Chapter 4, continued

particle in 3D box, V = 0 for 0 < x < a,
0 < y < b,
0 < z < c
= ∞,   otherwise

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

assume the problem separates: $\psi(x,y,z)=X(x)Y(y)Z(z)$

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

$$\frac{-\hbar^2}{2m}\left[\underbrace{\frac{1}{X}\frac{d^2X}{dx^2}}_{\text{depends only on x}}+\underbrace{\frac{1}{Y}\frac{d^2Y}{dy^2}}_{\text{depends only on y}}+\underbrace{\frac{1}{Z}\frac{d^2Z}{dz^2}}_{\text{depends only on z}}\right]=\underbrace{E}_{\text{a constant}}$$

depends only on x   depends only on y   depends only on z   a constant

Tells us that this separates into three different equations

$$\Rightarrow \quad \left.\begin{aligned} \frac{-\hbar^2}{2m}\frac{d^2X}{dx^2} &= E_x X \\ \frac{-\hbar^2}{2m}\frac{d^2Y}{dy^2} &= E_y Y \\ \frac{-\hbar^2}{2m}\frac{d^2Z}{dz^2} &= E_z Z \end{aligned}\right\} E = E_x + E_y + E_z$$

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right), \quad n_x, n_y, n_z = 1, 2, \ldots$$

$$\psi(x, y, z) = N \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

let a = b = c

$$E = \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$$

$$E(1,1,1) = \frac{h^2}{8ma^2}(3)$$

$$\left.\begin{array}{l} E(2,1,1) = \dfrac{h^2}{8ma^2}(6) \\ E(1,2,1) \\ E(1,1,2) \end{array}\right\}$$

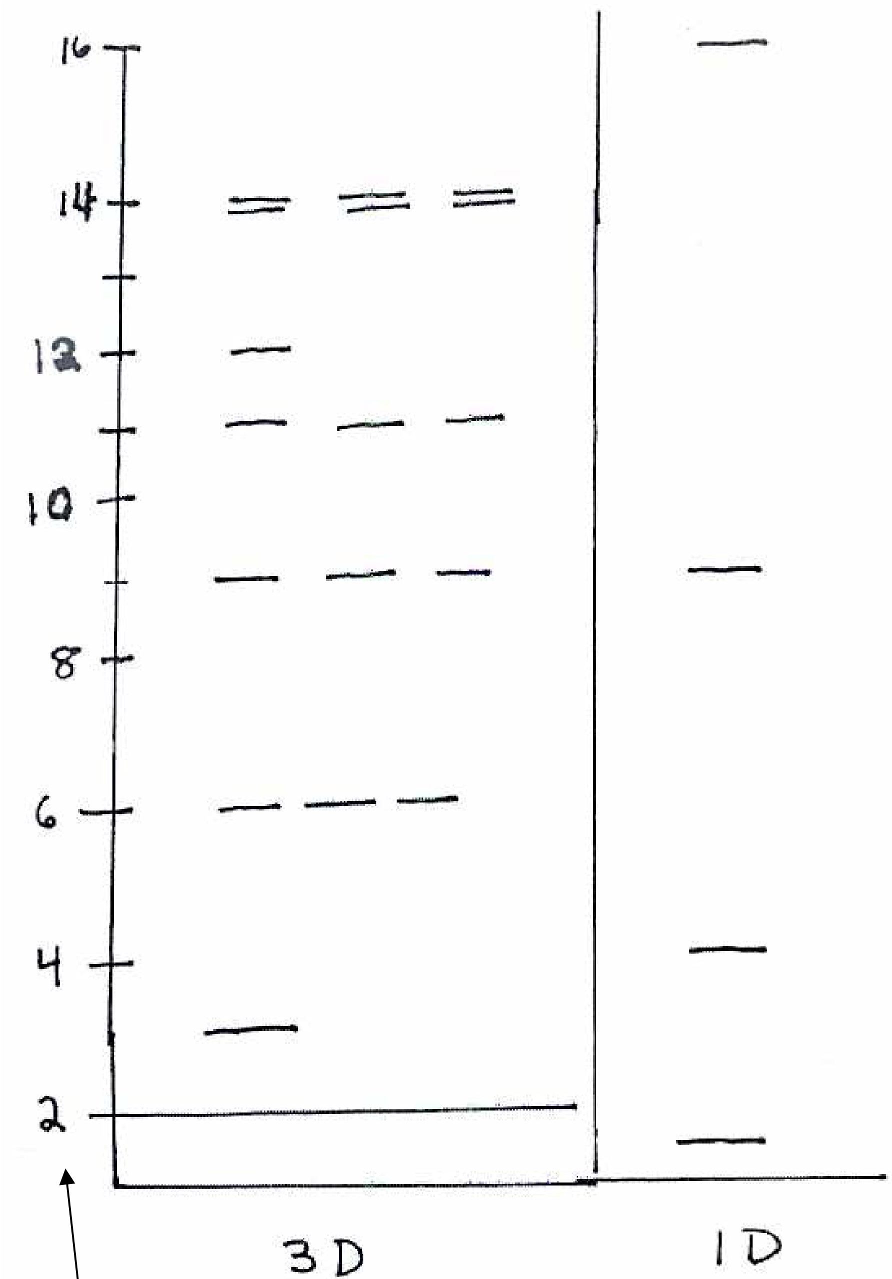
$$\left.\begin{array}{l} E(2,2,1) = \dfrac{h}{8ma^2}(9) \\ E(2,1,2) \\ E(1,2,2) \end{array}\right\}$$

