Let’s learn more QM from the simplest problem

(b) Looking into the Physics of the solutions

- $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$ discrete energies (selected by physics)

$$\propto \frac{1}{m} \text{ and } \propto \frac{1}{a^2}$$

$\underbrace{\text{"Confinement"}}_{\text{size } a \text{ in which particle lives}}$ leads to discrete energies

[behind the scene it is the boundary conditions due to confinement]
that matter

Quantum Size Effects : Beginning of Nanoscience and Technology

E.g. absorption/emission of nanoparticles tunable by size (why?)

$\propto \frac{1}{m}$ $\Rightarrow$ smaller mass particle has more noticeable discrete-energy effect

Where are discrete energies noticeable?

$\underbrace{\text{Atoms!}}$ Atomic spectrum

lightest particle → electrons confined to vicinity of nucleus

$m \rightarrow m_e$ (electron mass) $\frac{\hbar^2}{m_e} \approx 7.62 \text{ eV}\cdot\text{Å}^2$ Keep number in mind

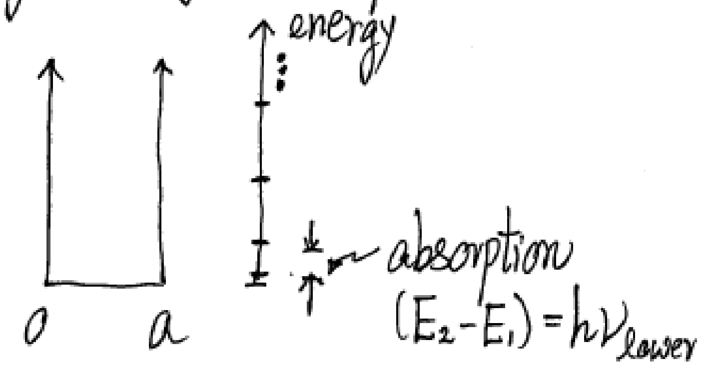
Size ~ Å

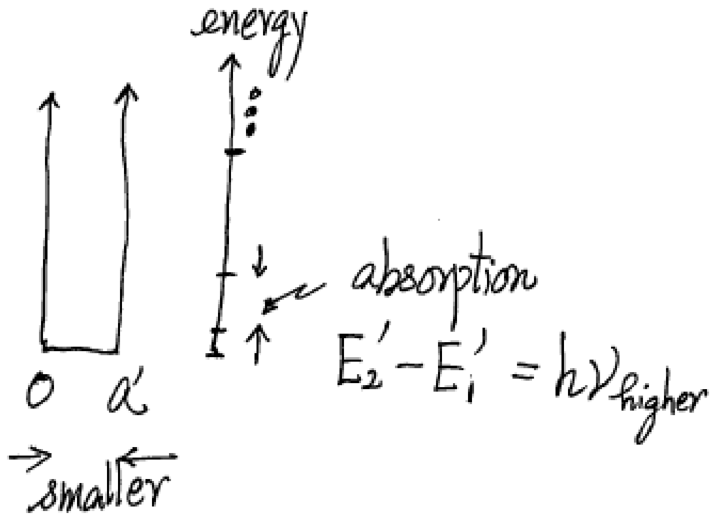
$\therefore$ Particle-in-a-1D-box predicts energies (energy separation) of order of $\frac{\hbar^2}{m_e \text{Å}^2} \approx$ a few eV (which is right!)

- Atomic energies are always about eV to tens of eV
- 1D Well is a simple picture to think about atoms
- Could consider 2D/3D boxes/wells
  - more realistic OK
  - but $\frac{\hbar^2}{ma^2}$ is always there in the results

    $\Rightarrow$ the same energy order!

- Engineering absorption





Someone comes to you and ask: I want absorption at 7.13 eV. Can you design a system delivering this specification?

Yes! This is done using semiconductors.

- Extend application to neutron/proton confined in nucleus. (Ex.)

