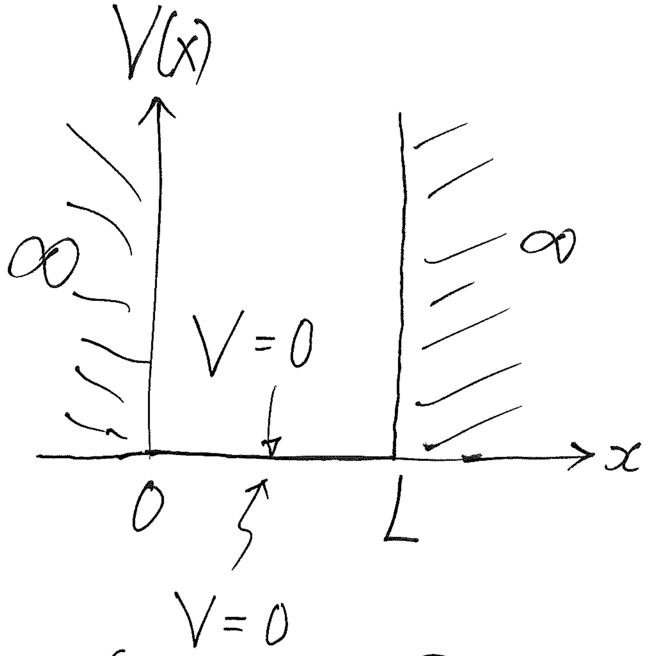
A. How to describe something Traveling: Beyond Standing Waves

- Problems handled so far: Solutions to Schrödinger Equation are standing waves

Particle-in-a-box



(no force ⇒ Free particle)

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad (0 < x < L)$$

$$\psi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar} \; ; \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Standing waves (bound states)

doesn't look like something is traveling freely

▪ "Simplest" Free Particle Problem (1D)

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} \qquad [V=0 \Rightarrow \text{free}] \qquad (1)$$

"free over all x" $[-\infty < x < \infty]$

- Easy to solve: $\hat{H}\psi = E\psi$

$$\psi \sim e^{ikx} \text{ works}, \quad e^{-ikx} \text{ works} \qquad (2)$$

$$\text{with} \quad \frac{\hbar^2 k^2}{2m} = E(k) \qquad (3)$$

[how $E(k)$ behaves is called dispersion relation]

- Time evolution:

$$\psi(x,t) \sim e^{ikx} e^{-i\frac{E(k)}{\hbar}t} \sim e^{ikx} e^{-i\omega(k)t} \quad \text{works}$$

$$\sim e^{-ikx} e^{-i\frac{E(k)}{\hbar}t} \sim e^{-ikx} e^{-i\omega(k)t} \quad \text{works}$$

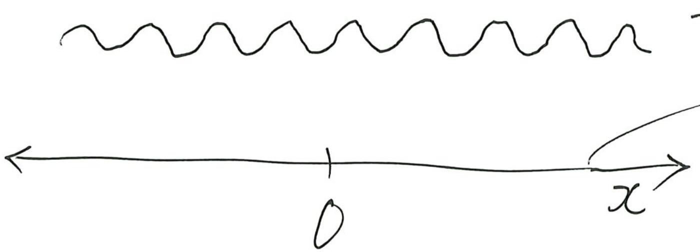
- Solutions have nice physical meaning $\left[\omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar k^2}{2m} \right]$

$e^{i(kx - \omega(k)t)}$ traveling to the right (+ve x) as time evolves

$e^{i(-kx - \omega(k)t)}$ traveling to the left (-ve x) as time evolves

$\therefore$ Finally, some freely traveling $\psi(x,t)$!

- Any $E > 0$ works (no discrete value requirement on E)
  - makes sense: No boundary (thus exercising boundary conditions) to select specify energies



Any $E>0$ works

$V=0$ all x

$\underbrace{\text{Any } E>0 \text{ works}}$ gives $k = \pm\sqrt{\frac{2mE}{\hbar}}$ to travel right (+) and left (−)

- All is so easy and well! Why didn't we introduce them earlier?

