ECE 162A
Mat 162A

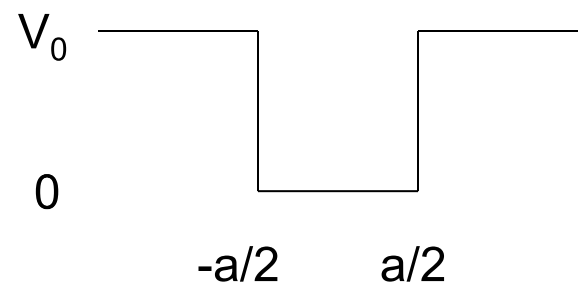
Lecture #7
Read Chapter 6 of Eisberg,Resnick
Chapter 5 of French/Taylor

Solutions to SE

- Free particle
- Step potential
- Infinite box
- Finite box
- Harmonic oscillator

Square Well

$$\frac{\hbar^2 k^2}{2m} = E \qquad \frac{\hbar^2 \kappa^2}{2m} = V_0 - E$$



$$For\ |x| < a/2$$

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

$$For\ x < -a/2$$

$$\psi(x) = C\exp(\kappa x) + D\exp(-\kappa x)$$

$$Boundary\ condition:\ \ D = 0$$

$$For\ x > a/2$$

$$\psi(x) = F\exp(\kappa x) + G\exp(-\kappa x)$$

$$Boundary\ condition:\ \ F = 0$$

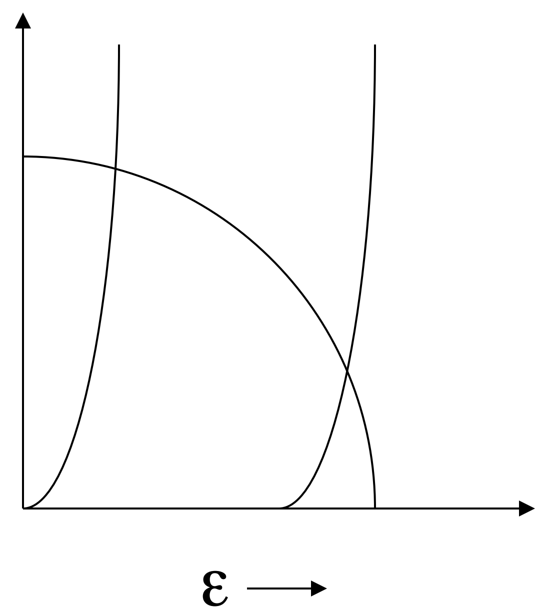
Solution in Appendix H

- 4 Equations (ψ and dψ/dx at two interfaces)
- 4 Unknowns (A,B,D,G)
- Solution for :

$$\varepsilon \tan \varepsilon = \sqrt{R^2 - \varepsilon^2}$$

where

$$E = \frac{2\hbar^2 \varepsilon^2}{ma^2} \qquad R^2 = \frac{mV_0 a^2}{2\hbar^2}$$



Harmonic Oscillator

- $V(x)=1/2\ C\ x^2$
- Very common because it represents any small vibration about a point of stable equilibrium
- Examples
  - Diatomic molecules
  - Atoms vibrating on a lattice.
  - Particle on a string.

Solution in Appendix I

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

Solution:

$$Let\ \alpha=\sqrt{\frac{Cm}{\hbar}} \quad \beta=\frac{2mE}{\hbar^2}$$

Then Schroedinger's Equation becomes

$$\frac{d^2\psi}{dx^2}+(\beta-\alpha^2x^2)\psi=0$$

$$Let\ u=\sqrt{\alpha}x$$

$$\frac{d^2\psi}{du^2}+(\frac{\beta}{\alpha}-u^2)\psi=0$$

For large u:

$$\frac{d^2\psi}{du^2} + (\frac{\beta}{\alpha} - u^2)\psi = 0$$

$$\frac{d^2\psi}{du^2} - u^2\psi \approx 0$$

$$\psi = Ae^{-u^2/2} + Be^{u^2/2}$$

$$Finite\,\psi \;\; means \;\; B = 0$$

$$\psi \approx Ae^{-u^2/2} \;\; f\,oru \rightarrow \infty$$

$$Try \;\; to \;\; f\,ind H(U) \;\; that \;\; satisf\,iesSE:$$

$$\psi = AH(u)e^{-u^2/2}$$

Solutions to Harmonic Oscillator

Substitute in SE to get the Hermite DE:

$$\frac{d^2H}{du^2} - 2u\frac{dH}{du} + (\frac{\beta}{\alpha} - 1)H = 0$$

$$H(u) = a_0 + a_1 u + a_2 u^2 + \ldots$$

Calculate the values of a_i:

$$\psi_0 = A_0 e^{-u^2/2}$$

$$\psi_1 = A_1 u e^{-u^2/2}$$

$$\psi_2 = A_2(1 - 2u^2)e^{-u^2/2}$$

where $\beta/\alpha = 2n + 1$ *causes the series to stop*

Where $E_n = (n+1/2)h\nu$ where $n = 0, 1, 2, \ldots$

Eigenvalues

E_n=(n+1/2)hν where n=0,1,2,…
And

$$\nu = \frac{1}{2\pi}\sqrt{\frac{C}{m}}$$

- The series H(u) are called Hermite polynomials.

