# More 1D Potentials with Bound States

- Piecewise potential review
- Finite square well
- Computational/numerical solution
- Delta function

# The Schrodinger Equation

$$\hat{H}\psi = \hat{E}\psi$$

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

and if V(x) is constant in time,

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

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + (E-V)\psi(x) = 0$$

# Piecewise potentials 1

- Many quantum physics problems can be solved by using the solutions for constant potential in each region and then matching up the solutions and derivatives at the boundaries.
  - Wavefunctions must always be matched.
  - Derivatives must be matched if the are no infinite potential steps in the problem.

# Piecewise potentials 2

Solution to the TISE in a region where V is a constant and E>V:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + (E-V)\psi(x) = 0$$

Guess: $\psi = e^{ikx}$

$$-\frac{\hbar^2 k^2}{2m} = (E-V) \Rightarrow k = \pm\sqrt{\frac{2m(E-V)}{\hbar^2}}$$

$$\psi = Ae^{ikx} + Be^{-ikx}$$

# Piecewise potentials 3

Solution to the TISE in a region where V is a constant and E<V:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} - |E - V|\psi(x) = 0$$

Guess: $\psi = e^{ikx}$

$$\frac{\hbar^2 k^2}{2m} = -|E - V| \qquad \Rightarrow \qquad k = \pm i\sqrt{\frac{2m|E - V|}{\hbar^2}}$$

Let $K = ik = \pm\sqrt{\dfrac{2m|E - V|}{\hbar^2}}$ ($\therefore$ K is a real number)

$\psi = Ae^{Kx} + Be^{-Kx}$ (exponential growth or decay)

# Some “intuitive” rules for sketching wavefunctions*

1. Solutions for the Schrodinger equation curve toward the x-axis in classically allowed $(E > V\ )$ regions and away from the axis in classically forbidden regions.
2. For bound states, the wavefunction must go to zero for large distances outside the well. (must be normalizable)
3. Curvature increases for larger $|E - V(x)|$.
4. Solutions are continuous and smooth if the potential has no infinite steps.
5. Energy eigenfunctions have an integer number of antinodes on classically allowed regions.
6. The  wavefunction amplitude is usually larger in regions with small E>V.

* From https:’’www.asc.ohio-state.edu/physics/ntg/H133/handouts/wavefunctions.pdf