Problem with Normalizing e^{ikx} (and e^{-ikx})

Consider $\psi(x) = A e^{ikx}$ (4)

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = |A|^2 \int_{-\infty}^{\infty} dx = \infty \Rightarrow \boxed{\text{Can't find } A \text{ that can normalize (4) in usual way}}$$

- Typical of $\underbrace{\text{continuum spectrum}}$,

any E is allowed $\Rightarrow$ any k is allowed $\left(E = \frac{\hbar^2 k^2}{2m}\right)$

continuum (not discretized)

[Same problem exists for e^{-ikx}]

- Meaning of the Problem

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} = \frac{\hat{p}^2}{2m}$$

$\therefore$ e^{ikx} & e^{-ikx} are also eigenstates of momentum operator $\hat{p}$

$$\hat{p}(Ae^{ikx}) = \frac{\hbar}{i}\frac{d}{dx}[Ae^{ikx}] = \underbrace{\hbar k}_{\text{eigenvalue}}(Ae^{ikx}) \quad (5)$$

$\therefore$ $\sim e^{ikx}$ is an eigenstate of $\hat{p}$ corresponding to $p = \hbar k$

[traveling freely with momentum $\hbar k$ to the right]

Normalization Problem

$\Rightarrow$ No way to have a wavefunction representing a particle of definite momentum that obeys standard normalization condition

Surprising? Not Really! Recall uncertainty Relation.

- Ways out?

(a) Get fancy [but problem actually remains]

- Consult Fourier transform

If label state by k, i.e. $\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$ (6)

then these states obey the "orthonormal" condition

$$\int_{-\infty}^{\infty} \psi_{k'}^*(x)\, \psi_k(x)\, dx = \underbrace{\delta(k-k')}_{\text{Dirac } \delta\text{-function}} \quad (7)$$

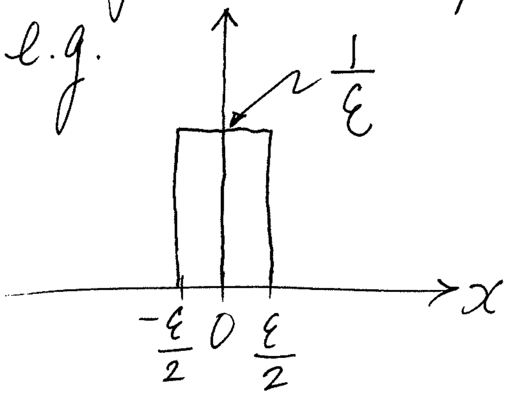
[δ-function "normalization"]

The δ-function : $\delta(x) = 0$ for $x \neq 0$

and $\displaystyle\int_{-\infty}^{\infty} \delta(x)\,dx = \int_{-\varepsilon}^{\varepsilon} \delta(x)\,dx = 1$

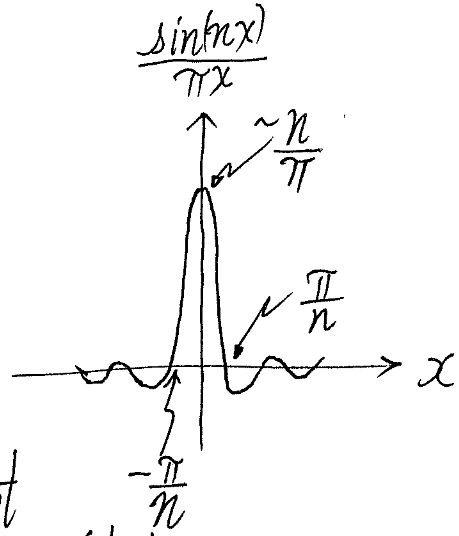
- Any x, $\delta(x) = 0$ except $x = 0$
- $\underbrace{\text{Very sharp}}_{(\text{to } \infty)}$ at $x = 0$ [area under sharp peak is 1]
- δ-fn can be represented in different ways

e.g.



(take $\varepsilon \to 0$)

OR $\underbrace{\displaystyle\lim_{n \to \infty} \frac{\sin(nx)}{\pi x}}_{\text{saw this in time-dependent perturbation theory}} = \delta(x)$



(take $n \to \infty$)

But Eq. (7) does <u>not</u> solve the normalization problem.
It <u>extends</u> the normalization condition.

If we focus on momentum eigenstates, then label them by p

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} \qquad (8) \qquad (\because p = \hbar k)$$

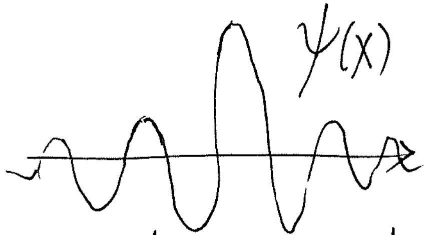
$$\int_{-\infty}^{\infty} \psi_{p'}^*(x)\, \psi_p(x)\, dx = \delta(p'-p) \qquad (9)$$

- For eigenvalues take on continuous values, <u>δ-function normalization</u> is a way out.

