

(14)

particle in 3D box, $V=0$ for $\begin{cases} 0 < x < a, \\ 0 < y < b, \\ 0 < z < c \end{cases}$
 $=\infty$, 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 problem separates:

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

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

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

$\sim \sim \sim$ a constant

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} = E_x X \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} E = E_x + E_y + E_z$$

$$-\frac{\hbar^2}{2m} \frac{d^2 Y}{dy^2} = E_y Y \quad \left. \begin{array}{l} \\ \\ \end{array} \right\}$$

$$-\frac{\hbar^2}{2m} \frac{d^2 Z}{dz^2} = E_z Z \quad \left. \begin{array}{l} \\ \\ \end{array} \right\}$$

$$E = \frac{\hbar^2}{8m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right), \quad n_x, n_y, n_z = 0, 1, 2, \dots$$

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

let $a = b = c$

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

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

$$\begin{cases} E(2,1,1) = \frac{h^2}{8ma^2} (6) \\ E(1,2,1) \\ E(1,1,2) \end{cases}$$

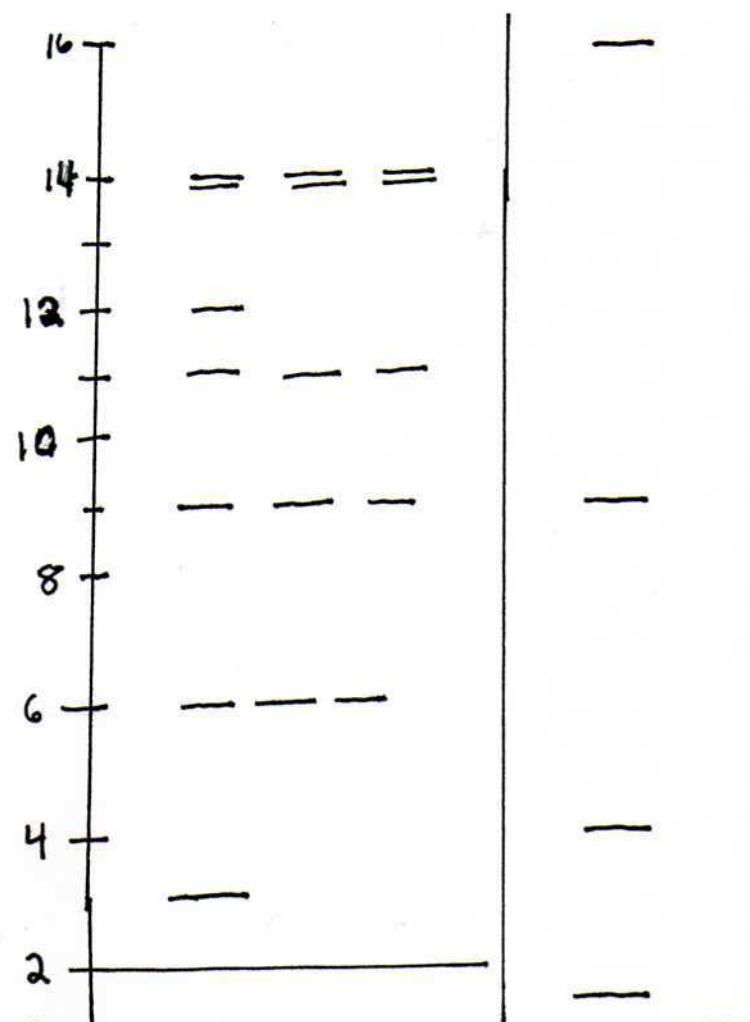
$$\begin{cases} E(2,2,1) = \frac{h^2}{8ma^2} (9) \\ E(2,1,2) \\ E(1,2,2) \end{cases}$$

$$\begin{cases} E(3,1,1) = \frac{h^2}{8ma^2} (11) \\ E(1,3,1) \\ E(1,1,3) \end{cases}$$