(c) Picking up better sense on Quantum Mechanics

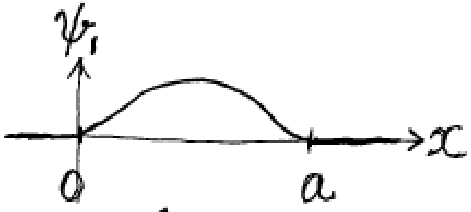
(i) Why does $\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$ have lower energy than $\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$?

Inside the box: $\underbrace{\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}}_{\text{kinetic energy term}}\psi = E\psi$ TISE (U = 0 in box)

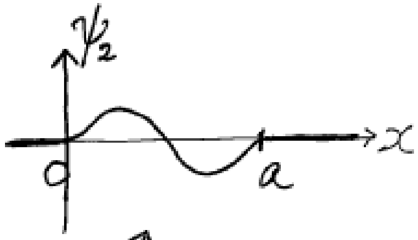
$$\therefore \boxed{\text{kinetic energy term} \sim \underbrace{\frac{d^2}{dx^2}\psi}_{}}$$

Same range "a": more wriggling around
(more turns/twist)
⇒ higher kinetic energy

This is true even when $U(x) \neq 0$



<u>vs</u>

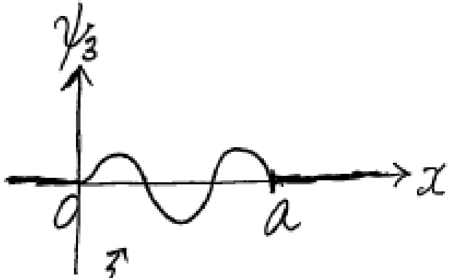


$\psi_2(x)$ has 1 node
(1st excited state)

gradual (energy E_1)

more turn & twist $\Rightarrow$ higher energy E_2

Ground state
ψ_1 has <u>no node</u>
[not counting the two ends]

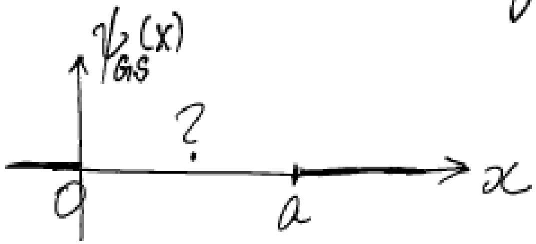


$\psi_3(x)$ has 2 nodes
(2nd excited state)

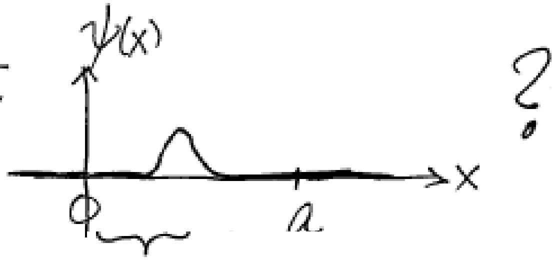
even more turns & twists $\Rightarrow$ even higher energy E_3

How about $\psi_{48}(x)$?
47 nodes (47th excited state)
E_{48} ? $\psi_{48}(x)$? Sketch it

Q: Could we have guessed what $\psi_1(x)$ is like?



How about

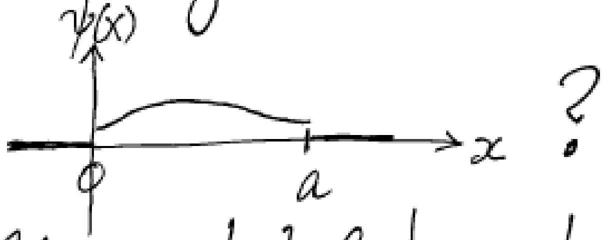


turn around in a maller interval

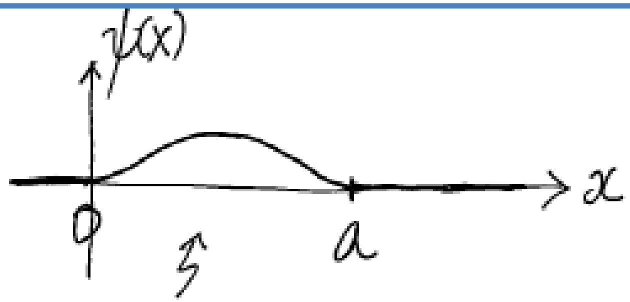
bigger $\frac{d^2\psi}{dx^2} \Rightarrow$ higher energy

No good!