# Illustrated “intuitive” rules

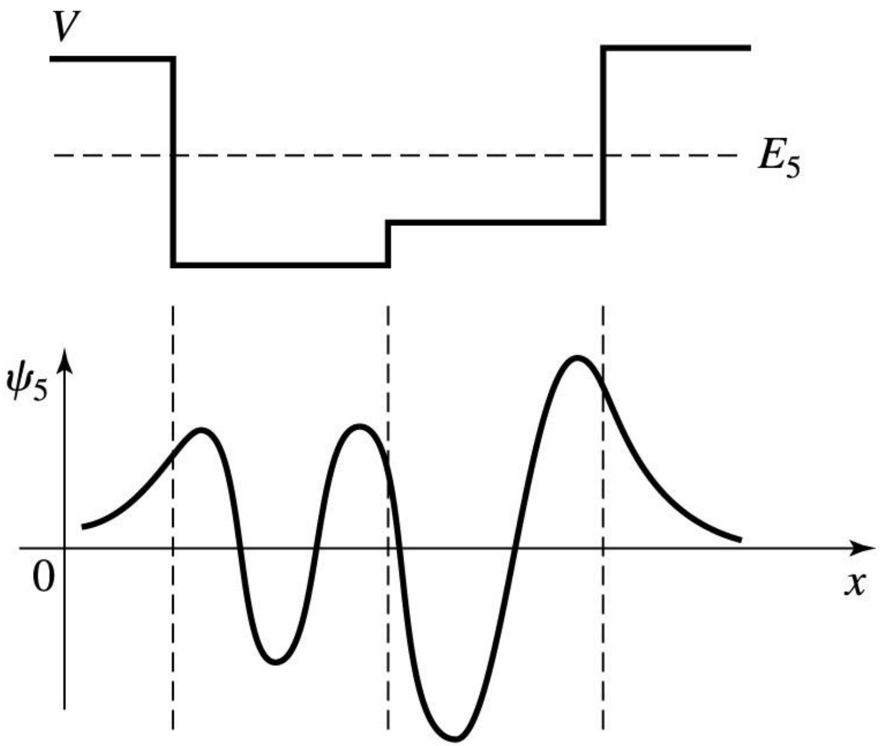
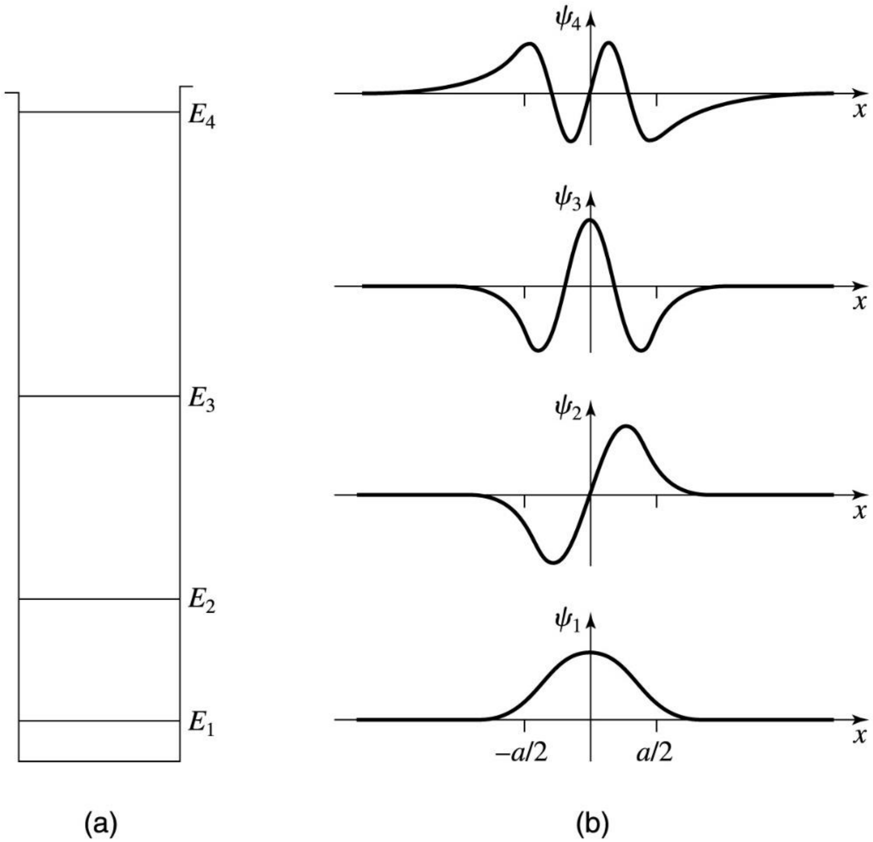



Figure 4.10 copyright 2009 University Science Books

1. Curvature direction.
2. Goes to zero outside well.
3. Curvature magnitude.
4. Continuity/smoothity.
5. Integer antinodes.
6. Wavefunction amplitude

* from Townsend Ch 4

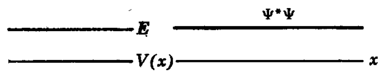
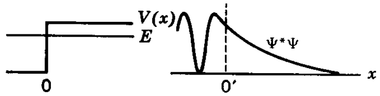
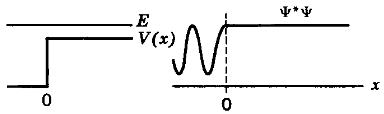
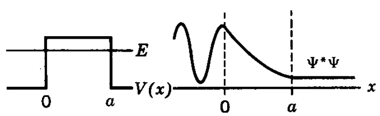
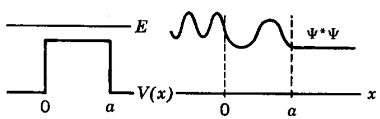
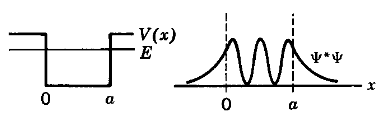
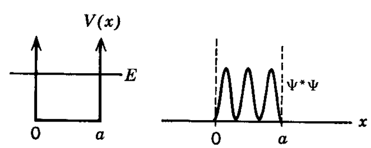
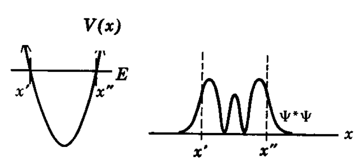
# Bound state wavefunctions for symmetric potentials






