Physics 48 - February 11, 2008

- Prelude
- The analytic solution to the Harmonic oscillator Schrödinger equation

Prelude

- Show film loop of a time-dependent superposition of waves for the particle in a box.
- Discuss probability for the reflection off of a cliff problem. Distinguish probability and probability flux.
- Show film loop for reflection from a well with different slopes of edges.
- Wave packet evolution in a potential well http://www.falstad.com/mathphysics.html#qm

The Analytic Method: (Power Series)

We again begin with the Schrodinger Equation

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

We introduce the dimensionless displacement $\xi=\sqrt{\frac{m\omega}{\hbar}}x$

Thus $\frac{d^2}{dx^2}=\left(\frac{m\omega}{\hbar}\right)\frac{d^2}{d\xi^2}$ and $\frac{1}{2}m\omega^2x^2=\frac{1}{2}m\omega^2\left(\frac{\hbar}{m\omega}\right)\xi^2$

Yielding

$$-\frac{\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)\frac{d^2\psi}{d\xi^2}+\frac{1}{2}\hbar\omega\xi^2\psi=E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)\frac{d^2\psi}{d\xi^2}+\frac{1}{2}\hbar\omega\xi^2\psi=E\psi$$

$$-\frac{d^2\psi}{d\xi^2}+\xi^2\psi=\frac{2E}{\hbar\omega}\psi\equiv E'\psi \quad \text{where} \quad E'\equiv\frac{2E}{\hbar\omega}$$

$$\frac{d^2\psi}{d\xi^2}=(\xi^2-E')\psi$$

Now for $\xi^2 >> E'$ we have the approximate asymptotic equation

$$\frac{d^2\psi}{d\xi^2}=\xi^2\psi$$

Thus for large values of ξ we have the solutions

$$\psi(\xi)\approx Ae^{-\xi^2/2}+Be^{\xi^2/2}$$

Lets verify that this is indeed a solution

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{\xi^2/2}$$

Note that $$d\psi/d\xi \approx -A\xi e^{-\xi^2/2} + B\xi e^{\xi^2/2}$$

And hence $$d^2\psi/d\xi^2 \approx A(\xi^2 - 1)e^{-\xi^2/2} + B(\xi^2 + 1)e^{\xi^2/2}$$

But $\xi^2 >> E' \geq \frac{1}{2}$

Which yields $d^2\psi/d\xi^2 \approx A\xi^2 e^{-\xi^2/2} + B\xi^2 e^{\xi^2/2} \approx \xi^2\psi$ as we hoped.

Now the increasing exponential is not a normalizable solution. So we will be looking for a solution with the asyptotic limit:

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}$$

Note that I now write this as an equality. What we did above is simply to motivate the functional form. We are "peeling off" the asymptotic limit in the hope that the remaining part of the solution will be simpler. Let's see what we now require for $h(\xi)$.

$$\psi(\xi) = h(\xi) e^{-\xi^2/2}$$

$$d\psi/d\xi = \frac{dh}{d\xi} e^{-\xi^2/2} - \xi h e^{-\xi^2/2}$$

$$d^2\psi/d\xi^2 = \frac{d^2h}{d\xi^2} e^{-\xi^2/2} - \xi \frac{dh}{d\xi} e^{-\xi^2/2} - h e^{-\xi^2/2} - \xi \frac{dh}{d\xi} e^{-\xi^2/2} + \xi^2 h e^{-\xi^2/2}$$

So
$$d^2\psi/d\xi^2 = \left(\frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (\xi^2 - 1) h \right) e^{-\xi^2/2}$$

Thus the Schrodinger Equation $\frac{d^2\psi}{d\xi^2} = (\xi^2 - E')\psi$ becomes

$$\left(\frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (\xi^2 - 1) h \right) e^{-\xi^2/2} = \left(\xi^2 - E' \right) h e^{-\xi^2/2}$$

$$\left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right)e^{-\xi^2/2} = \left(\xi^2 - E'\right)he^{-\xi^2/2}$$

or
$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (E'-1)h = 0$$

We will look for a solution to the SE for h in the form of a power series (Taylor's theorem says that this is OK for any smooth function). We assume

