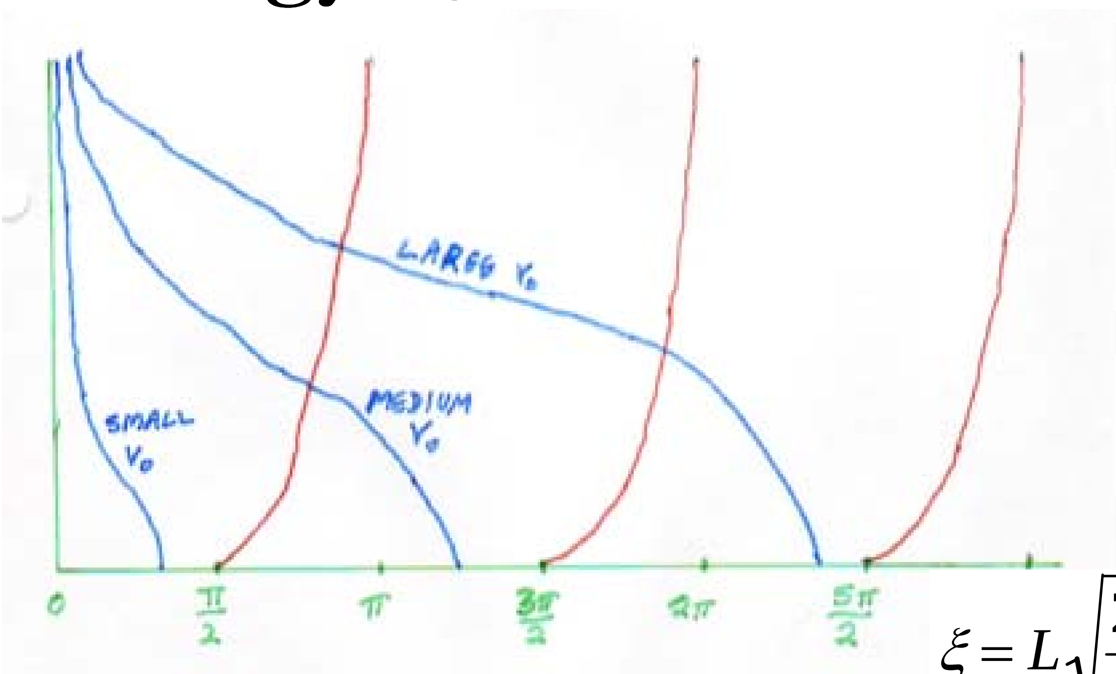
$$\psi_3 = A \sin\xi \, e^{\eta} e^{-\kappa_1 x} \qquad (x > L)$$

- Whenever the potential is symmetric, V(-x)=V(x), eigenfunctions must have definite parity, i.e. Ψ(-x) = ±Ψ(x)
  - Symmetric V implies symmetric probabilities

    $P(-x)=P(x)$ but $P(x)=|\Psi(x)|^2$ so $\Psi(-x) = \pm\,\Psi(x)$



Energy Quantization :Graphical Solution



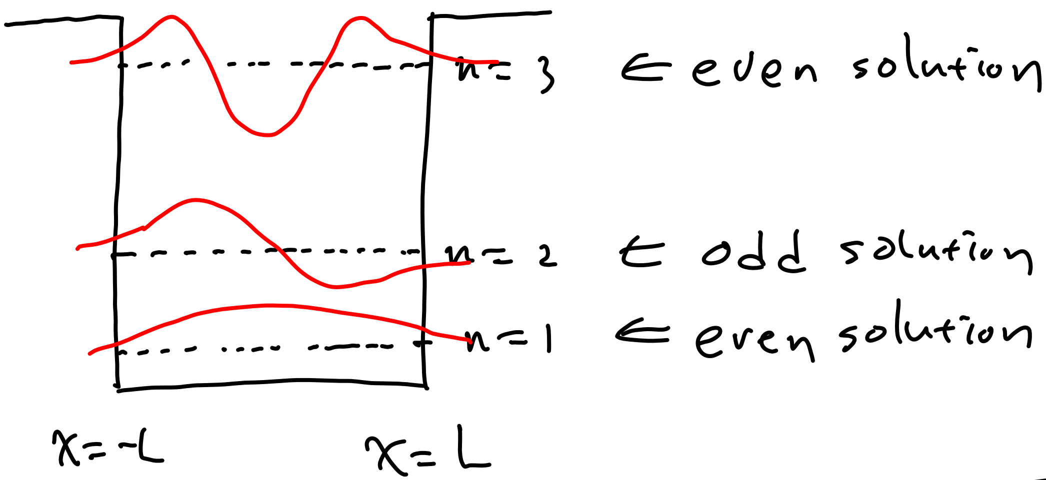
$$-\cot(L\sqrt{\frac{2mE}{\hbar^2}}) = -\cot(\xi) = \sqrt{\frac{V_0 - E}{E}}$$