Same rules: +

- Ground state has one antinode, centered
- Alternating odd and even functions.

| Name of System | Physical Example | Potential and Total Energies | Probability Density | Significant Feature |
|---|---|---|---|---|
| Zero potential | Proton in beam from cyclotron |  | | Results used for other systems |
| Step potential (energy below top) | Conduction electron near surface of metal |  | | Penetration of excluded region |
| Step potential (energy above top) | Neutron trying to escape nucleus |  | | Partial reflection at potential discontinuity |
| Barrier potential (energy below top) | α particle trying to escape Coloumb barrier |  | | Tunneling |
| Barrier potential (energy above top) | Electron scattering from negatively ionized atom |  | | No reflection at certain energies |
| Finite square well potential | Neutron bound in nucleus |  | | Energy quantization |
| Infinite square well potential | Molecule strictly confined to box |  | | Approximation to finite square well |
| Simple harmonic oscillator potential | Atom of vibrating diatomic molecule |  | | Zero-point energy |

from Eisberg and Resnick

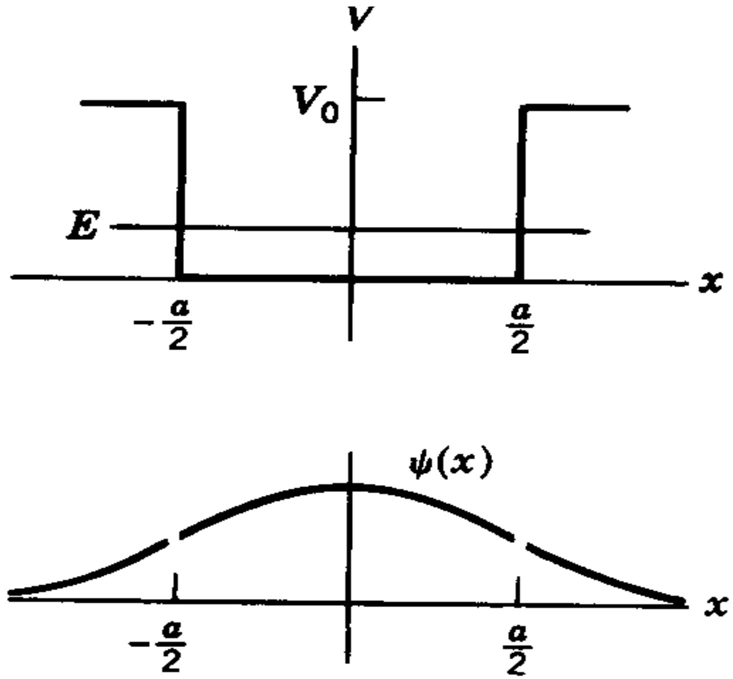
# The Finite Square Well

$$V(x)=\begin{cases}0\,; & -\frac{a}{2}<x<\frac{a}{2}\\ 1; & |x|>\frac{a}{2}\end{cases}$$

$$\psi(x)=\begin{cases}Ce^{Kx}+De^{-Kx}\ \ for\ \ x<-\dfrac{a}{2}\\ A\sin k\,x+B\cos k\,x\ \text{ for }\ -\dfrac{a}{2}<x<\dfrac{a}{2}\\ Fe^{Kx}+Ge^{-Kx}\ for\ \ x>\dfrac{a}{2}\end{cases}$$

where $k=\left|\frac{\sqrt{2mE}}{\hbar}\right|$ and $K=\left|\frac{\sqrt{2m(V_0-E)}}{\hbar}\right|$

We can guess that the solutions will look like those of the infinite square well, but with relaxed decay at the boundaries



The physical requirement that the wavefunction must be normalizable means that it cannot blow up at $\pm\infty, so$

$$\psi(x) = \begin{cases} Ce^{Kx} \ for \ \ x < -\frac{a}{2} \\ A\sin k\,x + B\cos k\,x \text{ for } -\frac{a}{2} < x < \frac{a}{2} \\ Ge^{-Kx} \ for \ \ x > \frac{a}{2} \end{cases}$$

Symmetry of the potential leads to the requirement that the probability density for an eigenfunction be an even function of x. This leads to the requirement that the eigenfunctions be either even or odd.

$$\psi_{even}(x) = \begin{cases} Ce^{Kx} \;\; for \;\; x < -\frac{a}{2} \\ B\cos k\,x \;\; \text{for} \;\; -\frac{a}{2} < x < \frac{a}{2} \\ Ce^{-Kx} \; for \;\; x > \frac{a}{2} \end{cases}$$ (Note that we set C=G.)

$$\psi_{odd}(x) = \begin{cases} Ce^{Kx} \;\; for \;\; x < -\frac{a}{2} \\ B\sin kx \;\; \text{for} \;\; -\frac{a}{2} < x < \frac{a}{2} \\ -Ce^{-Kx} \; for \;\; x > \frac{a}{2} \end{cases}$$ (Note that we set C=-G.)