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j = a_0 + a_1\xi + a_2\xi^2 + \cdots$$

Then
$$\frac{dh(\xi)}{d\xi} = \sum_{j=0}^{\infty} a_j j \xi^{j-1} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots$$

and
$$\frac{d^2h(\xi)}{d\xi^2} = \sum_{j=0}^{\infty} a_j j(j-1)\xi^{j-2} = 2a_2 + 6a_3\xi + 12a_4\xi^2 + \cdots$$

$$\frac{d^2h(\xi)}{d\xi^2} = \sum_{j=0}^{\infty} a_j j(j-1)\xi^{j-2} = 2a_2 + 6a_3\xi + 12a_4\xi^2 + \cdots$$

Notice that the first two terms of this last series are zero so we could move the index up by 2. i.e.

$$\frac{d^2h(\xi)}{d\xi^2} = \sum_{j=0}^{\infty} a_{j+2}(j+2)(j+1)\xi^{j} = 2a_2 + 6a_3\xi + 12a_4\xi^2 + \cdots$$

Putting this into the S.E. for *h* $\quad \frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (E'-1)h = 0 \quad$ yields

$$\sum_{j=0}^{\infty} a_{j+2}(j+2)(j+1)\xi^{j} - 2\xi\sum_{j=0}^{\infty} a_j j\xi^{(j-1)} + (E'-1)\sum_{j=0}^{\infty} a_j\xi^{j} = 0$$

$$\sum_{j=0}^{\infty} [a_{j+2}(j+2)(j+1) - 2a_j j + (E'-1)a_j]\xi^{j} = 0$$

$$\sum_{j=0}^{\infty}[a_{j+2}(j+2)(j+1)-2a_j j+(E'-1)a_j]\xi^j=0$$

To be true for arbitrary values of ξ^j it must be true that the coefficient of each term must vanish. ie.

$$a_{j+2}(j+2)(j+1)-2a_j j+(E'-1)a_j=0$$

This yields the recursion relation for the coefficients:

$$a_{j+2}=\frac{2j+1-E'}{(j+1)(j+2)}a_j$$

Given an a_0 and an a_1 we can in principle find all the coefficients of the power series expansion! These first two terms are the 2 arbitrary constants required for the solution of a second order differential equation.

Theorem: Solutions to Symmetric Potentials can always be taken to be either even or odd.

Proof: Assume $\psi(x)$ is a solution to the S.E.

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

Let x => -x

$$Note: \partial^2 / \partial(-x)^2 = \partial^2 / \partial x^2$$

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

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

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

So $\psi(-x)$ is also a solution to the S.E.

Hence we can construct even and odd solutions that must also satisfy the S.E.