$$-\cot(\xi) = \tan(\xi \pm \frac{\pi}{2})$$

$$\xi = L\sqrt{\frac{2mE}{\hbar^2}}$$

- So the graphical solution is the same as for the even parity solutions, except that the tangent curves are displaced by $\pi/2$!
- This time if V_0 is small enough, we may get no solutions.
  - As V_0 increases we get more solutions, but always a finite number
  - In general, for a given V_0, the particle will have a mixture of both classes even and odd parity (A=0 and B=0).

One page summary of the finite rectangular well



$$\eta = k_1 L$$

$$\xi = k_2 L$$

$$\eta^2 + \xi^2 = K^2 = \frac{2 m V_0 L^2}{\hbar^2}$$

even solution : $\tan(\xi) = \dfrac{\sqrt{K^2 - \xi^2}}{\xi}$

odd solution : $\tan(\xi \pm \frac{\pi}{2}) = \dfrac{\sqrt{K^2 - \xi^2}}{\xi}$

Important things to note

- For a finite potential well:
  - **There is some probability of finding the particle beyond the walls of the well!**
  - Classically: it cannot be found there
- This is called **tunneling** or **barrier penetration**
- A **characteristic tunneling length** is given by the reciprocal of k_1

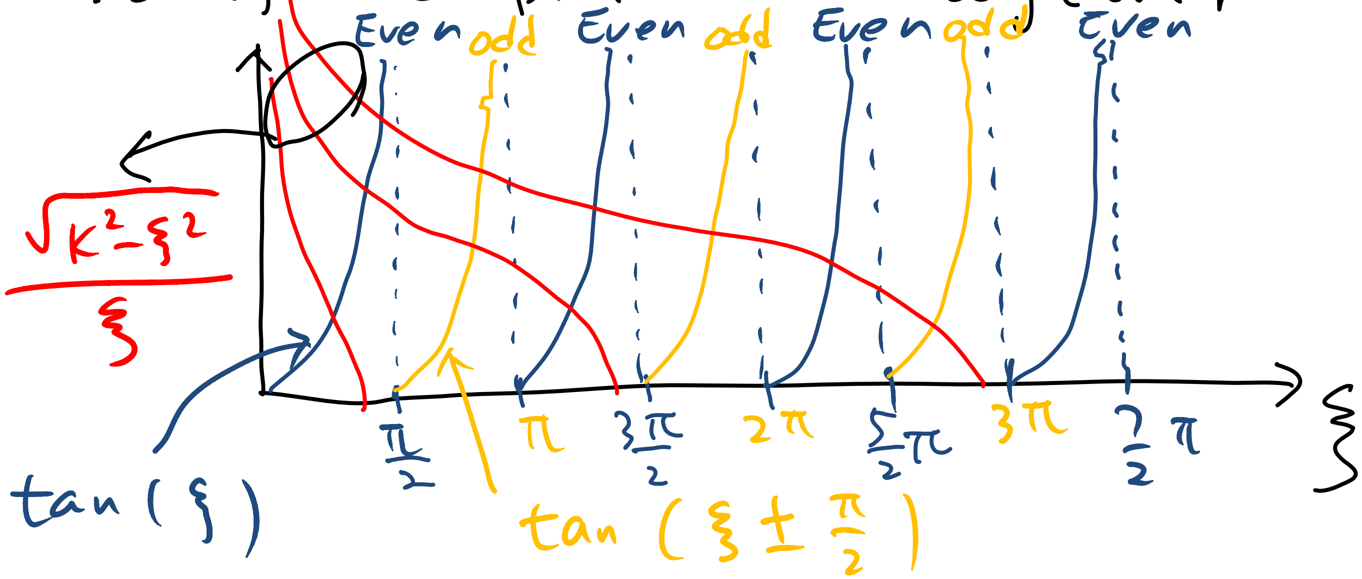
Number of bound states in a finite potential well