$$\left.\begin{array}{l} E(3,1,1) = \dfrac{h^2}{8ma^2}(11) \\ E(1,3,1) \\ E(1,1,3) \end{array}\right\}$$

$$E(2,2,2) = \frac{h^2}{8ma^2}(12)$$

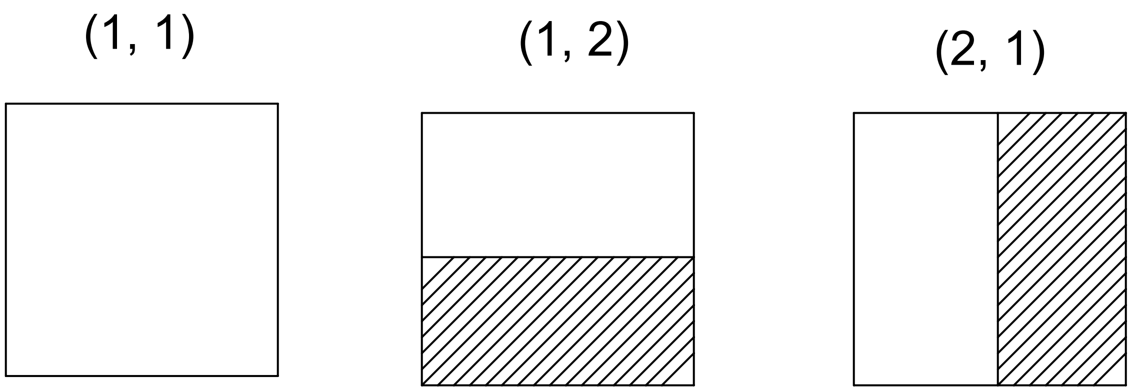
$$E(1,2,3) = \frac{h^2}{8ma^2}(14)$$

6-fold degenerate



Energy in units of $h^2/8ma^2$

- Note how much more rapidly energy levels grow for 3D *vs.* 1D
- Degeneracies are a result of symmetry
  - In general if a ≠ b, no degeneracies



Imagine looking at the wavefunction from above: white is where it is above the xy plane and shaded indicates where it is below