$$\psi_+(x)\equiv\psi(x)+\psi(-x) \qquad \text{(even in } x\text{)}$$

$$\psi_-(x)\equiv\psi(x)-\psi(-x) \qquad \text{(odd in } x\text{)}$$

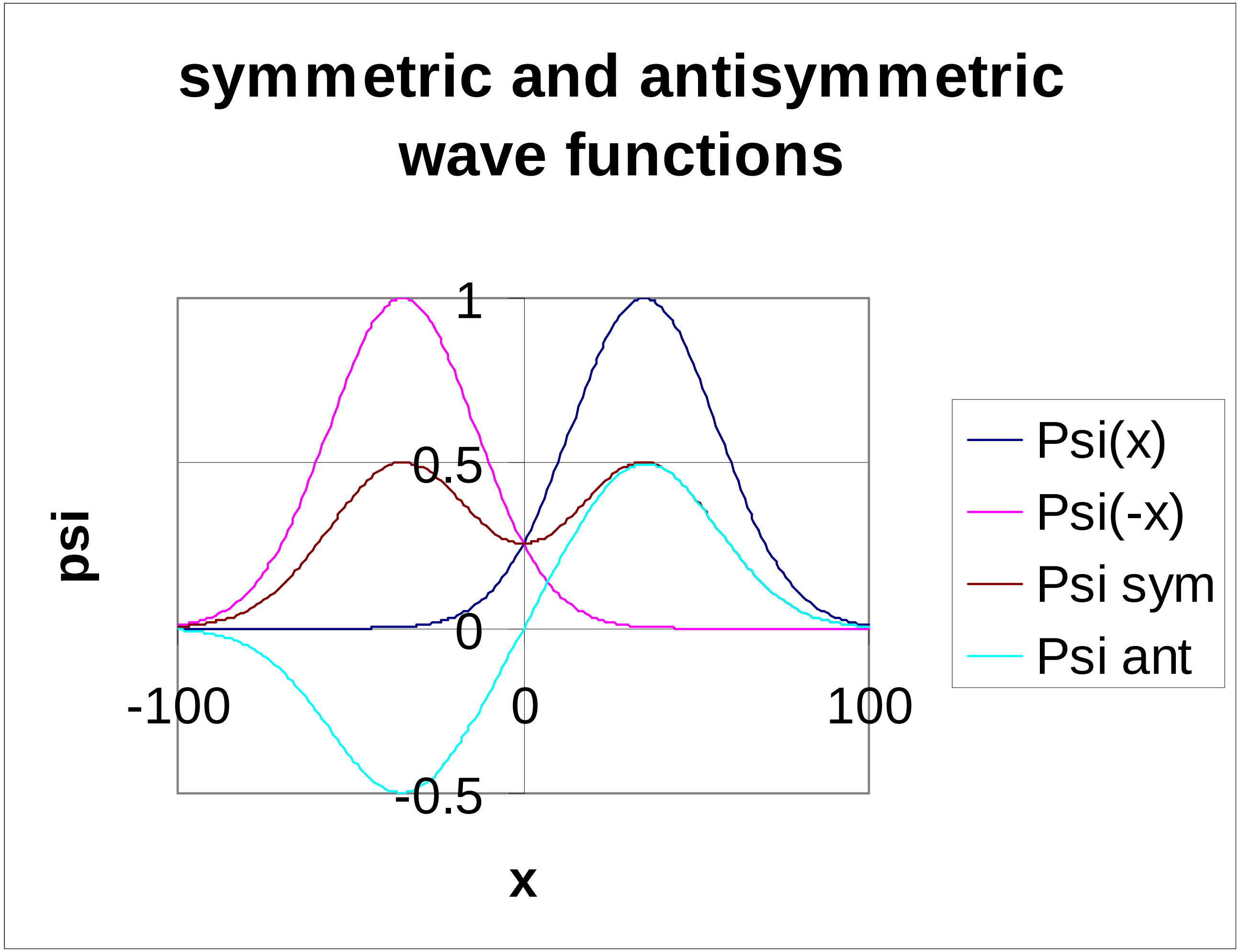
But $$\psi(x)=\tfrac{1}{2}(\psi_+(x)+\psi_-(x))$$

Hence any solution to the S.E. with a symmetric potential can be expressed as a linear combination of even and odd solutions (QED).

Square well from x = -100 to 100 ,V(-x) = V(x).

$\psi(-x)$ is a solution to the SE.