Now we use the physical properties of the wavefunction at the boundaries to find the constants B and C, and the energies.

Considering the even solutions first:

1) The wavefunction must be continuous at the boundary at +a/2 and –a/2.

For x=-a/2 and +a/2: $B\cos\frac{ka}{2} = Ce^{-\frac{Ka}{2}}$

2) The derivative of the wavefunction must be continuous at the boundaries.

For x=-a/2 and +a/2: $Bk\sin\frac{ka}{2} = CKe^{-\frac{Ka}{2}}$

And dividing eq 2 by eq 1:

$$\left(k \sin \frac{ka}{2}\right) / \left(\cos \frac{ka}{2}\right) = K$$

$$k \tan \frac{ka}{2} = K$$

Similarly, for the odd parity states,

$$\left(k \cos \frac{ka}{2}\right) / \left(-\sin \frac{ka}{2}\right) = K$$

$$k \cot \frac{ka}{2} = -K$$

These equations are transcendental equations that cannot be solved in closed form, but can be solved numerically. A graphical approach yields insight.

From these equations alone, we can find the allowed energies:

$$\frac{\mathrm{K}}{\mathrm{k}} = \tan\left(\frac{kL}{2}\right) \text{ for odd n (even parity)}$$

$$\frac{\mathrm{K}}{\mathrm{k}} = -\cot\left(\frac{kL}{2}\right) \text{ for even n (odd parity)}$$

The even parity state will be the lowest energy state.

These equations cannot be solved in closed form, but we can find the numerical solutions using "solve" in Maple

or by plotting each side as a function of k.

On the next slide we'll switch to terms of energy because everyone does.

Let

$\xi = \frac{ka}{2}$ (a measure of kinetic energy in the well)

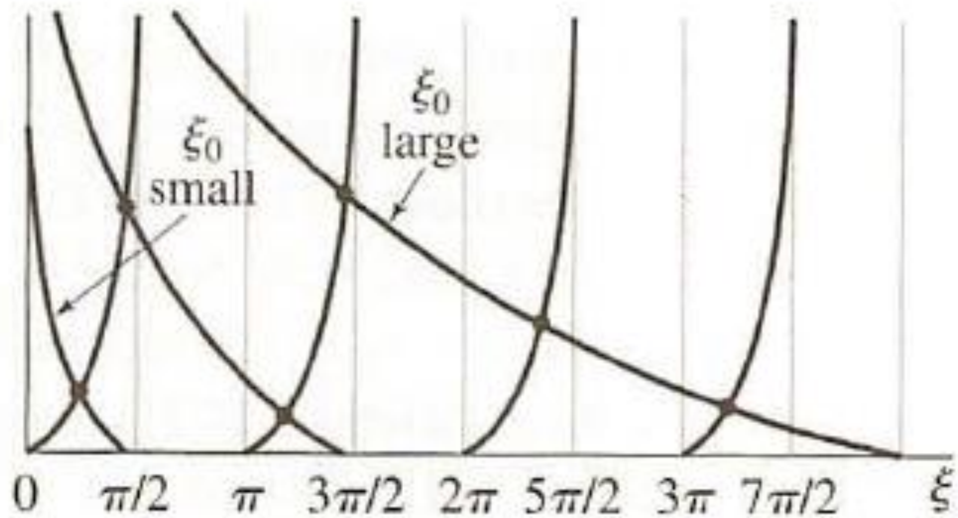
$\xi_0 = \frac{a}{\hbar}\sqrt{\frac{mV}{2}}$ (a measure of the depth of the well)