You will see more of it in more advanced QM courses.

(b) Be strict and formal

- QM wavefunctions must obey normalization condition
- Must use $\underbrace{\text{wave packet}}_{\text{form by superposition of } e^{ikx} \text{ of different } k\text{'s}}$ (not just $\sim e^{ikx}$)

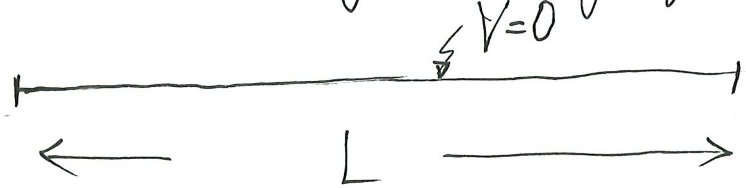


Can be normalized!

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underbrace{\phi(k)}_{\text{different } k\text{-components to give } \psi(x)} e^{ikx} dk$$

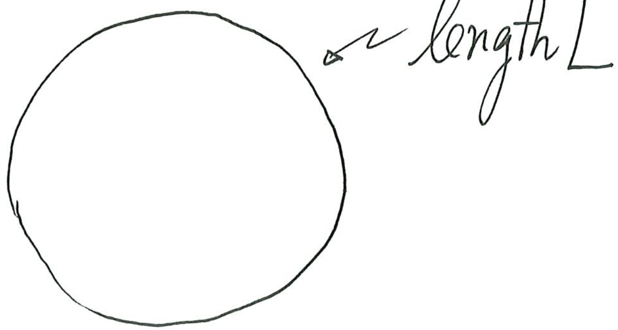
- This really solves the normalization problem
- But it makes calculations harder to do.

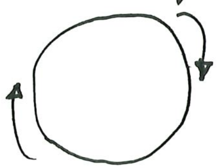
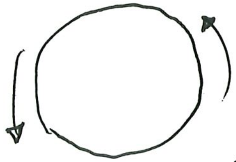
(c) Mimicing traveling freely in infinite space by a large finite space



"Particle-in-a-box" Again? No!

Periodic boundary condition: Hook up two ends



- traveling around ($\approx$ infinite system)
- e^{ikx} (going around )
- e^{-ikx} (going around )

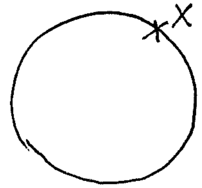
$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx}$ is normalized in ordinary sense

[always think that L is large]

$$\int_{-L/2}^{L/2}\left(\frac{1}{\sqrt{L}}e^{-ikx}\right)\left(\frac{1}{\sqrt{L}}e^{ikx}\right)dx = \frac{1}{L}\int_{-L/2}^{L/2}dx = \frac{1}{L}\cdot L = 1$$

$$\Rightarrow \boxed{\psi_k(x) = \frac{1}{\sqrt{L}}e^{ikx} \text{ is properly normalized}} \quad (10)$$

But there is a price to pay!



x and x+L refer to the same place

$$\psi_k(x+L) \overset{\text{[same place]}}{=} \psi(x)$$

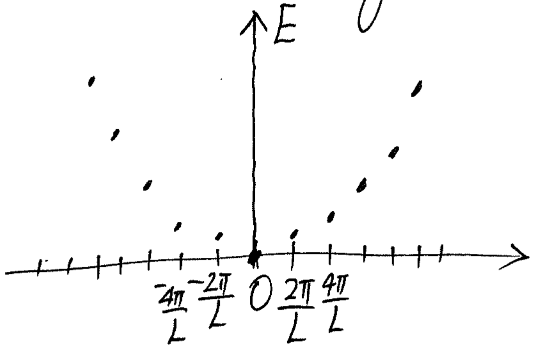
$$\Rightarrow e^{ikx}e^{ikL} = e^{ikx} \Rightarrow e^{ikL} = 1 \Rightarrow kL = 2\pi n \quad (n = 0, \pm 1, \pm 2, \cdots)$$

$$\Rightarrow \boxed{k_n = \frac{2\pi}{L}\cdot n} \quad (11) \quad (\because \text{There is a "boundary" set by } L)$$

k is discretized $\Rightarrow$ p is discretized $(\hbar k)$ $\Rightarrow$ $E = \frac{\hbar^2 k^2}{2m}$ is discretized

This is called "Box Normalization"

