ECE 162A
Mat 162A

Lecture #8: Stationary Solutions
Read Chapter 5,6 of Eisberg,Resnick
Appendix H,I
Read French/Taylor Chapter 3

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

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

$Solution:$

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

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:

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

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

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

What Boundary condition can be applied?

For large u:

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

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

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

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

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

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

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

Solutions to Harmonic Oscillator

$$Substitute\ in\ SE\ to\ get\ the\ Hermite\ DE:$$

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

$$H(u) = a_0 + a_1u + a_2u^2 + \ldots$$

$$Calculate\ the\ values\ of\ a_i:$$

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

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

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

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

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

Eigenvalues

$E_n=(n+1/2)h\nu$ where n=0,1,2,…
And

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

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

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Harmonic oscillator 13th mode

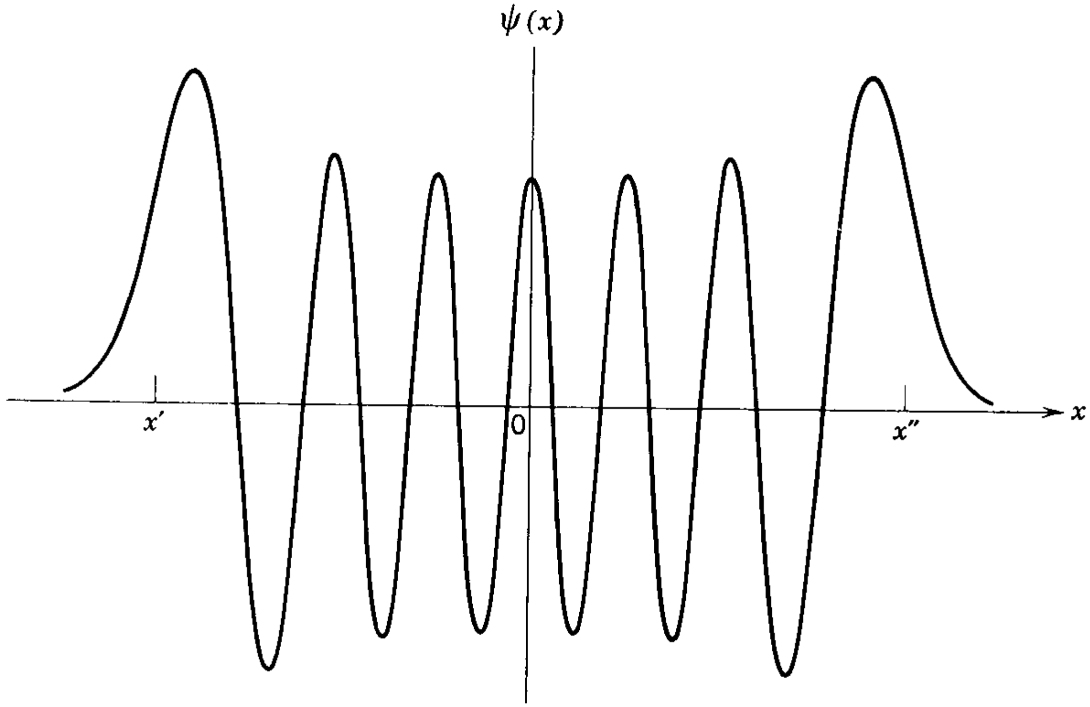


Figure 5-18 The eigenfunction for the thirteenth allowed energy of the simple harmonic oscillator. The classical limits of motion are indicated by x' and x''.

3 Dimensional Time Independent Schroedinger Equation

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)+V(x,y,z)\psi(x,y,z)$$

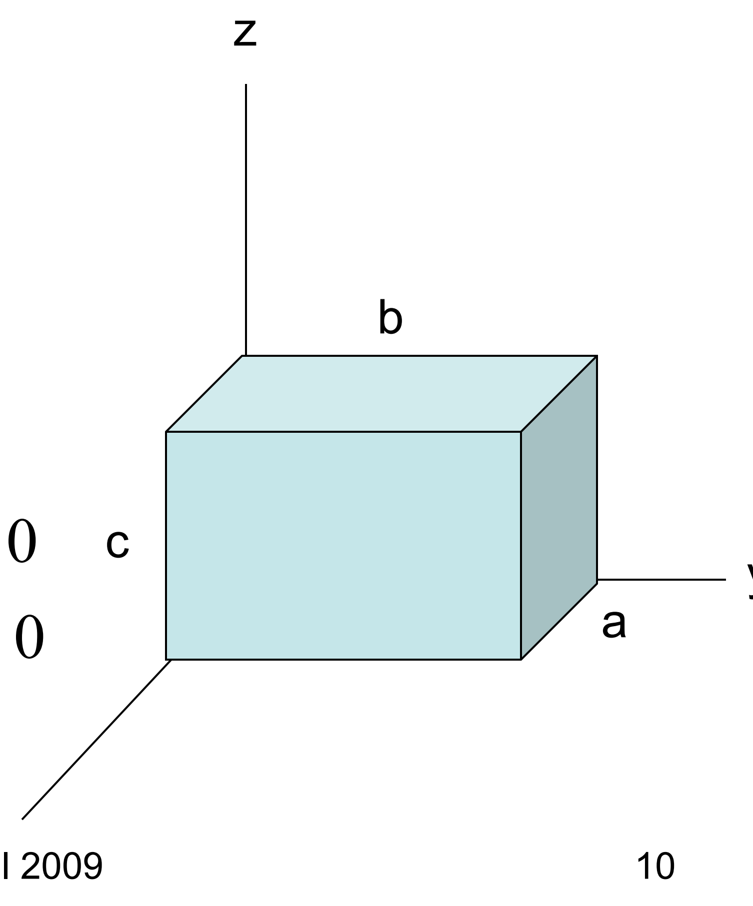
$$=E\psi(x,y,z)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi$$