How about



More gradual: looks good. But discontinuous!



this is as gradual as ψ can be and be continuous!

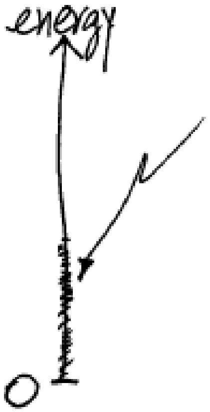
(ii) "Think like a Computer"

Another way to understand why Boundary Conditions select specific energies

In solving TISE, at one point we have (after considering $\psi(0) = 0$)

$$\psi(x) = A \sin kx \qquad (0 < x < a) \qquad \text{and } E = \frac{\hbar^2 k^2}{2m}$$

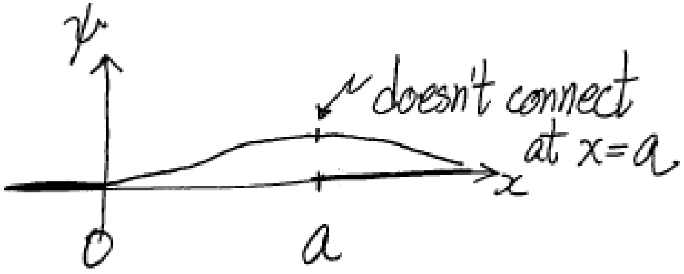
Why couldn't we have $E < E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$ (Ground state energy)?



Let's try different values of E and see what happens

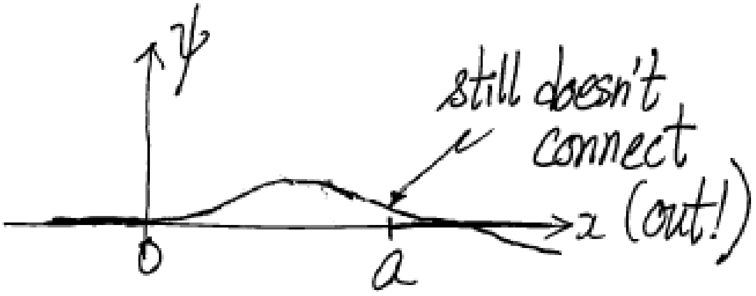
Pick $E \Rightarrow$ try $k = \sqrt{\frac{2mE}{\hbar^2}}$

Try a $E \gtrsim 0$ ($< E_1$), $k \approx 0$ meaning

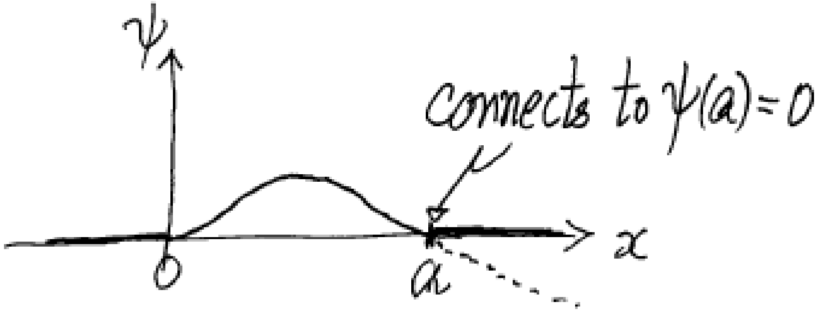


$\Rightarrow$ Not QM acceptable (out!)