Note : $\xi^2 + \eta^2 = K^2 \left(\equiv \frac{2mV_0L^2}{\hbar^2}\right)$

Even solution : $\tan(\xi) = \frac{\eta}{\xi} = \frac{\sqrt{K^2 - \xi^2}}{\xi}$

odd solution ; $\tan\left(\xi \pm \frac{\pi}{2}\right) = \frac{\eta}{\xi} = \frac{\sqrt{K^2 - \xi^2}}{\xi}$

So if we plot them together



Number of bound states Cont'd

\# of Bound states $\equiv N$

If $0 \leq K < \frac{\pi}{2}$ $\left(\Leftrightarrow 0 \leq \frac{2K}{\pi} < 1 \right) \Rightarrow N = 1$

$\frac{\pi}{2} \leq K < \pi$ $\left(\Leftrightarrow 1 \leq \frac{2K}{\pi} < 2 \right) \Rightarrow N = 2$

$\pi \leq K < \frac{3}{2}\pi$ $\left(\Leftrightarrow 2 \leq \frac{2K}{\pi} < 3 \right) \Rightarrow N = 3$

$\vdots$

$$\therefore \; N(K) = 1 + \underbrace{\left[\frac{2K}{\pi} \right]}$$

largest integer less than or equal to $\frac{2K}{\pi}$

Example: CCD

- Finite potential wells are used in everyday devices!
  - Digital cameras: two-dimensional grid of potential wells
    - This is called a charge-coupled-device or CCD
      - Each well can be thought of as a "pixel" or a picture element

- Example: We have a camera with "9micron pixels"; this means each potential well is 9 by 9microns in size (1micron = 10^{-6}m). Let's assume it can hold 60,000 electrons before becoming full (each energy level can hold two electrons of opposite spin). If we assume that the pixels are one-dimensional finite square wells, what must be their depth V_0?

Number of eigenvalues $N = 30{,}000$

$$\therefore \quad N = 1 + \frac{2K}{\pi} \approx \frac{2K}{\pi}$$

$$\Rightarrow K = \frac{\pi}{2} N = \sqrt{\xi^2 + \eta^2} = \sqrt{\frac{2mV_0 L^2}{\hbar^2}}$$

$$\left(\frac{\pi}{2} N\right)^2 = \frac{2mV_0 L^2}{\hbar^2}$$

½ the width of well

$$V_0 = \frac{(N\pi\hbar)^2}{8mL^2} \quad ; \quad L = \frac{9\,\text{microns}}{2} = 4.5\,\text{microns}$$

$$V_0 = \frac{\left((30{,}000)\pi \cdot 1.055\times10^{-34}\,\text{J}\cdot\text{s}\right)^2}{8(9.11\times10^{-31}\,\text{kg})(4.5\times10^{-6}\,\text{m})^2} = 6.7\times10^{-19}\,\text{J}$$

$$\approx \underline{4.2\,\text{eV}}$$

- Which is a device that can be easily powered with batteries!

Example 2

- Do the previous CCD camera problem, using the infinite well formula we found earlier, but simply using the approximate criterion that $E_N < V_0$.

Summary/Announcements

- The Finite Potential Well

- Next time:
  - Sketches of Wavefunctions,
  - Potential Barriers and Scattering
- Next homework due on Monday Sept 26
- Now it's time for Quiz: Closed note and Closed book, and No Calculator!