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

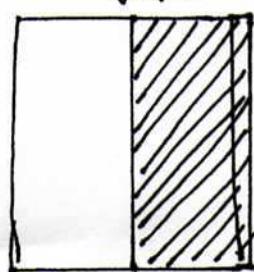
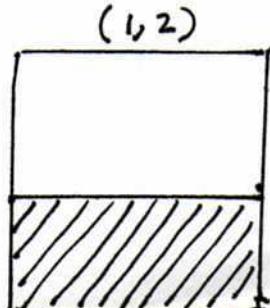
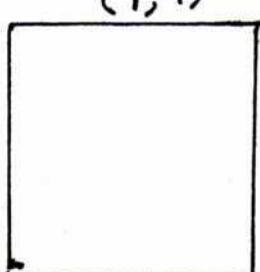
$$E(1,2,3) = \frac{h^2}{8ma^2} (14)$$

\uparrow
6-fold degenerate



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

- Note how rapidly energy levels grow for 3D vs 1D.
- Degeneracies are a result of symmetry



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

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back to the 1D particle-in-a-box problem.

example 4.2.

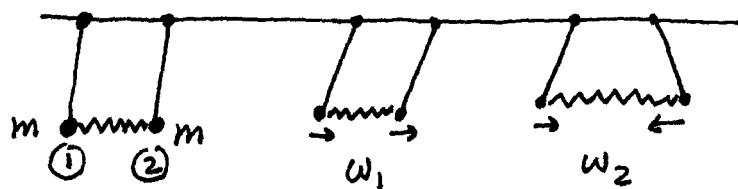
$$\psi = c \sin\left(\frac{\pi x}{a}\right) + d \sin\left(\frac{2\pi x}{a}\right) \quad \leftarrow \text{Not an e.f. of } H \text{ unless } c \text{ or } d = 0$$

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

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

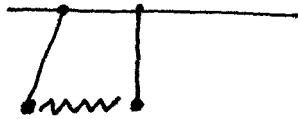
\Rightarrow Not a standing wave

Classical analog.

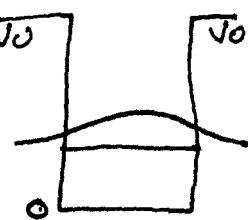


two fundamental frequencies ω_1, ω_2

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



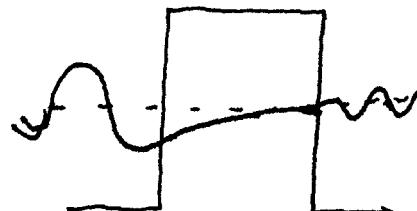
What happens if the box is finite?



The wavefunction now leaks (tunnels) outside the box.

What if there is a barrier?

The particle can tunnel through the barrier.



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Some additional exercises

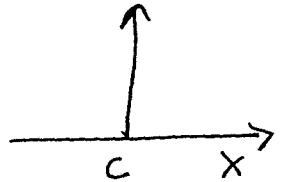
if $\psi(x) = \sqrt{\frac{2}{a}} \left[c \sin \frac{\pi x}{a} + d \sin \frac{2\pi x}{a} \right]$, $c^2 + d^2 = 1$

What is $\langle \hat{H} \rangle$? $c^2 E_1 + d^2 E_2 = c^2 \frac{\hbar^2}{8ma^2} + d^2 \frac{4\hbar^2}{8ma^2}$

$$\begin{aligned}\langle \psi | \hat{H} | \psi \rangle &= \frac{2}{a} \int_0^a \left(c \sin \frac{\pi x}{a} + d \sin \frac{2\pi x}{a} \right) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \left(c \sin \frac{\pi x}{a} + d \sin \frac{2\pi x}{a} \right) \\ &= \frac{2}{a} \left[\int_0^a \left(c \sin \frac{\pi x}{a} + d \sin \frac{2\pi x}{a} \right) \left(\frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \right) \left(c \sin \frac{\pi x}{a} + d \sin \frac{2\pi x}{a} \right) \right] \\ &= \frac{\hbar^2}{4ma^3} \left[c^2 \int_0^a \sin^2 \frac{\pi x}{a} dx + 4d^2 \int_0^a \sin^2 \frac{2\pi x}{a} dx \right] \\ &= \frac{\hbar^2}{8ma^2} [c^2 + 4d^2]\end{aligned}$$

$$\delta(x-c) = \text{delta function} = \begin{cases} 0 & x \neq c \\ \infty & x = c \end{cases}$$

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



This is a strange function, and it is beyond the scope of our course to pursue this further.

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

\Rightarrow momentum ranges over all possible values.