Free Particle in a 3D Box

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial x^2}\right)\psi(x,y,z)+V(x,y,z)\psi(x,y,z)$$

$$= E\psi(x,y,z)$$



$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$Boundary\,Conditions:$$

$$\psi(0,y,z)=\psi(x,0,z)=\psi(x,y,0)=0$$

$$\psi(a,y,z)=\psi(x,b,z)=\psi(x,y,c)=0$$

Separation of Variables

- Voltage is separable
- Boundary conditions are separable

So try:

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

3D Particle in a Box

$$-\frac{\hbar^2 YZ}{2m}\frac{d^2X}{dx^2}-\frac{\hbar^2 XZ}{2m}\frac{d^2Y}{dy^2}-\frac{\hbar^2 XY}{2m}\frac{d^2Z}{dz^2}=EXYZ$$

$Divide \quad by \quad XYZ$

$$-\frac{\hbar^2}{2mX}\frac{d^2X}{dx^2}-\frac{\hbar^2}{2mY}\frac{d^2Y}{dy^2}-\frac{\hbar^2}{2mZ}\frac{d^2Z}{dz^2}=E$$

$FunctionofX \;\; FunctionofY \;\; FunctionofZ = Const.$

$$E_x + E_y + E_z = E$$

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2}=E_x X$$

$$X = e^{ikx}$$

$$\psi = e^{ikx}e^{iky}e^{ikz} = e^{ikx+iky+ikz}$$

Simplest to use Sines and Cosines to match boundary conditions

$$X(x) = \sin\frac{n_x \pi x}{a} \quad n_x = 1,2,3,...$$

$$Y(y) = \sin\frac{n_y \pi y}{b} \quad n_y = 1,2,3,...$$

$$Z(z) = \sin\frac{n_z \pi z}{c} \quad n_z = 1,2,3,...$$

$$E = \frac{\hbar^2}{2m}\left(\left(\frac{n_x \pi}{a}\right)^2 + \left(\frac{n_y \pi}{b}\right)^2 + \left(\frac{n_z \pi}{c}\right)^2\right)$$

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

Time Dependence of Solution

- Solve for stationary solutions $\psi_n(x)$ with energies E_n

$$\Psi(x,t) = \sum_n A_n \psi_n(x) e^{-i\omega_n t}$$

$$\omega_n = E_n / \hbar$$

- Find the values for A_n that satisfy the intial conditions.

Motion of a Particle in a Box

$$\psi(x) = A_1 \sin(\frac{\pi x}{L}) + A_2 \sin(\frac{2\pi x}{L}) + \cdots$$

$$E_n = E_0 n^2$$

$$Special\ case A_1 = A_2 = 1; others\ \ 0$$

$$\Psi(x,t) = \sin(\frac{\pi x}{L}) e^{i\omega t} + \sin(\frac{2\pi x}{L}) e^{4i\omega t}$$

Wave function evolution

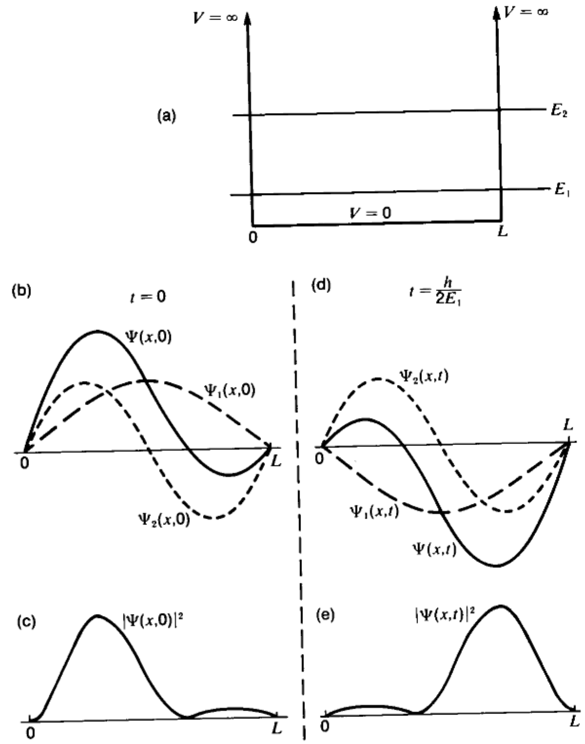


Fig. 8-1 Superposition of the lowest stationary states of an infinite square well. (a) Potential energy function for the well, with the two lowest energy eigenvalues shown. (b) Eigenfunctions for the two lowest energy states (broken lines) and the superposition of these functions (solid line), at $t = 0$. (c) Probability density function at $t = 0$ for the superposition shown in (b). (d) and (e) Plots corresponding to (b) and (c) for the later time $t = h/(2E_1)$.

ing $E = 0$ at the bottom of the well)

$$E_n = \frac{n^2h^2}{8mL^2}$$

Therefore,

$$\omega_2 = \frac{E_2}{\hbar} = 4\frac{E_1}{\hbar} = 4\omega_1$$

Thus one half-cycle for ω_1 occupies the same time as two complete cycles for ω_2. This means that between $t = 0$ and $t = h/2E_1$ the relative signs of the two components reverse, as

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Time Evolution

$$\psi(x) = \sin(\frac{\pi x}{L}) + \sin(\frac{2\pi x}{L}) = f_1 + f_2$$

$$\Psi(x,t) = f_1 e^{i\omega t} + \ f_2 e^{4i\omega t}$$

$$\left|\Psi(x,t)\right|^2 = f_1^2 + f_2^2 + 2 f_1 f_2 \cos((E_2 - E_1)t/\hbar)$$