Then

$$\tan\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$$

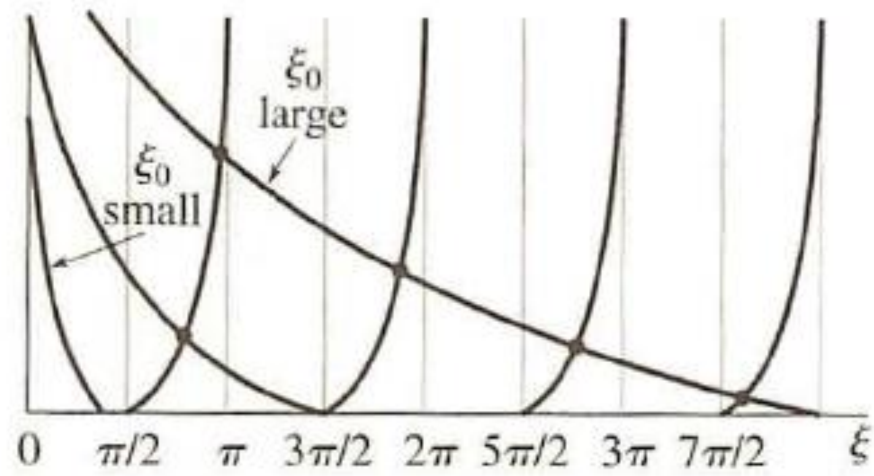
$$-\cot\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$$

Even solutions: Plot both the left hand and right hand side of $\tan\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$ as a function of $\xi$.



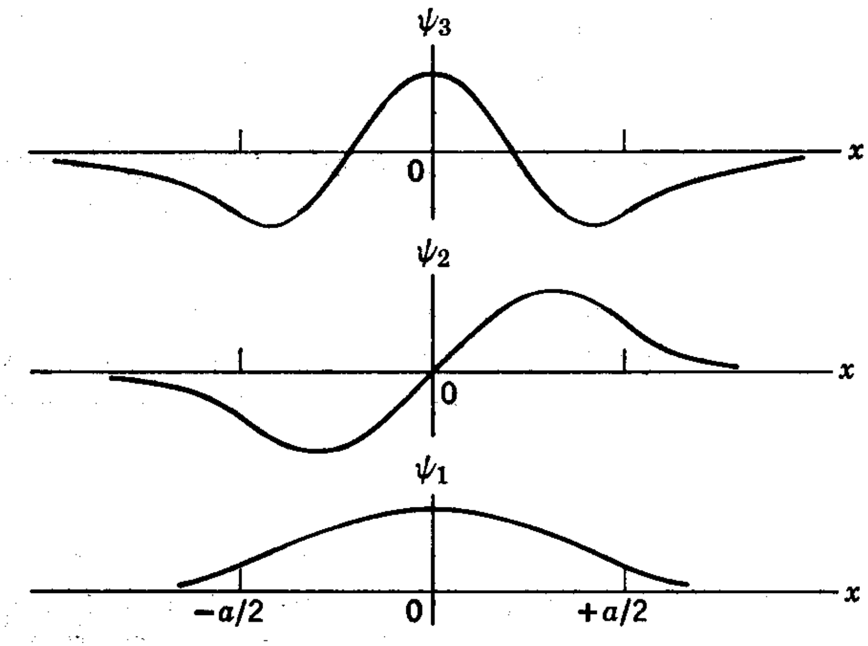

- Intersections are allowed energies
- $\tan\xi$ goes to $\infty$ each time $\xi$ goes through odd $\frac{\pi}{2}$.
- If well depth is small, then only one solution can be found.
- If well depth is large, solutions approach infinite well.

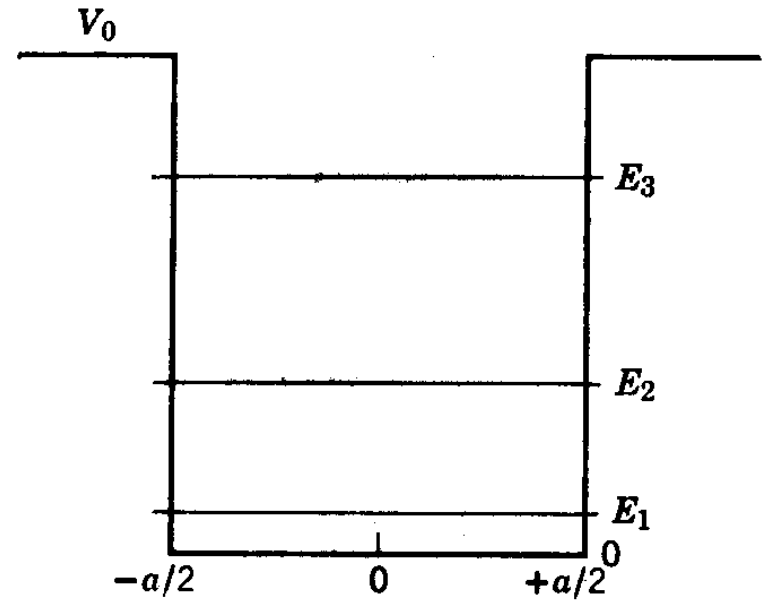
Odd solutions: Plot both the left hand and right hand side of $-\cot\xi = \frac{\sqrt{\xi_0^2-\xi^2}}{\xi}$ as a function of $\xi$.