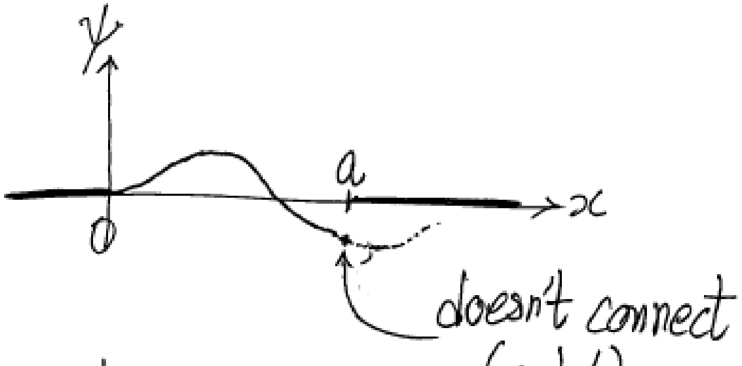
Try a higher one ($E < E_1$),



Until $E = E_1$, $\underbrace{\text{first acceptable energy}}_{\text{giving physically well-behaved wavefunction}}$

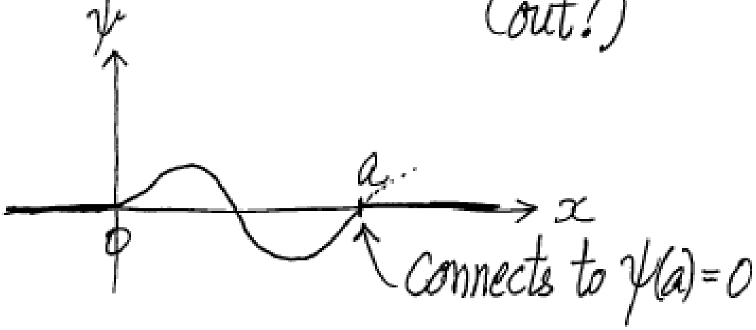


Try $E_1 < E < E_2 \left(= \frac{4\pi^2\hbar^2}{2ma^2}\right)$



doesn't connect (out!)

Until $E = E_2$, $\underbrace{\text{second acceptable energy}}_{\text{giving physically well-behaved wavefunction}}$



connects to $\psi(a)=0$

and so on...

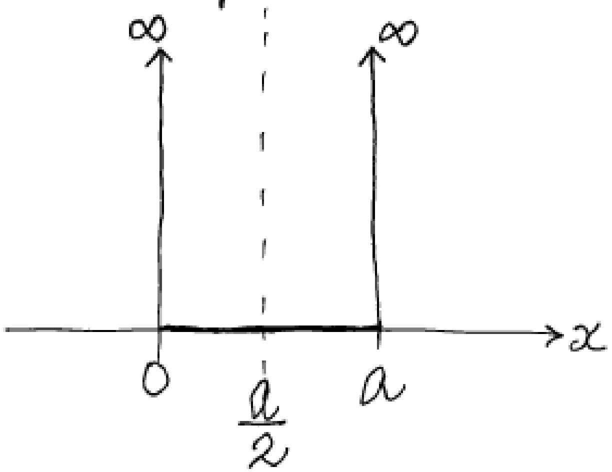
- Think like a computer helps understand how B.C. works to select E

The idea here is general, although we are discuss 1D box problem

- Better strategy: Let computer think like a computer!
  This is how a program solving TISE numerically works.

(iii) Symmetry of $U(x)$ restricts how $|\psi(x)|^2$ looks like

Inspect $U(x)$



Origin: $U(x)$ is symmetric about the center

Student A: Watching it in front of page

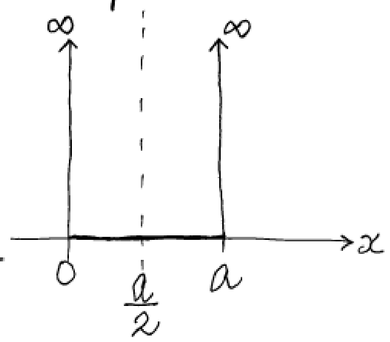
Student B: Watching it from back of page

A's left is B's right

A's right is B's left

If A says the probability of finding the particle is more (biased) on the left side (if it were true), B will say it is more on the right side. There are <u>contradictory views</u>.