Nodal patterns for (1,1), (1,2), (2,1) eigenfunctions of 2D particle-in-box problem

back to the 1D particle-in-box problem: example 4.2

Consider a wavefunction which a a superposition of two eigenfunctions

$$\psi = c\sin\left(\frac{\pi x}{a}\right) + d\sin\left(\frac{2\pi x}{a}\right) \longleftarrow$$

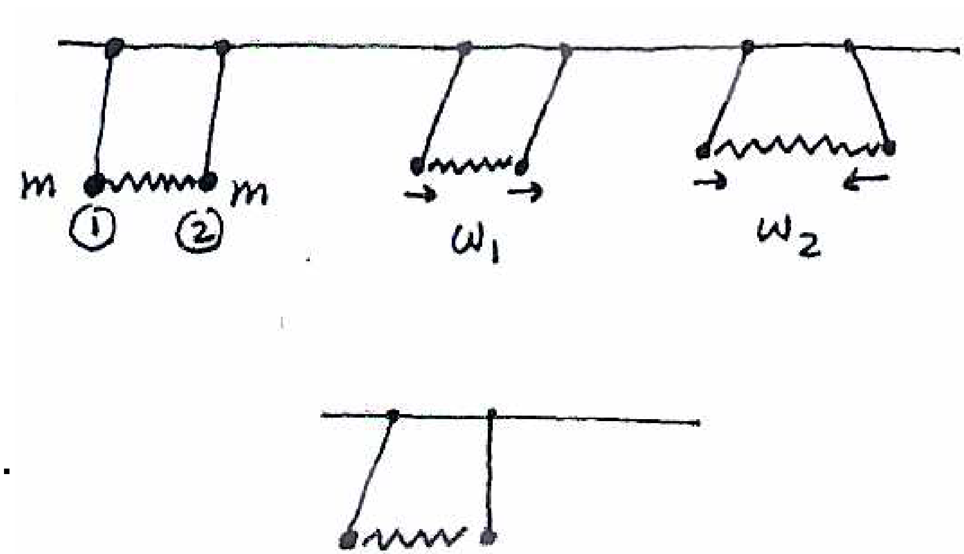
Not an e.f. of H unless c or d = 0

$$\Psi(x,t) = c\ e^{-iE_1 t/\hbar}\sin\left(\frac{\pi x}{a}\right) + d\ e^{-iE_2 t/\hbar}\sin\left(\frac{2\pi x}{a}\right)$$

$$\neq \psi(x)\, f(t)$$

$$\Rightarrow \text{ Not a standing wave}$$

Classical analog



two fundamental frequencies

ω_1, ω_2

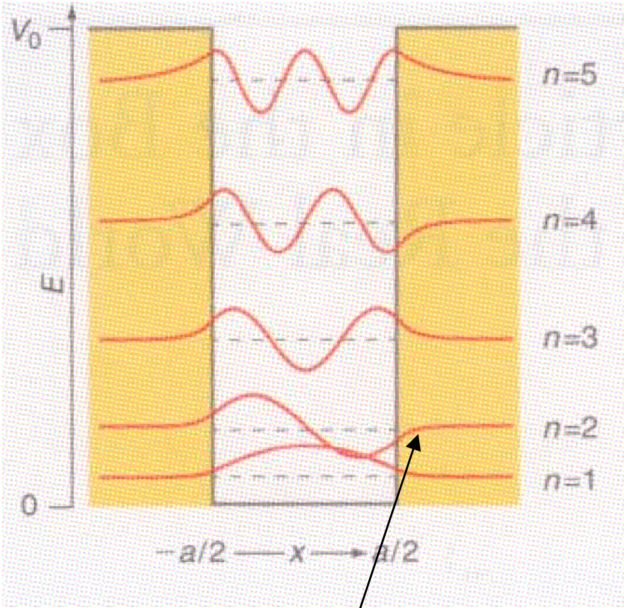
As discussed in class, both motions and frequencies are present, when the initial condition is that to the right.