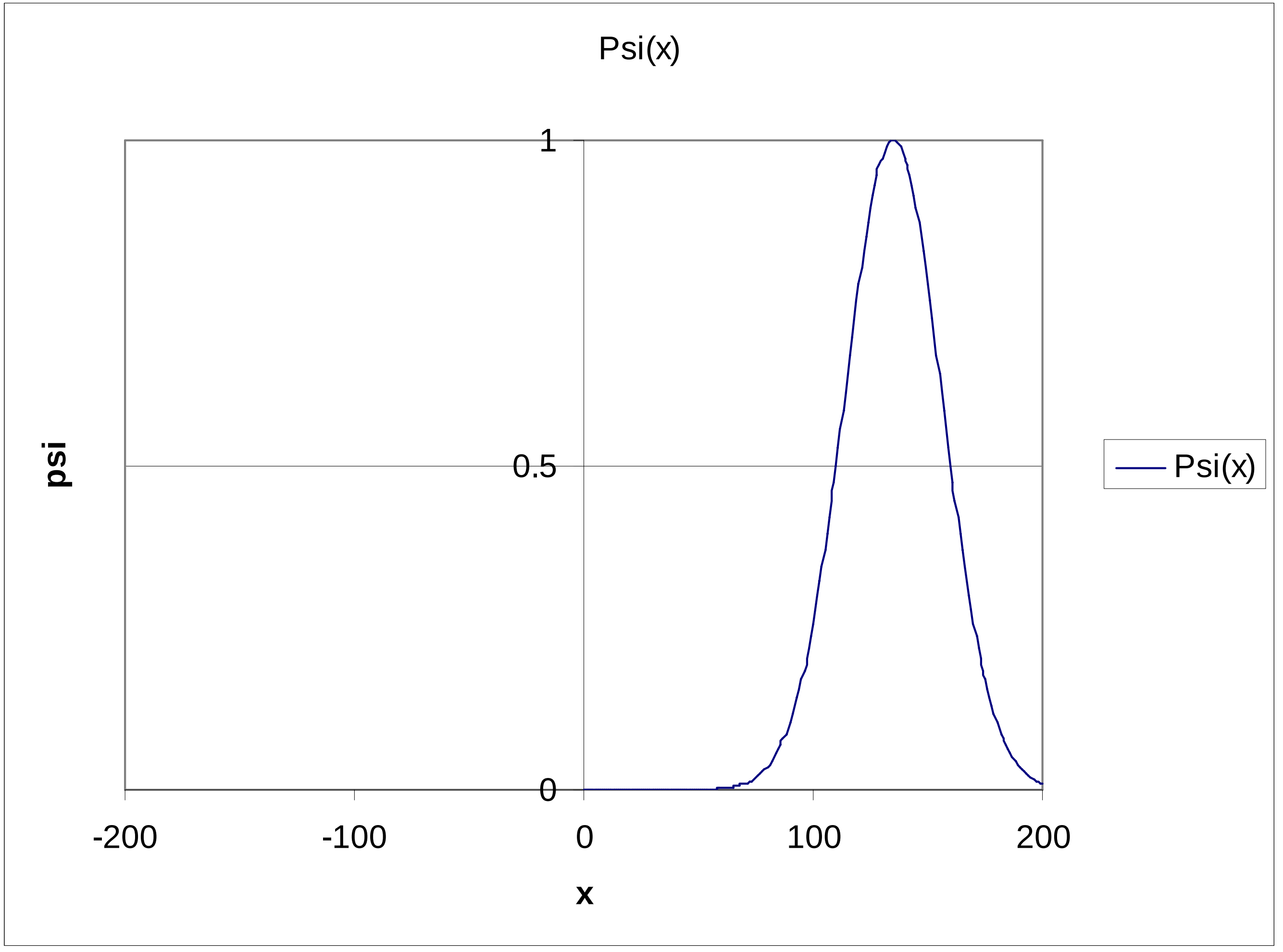
$\psi(x)$ can be written in terms of symmetric and anti-symmetric solutions to the SE.



Square well from x = 0 to 200 ,(V(-x) is not equal to V(x).

ψ(-x) is not a solution to the SE.

ψ(x) can not be written in terms of symmetric and anti-symmetric solutions to the SE.



Note: Also useful for numerical solutions

- One can use this theorem to simplify numerical solutions.
- For a symmetric potential, one may always begin at the origin with either

  $\psi = 0$ (anti-symmetric solutions)

  or $d\psi/dx = 0$ (symmetric solution).