Inspect $U(x)$



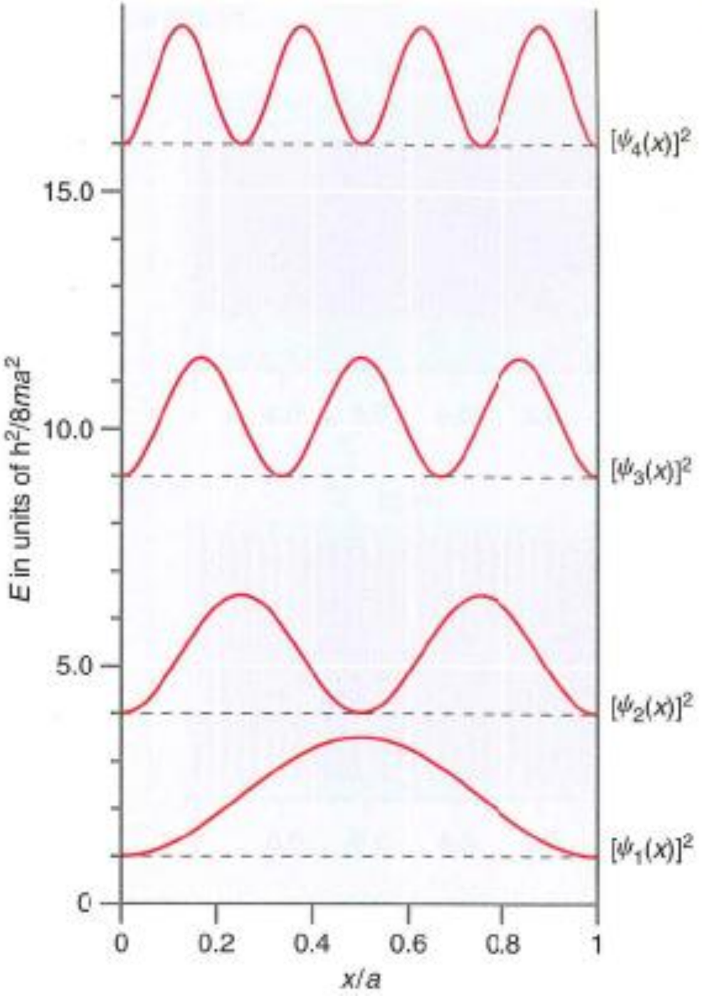
Alternatively, if you were the particle, how could you decide which side is the "left" or the "right" (about the point that $U(x)$ is symmetric)?

$\underbrace{|\psi(x)|^2}$ should be symmetric about the point that $U(x)$ is symmetric

physical interpretation of ψ is about $|\psi|^2$ (not ψ itself)

Inspect $|\psi_n(x)|^2$

It is symmetric about the mid-point of the box/well
(or x/a = 0.5)



Implication on $\psi_n(x)$?

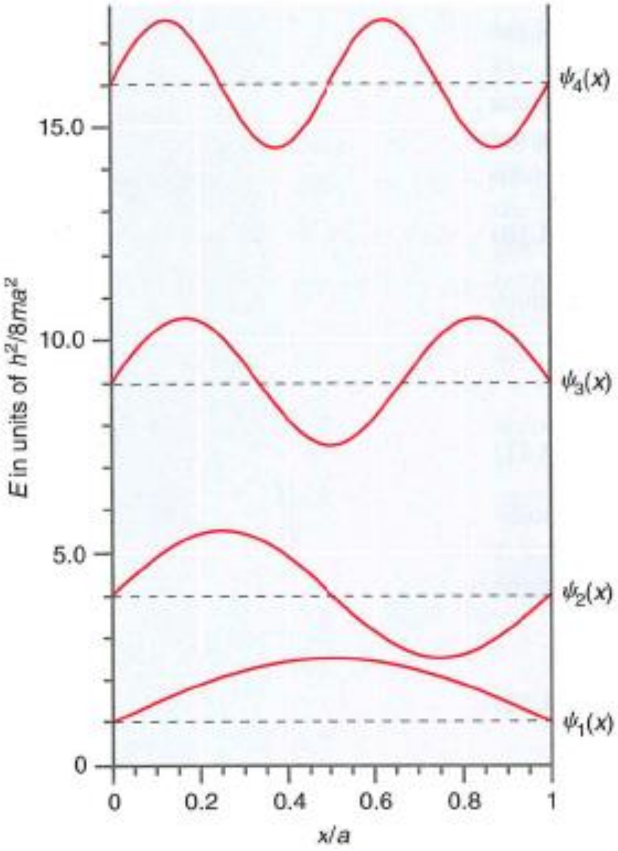
$\psi_n(x)$ can either be symmetric OR anti-symmetric