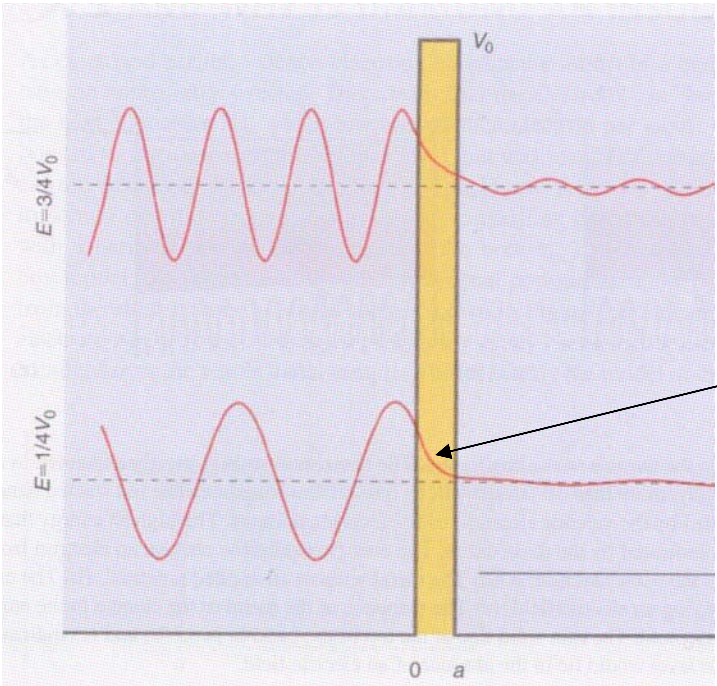
What happens if the box is finite?

The wavefunction now leaks (tunnels) outside the box

What if there is a barrier?

The particle can tunnel through the barrier





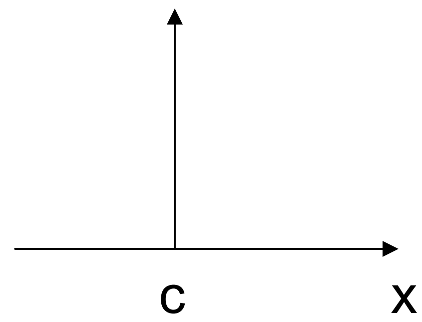
Classically forbidden region

exponential decay

Figures from Engel text.

δ(x-c) = delta function = 0, x ≠ c

= ∞, x = c



$$\int_{-\infty}^{\infty} f(x)\delta(x-c)dx = f(c)$$

Convince yourself that for the particle-in-box problem, δ(x-c) can be represented as a sum over all $\sin\left(\frac{n\pi x}{a}\right)$ functions.

⇒ momentum ranges over all possible values

Note the connection with the uncertainty principle

Some additional exercises:

$$\text{if } \psi(x) = \sqrt{\frac{2}{a}}\left[c\sin\frac{\pi x}{a} + d\sin\frac{2\pi x}{a}\right], \quad c^2 + d^2 = 1$$

What is $<\hat{H}>$? $\quad c^2E_1 + d^2E_2 = c^2\frac{h^2}{8ma^2} + d^2\frac{4h^2}{8ma^2}$

$$<\psi\left|\hat{H}\right|\psi> = \frac{2}{a}\int_o^a\left(c\sin\frac{\pi x}{a} + d\sin\frac{2\pi x}{a}\right)\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\left(c\sin\frac{\pi x}{a} + d\sin\frac{2\pi x}{a}\right)$$

$$= \frac{2}{a}\left[\int_o^a\left(c\sin\frac{\pi x}{a} + d\sin\frac{2\pi x}{a}\right)\left(\frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\right)\left(c\sin\frac{\pi x}{a} + 4d\sin\frac{2\pi x}{a}\right)\right]$$

$$= \frac{h^2}{4ma^3}\left[c^2\int_o^a\sin^2\frac{\pi x}{a}dx + 4d^2\int_o^a\sin^2\frac{2\pi x}{a}dx\right]$$

$$= \frac{h^2}{8ma^2}\left[c^2 + 4d^2\right]$$