Chapter 2, continued

particle in 3D box, $V = 0$ for $0 < x < a$, $0 < y < b$, $0 < z < c$
$= \infty$, 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 wavefunction 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

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

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right), \quad n_x, n_y, n_z = 1, 2, 3, \ldots$$

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

let a = b = c

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

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

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

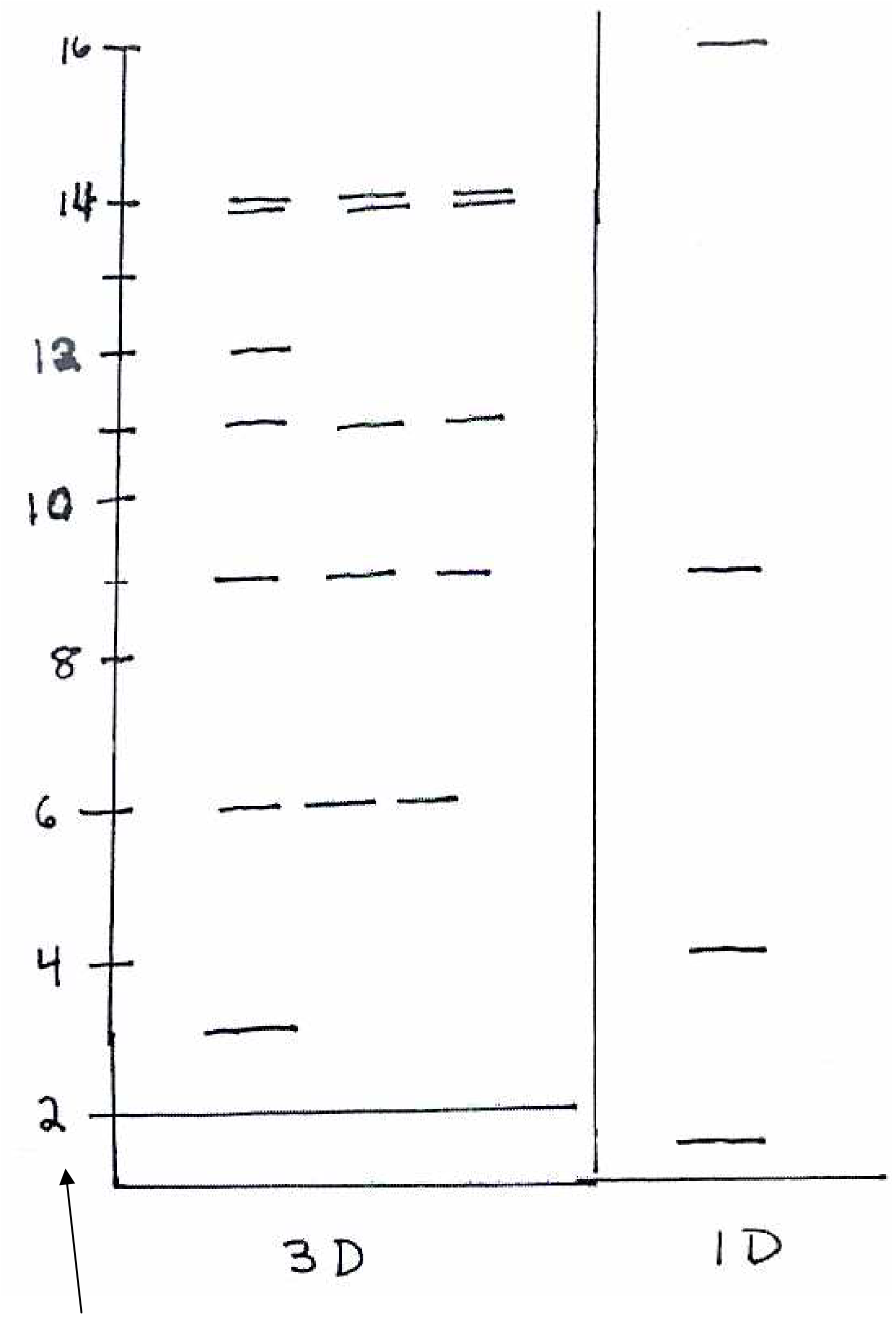
$$\left\{\begin{array}{l} E(2,2,1) = \dfrac{h}{8ma^2}(9) \\ E(2,1,2) \\ E(1,2,2) \end{array}\right.$$