For a box in $0 < x < a$,

$\psi(x) = \psi(a-x)$ symmetric (for $0 < x < \frac{a}{2}$)

$\psi(x) = -\psi(a-x)$ antisymmetric (for $0 < x < \frac{a}{2}$)

Could have also guessed the form of other ψ_n's.

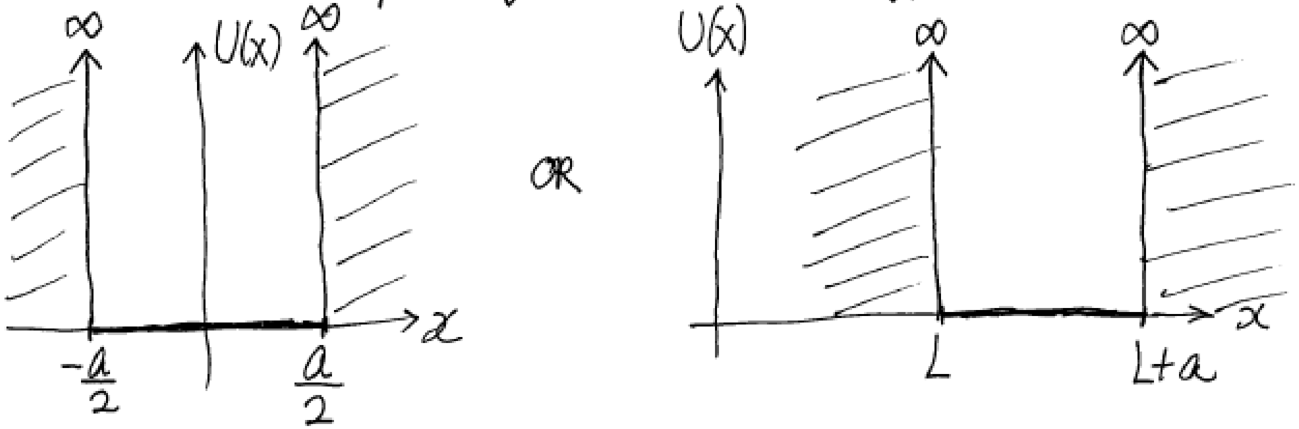


Inspect that the anti-symmetric (or odd) ones must be zero at the center of the box (point about which U(x) is symmetric). Why?

Important to note that the argument here is general for symmetric U(x), not only for the 1D box/well

Argument holds for other symmetric $U(x)$, e.g. 

(iv) How about putting the box at different locations?



Ex: Will energy eigenvalues E_n depend on location of box?

Will energy eigenfunctions $\psi_n(x)$ depend on location of box?

(v) Bound States and bound states can be normalized

What are bound states?

Generally, $\psi(x) \to 0$ as $x \to \pm\infty$

[so all energy eigenfunctions of 1D box are bound states]

(but NOT all energy eigenfunctions of other QM problems are bound states)

If $\psi_E(x)$ is an energy eigenfunction, a state of definite energy E, then it is a bound state if $E < U(x \to \pm\infty)$.

Bound states can always be normalized

Another implication:

There are energy eigenfunctions that are not bound states.

They cannot be normalized according to $\int_{\text{all space}} |\psi(x)|^2 dx = 1$

Their "normalization" is handled differently

E.g. free particle in $-\infty < x < +\infty$

The wavefunctions are plane wave of the form exp(ikx)