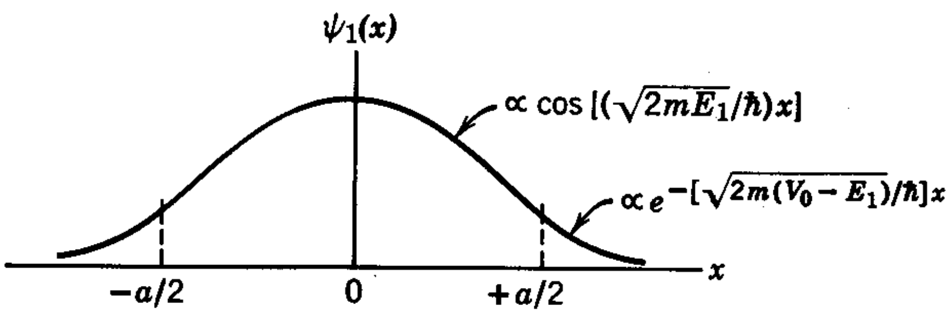



- Intersections are allowed energies
- $-\cot\xi$ goes to $\infty$ each time $\xi$ goes through even $\frac{\pi}{2}$.
- If well depth is small, then only no solution can be found.
- If well depth is large, solutions approach infinite well.

- Summary of eigenfunctions and eigenvalues



# Numerical Solutions

# Numerical approach

Letting $\hbar = m = 1$ in the TISE ,

$$\frac{\partial^2\psi(z)}{\partial z^2} = -2[E - V(z)]\psi.$$

*Convert the TISE to a finite difference equation*

a) $z \Rightarrow z_j = j\Delta z$

b) $\psi(z) \Rightarrow \psi(z_j) \equiv \psi_j$

c) $V(z) \Rightarrow V(z_j) \equiv W_j$

$$\psi'_{j+1/2} \equiv \frac{(\psi_{j+1} - \psi_j)}{\Delta z}$$

$$\psi''_j = \frac{\psi'_{j+1/2} - \psi'_{j-1/2}}{\Delta z} = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta z^2}$$

# Making a difference equation

Plugging in, we get:

$$\psi_{\mathrm{j+1}} = 2\psi_j - \psi_{j-1} + 2\Delta x^2[V_i - E]\psi_i$$

All we need to know to proceed is

1) whether the slope of the wavefunction at a known point is zero or finite.

2) The expected functional behavior of the wavefunction.

The only parameter with which to achieve agreement of the wavefunction with expected behavior is $E$.

# The starting point

- We can choose the starting point based on symmetry.
- For the finite well, even solutions have zero slope at the center. (Let's take $\psi_0 = \psi_1 = 1$.)
- Expected asymptotic behavior: For z growing to large values (outside the well) we expect the wavefunction to go to zero.

- Now we will go to the Jupyter Notebook: The+Shooting+Method+for+solving+finite+well.ipynb

# The Dirac Delta Function

- Definition: $\int_{-\infty}^{\infty} \delta(x - x_0) f(x) dx = f(x_0)$
- $\delta(x - x_0) = \begin{cases} 0 \; for \; x \neq x_0 \\ \infty \;\; for \; x = x_0 \end{cases}$
- $\int \delta(x - x_0) dx = 1$
- $\delta(x) \;\; is \, real$
- $\delta(x) \; is \; even$