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

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

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

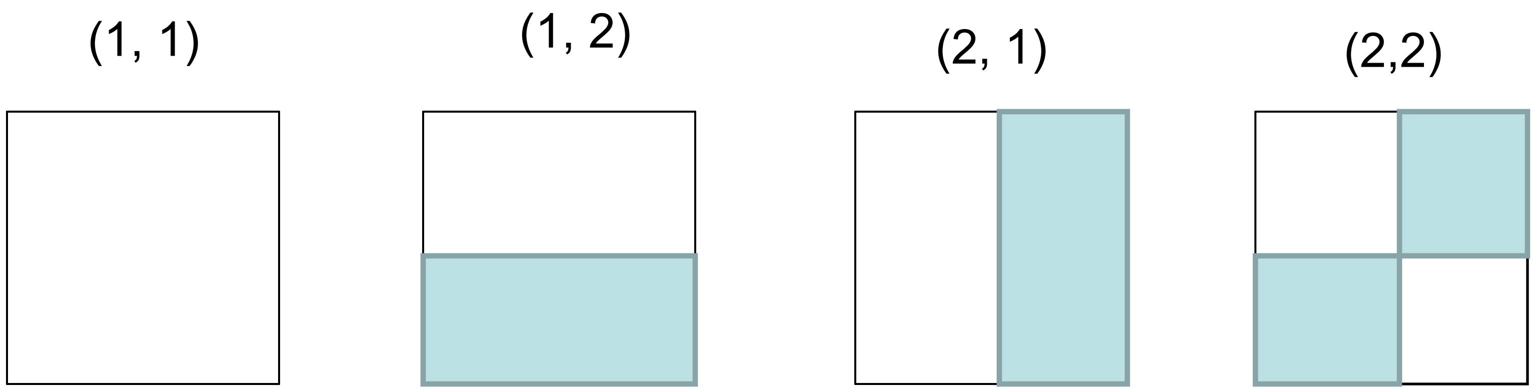
6-fold degenerate



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



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

example 4.2

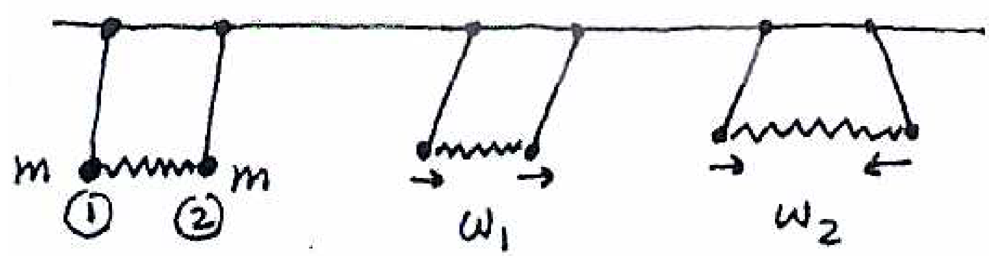
$$\psi = c\sin\left(\frac{\pi x}{a}\right) + d\sin\left(\frac{2\pi x}{a}\right)$$ ← Not an e.f. of H unless c or d = 0

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

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

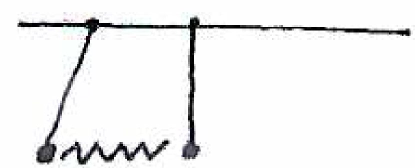
$\Rightarrow$ Not a standing wave

Classical analog



two fundamental frequencies
ω_1, ω_2

what happens with the initial condition shown to the right (① is displaced but ② is not)?

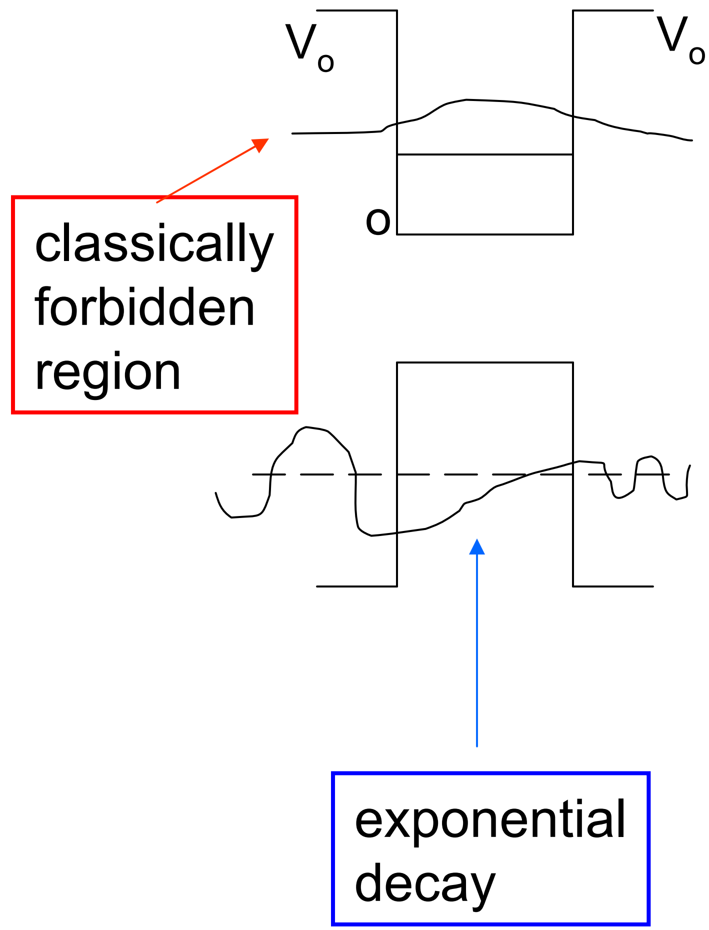


What happens if the box is finite?

The wavefunction now leaks (tunnels) outside the box

What if there is a barrier?

The particle can tunnel through the barrier



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

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

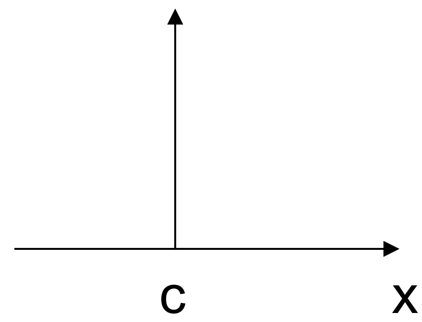
$$= \frac{2}{a}\left[\int_o^a\left(c\sin\frac{\pi x}{a} + d\sin\frac{2\pi x}{a}\right)\left(\frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\right)\left(c\sin\frac{\pi x}{a} + 4d\sin\frac{2\pi x}{a}\right)\right]$$

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

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

δ(x-c) = delta function = 0, $x \neq c$

= ∞, 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.

$\Rightarrow$ momentum ranges over all possible values

Note the connection with the uncertainty principle