- Page 223,224

Harmonic oscillator 13th mode

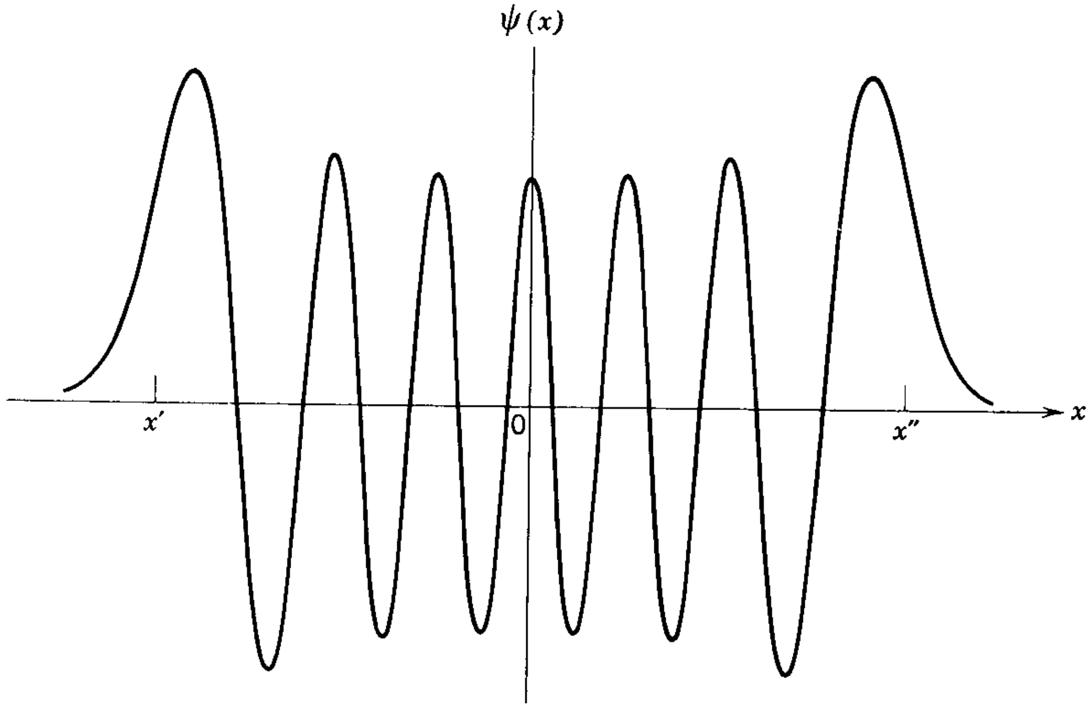


Figure 5-18 The eigenfunction for the thirteenth allowed energy of the simple harmonic oscillator. The classical limits of motion are indicated by x' and x''.

Qualitative Plots

- Lowest energy solution has no nodes.
- Successively higher energy solutions have additional nodes.
- Curvature related to E-V
- Decay rate related to V-E.
- For constant V:
  - sinusoid for E>V (k constant)
  - Exponential decay for E<V (κ constant)

$$\frac{\hbar^2 k^2}{2m} = E - V$$

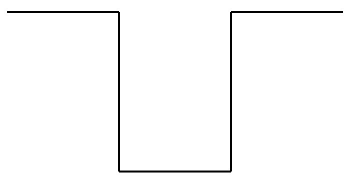
$$\frac{\hbar^2 \kappa^2}{2m} = V - E$$

- Amplitudes larger in smaller curvature regions.
  - (Classically, lower P means slower velocity, more likely to find there.)

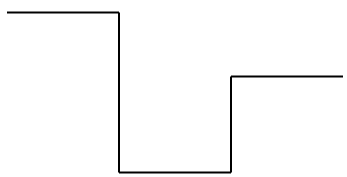
Symmetry

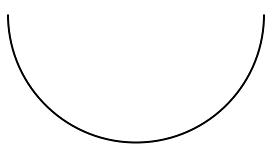
- If V(x) is symmetric, then all solutions are either
  – Symmetric (even parity)
  – Antisymmetric (odd parity)

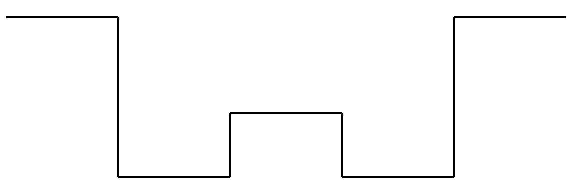
Sketch the solutions



How do they differ from infinite square well?







Computer Solutions

- French/Taylor page 174. Eisberg/Resnick Appendix G
- Convert SE to dimensionless units.
- Otherwise, you are dealing with very large quantities and get numeric overflow and inaccuracies.

- A dimensionless form is

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

- Where z is some appropriate natural unit z=x/L

$$\frac{d^2\psi}{dz^2} = (\varepsilon - v(x))\psi$$

Solve Numerically

- Divide z into a mesh with steps Δz

$$z \rightarrow z_j = j\Delta z$$

$$\psi(z) \rightarrow \psi(z_j) = \psi_j$$

$$W(z) \rightarrow W(z_j) = W_j$$

Calculate derivatives using finite difference

$$\frac{d\psi}{dz} = \frac{\psi_{j+1} - \psi_j}{\Delta z}$$

$$\frac{d^2\psi}{dz^2} = \left(\frac{\psi_{j+1} - \psi_j}{\Delta z} - \frac{\psi_j - \psi_{j-1}}{\Delta z}\right) / \Delta z$$

$$\frac{d^2\psi}{dz^2} = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta z^2}$$

This can be inverted and combined with SE to yield

$$\psi_{j+1} = (2 - \Delta z^2(\varepsilon - W_j))\psi_j - \psi_{j-1}$$

Numerical solutions (cont)

- W_j is known.
- Pick a value for $\varepsilon_{n.}$ Choose wisely.
- Start with a value for ψ_j and calculate across mesh. Choose wisely. (Use symmetric if possible and ignore normalization i.e. start with ψ_j =1.
- Adjust ε_n and recalculate until an appropriate solution is found (finite at infinity).