# Some Dirac Delta Representations

- $\delta(x) = \begin{matrix} lim \\ \alpha \to \infty \end{matrix} \sqrt{\frac{\alpha}{\pi}} e^{-\alpha x^2}$
- $\delta(x) = \begin{matrix} lim \\ \alpha \to 0 \end{matrix} \frac{1}{\pi} \frac{\alpha}{x^2+\alpha^2}$
- $\delta(x) = \begin{matrix} lim \\ \alpha \to 0 \end{matrix} \frac{1}{\pi} \frac{\sin\frac{x}{\alpha}}{x}$
- $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} dx$

# The delta function potential

$$\hat{H}\psi = \hat{E}\psi$$

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

with $\lambda$ negative, for an attractive potential.

http://galileo.phys.virginia.edu/classes/751.mf1i.fall02/OneDimSchr.htm

$\psi = Ae^{Kx} + Be^{-Kx}$

So for negative x, $\psi^{-} = Ae^{Kx}$

and for positive x, $\psi^{+} = Be^{-Kx}$

Continuity of the wavefunction gives $\psi^{-} = \psi^{+}\ so\ A = B$.

The slope on the two sides is discontinuous due to the infinite $\delta$ function.

$\left.\frac{d\psi}{dx}\right|_{-\beta} = KA;\quad \left.\frac{d\psi}{dx}\right|_{\beta} = -KA;$ for small $\beta,$ so $\left.\frac{d\psi}{dx}\right|_{-\beta} \quad \left.\frac{d\psi}{dx}\right|_{\beta} - \left.\frac{d\psi}{dx}\right|_{-\beta}$

$= -2KA;$

Returning to the Schrodinger equation,

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

We integrate both sides once in x, from $-\beta$ to $+\beta$.

$$-\int_{-\beta}^{\beta}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi dx + \int_{-\beta}^{\beta}\lambda\delta(x)\psi dx = \int_{-\beta}^{\beta}E\psi dx$$

The rhs goes to zero as $\beta \Rightarrow 0$ because the integrand is finite.

so, $\displaystyle\int_{-\beta}^{\beta} \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi dx = \int_{-\beta}^{\beta} \lambda\delta(x)\psi dx$

Doing both integrals separately, $\displaystyle\frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\bigg|_{-\beta}^{\beta} = \lambda\psi(0)$

and substituting $\displaystyle\frac{\partial\psi}{\partial x}\bigg|_{-\beta}^{\beta} = -2AK$ (from the previous slide),

we have $\displaystyle -\frac{\hbar^2 K}{m} = \lambda$

$$K = -\frac{\lambda m}{\hbar^2} \quad \Rightarrow \quad E = \frac{\hbar^2 K^2}{2m} = -\frac{m\lambda^2}{2\hbar^2}$$

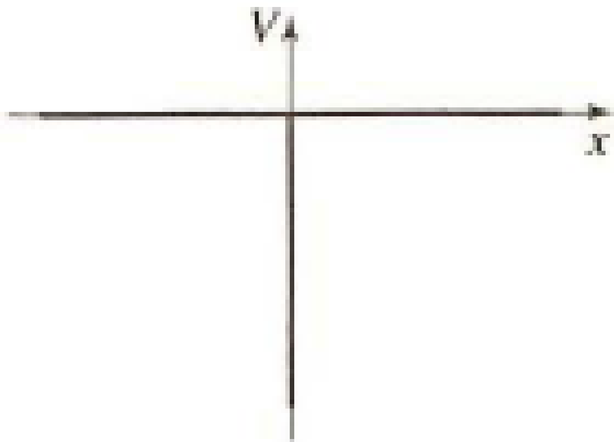



Figure 4.14 The Dirac delta function potential energy (4.77).

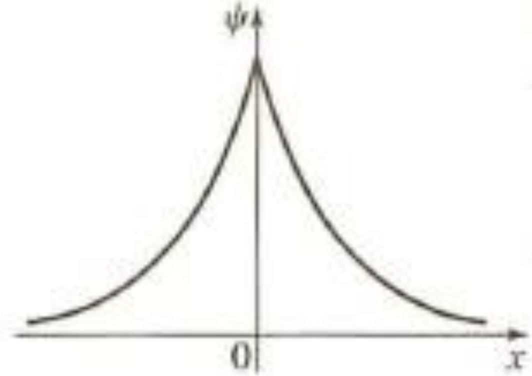



Figure 4.15 The wave function (4.85) for a particle bound in a Dirac delta function potential energy well.

$$\psi(x) = \mathrm{A}\exp\left(-\frac{\lambda m}{\hbar^2}|x|\right)$$

is the only bound state.