Box Normalization (length L)



$$E_n = \frac{\hbar^2 k_n^2}{2m}$$

But L is meant to be big

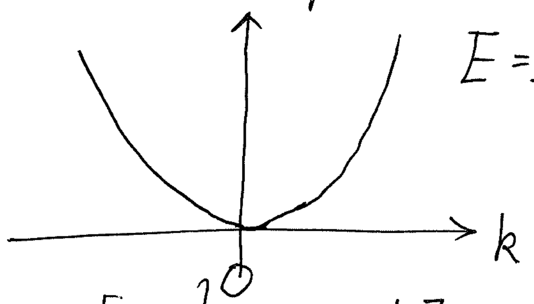
(Think $L \to \infty$) $\Rightarrow$ closely spaced k-values ($\approx$ continuum)

$$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx} \quad \text{(normalized)}$$

$$k_n = n \frac{2\pi}{L} \quad (n = 0, \pm 1, \pm 2, \cdots)$$

- Retains ideas on QM wavefunctions learned so far & has traveling waves

Infinite Space



$$E = \frac{\hbar^2 k^2}{2m}$$

[continuous k]

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

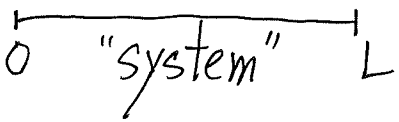
[δ-function normalization]

(any k)

- Needs new way for "normalization" that works for continuous spectrum (eigenvalues) & has traveling waves

$$\psi_k(x) = \frac{1}{\sqrt{L}}\, e^{ikx} \quad ; \quad \underbrace{k_n = n\,\frac{2\pi}{L}}_{\text{finite } L \text{ (finite "Box") leads to discrete } k\text{'s}} \quad (n = 0, \pm 1, \pm 2, \ldots)$$

- The bigger the box, the less noticeable is the discreteness of k
- Any way to visualize box normalization & Periodic boundary condition



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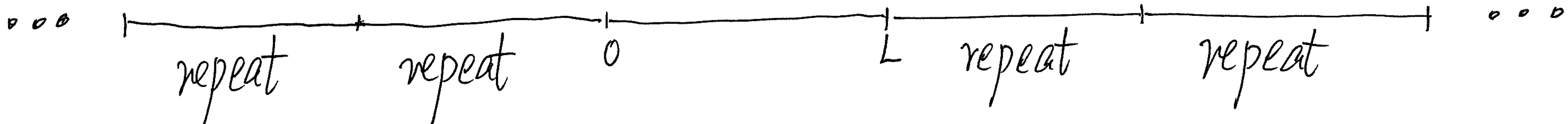
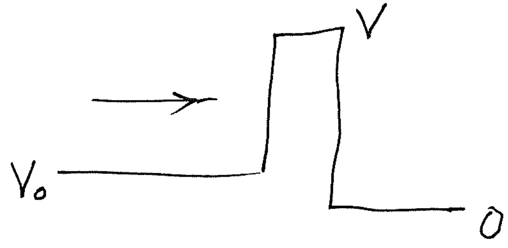


Mimicing an infinite system by repeating a finite system!

- Why do we want/need traveling waves?
  - incident wave upon a barrier in <u>tunneling problem</u>



and other <u>scattering problems</u>

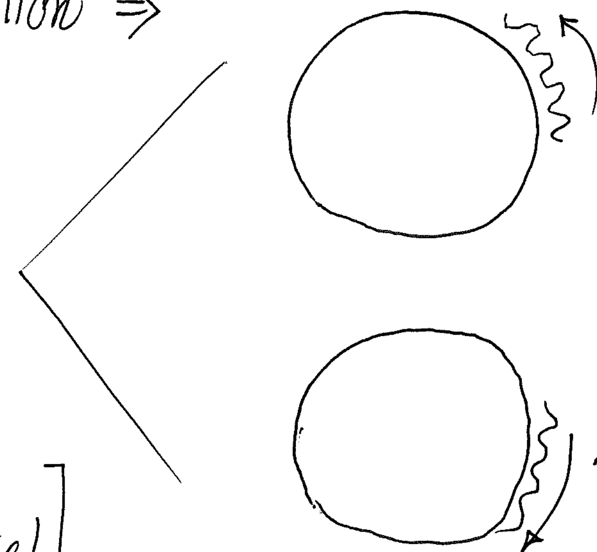
  - electrons travel in a metal to make it a conductor

metal wire

Box Normalization is often used in Solid State Physics

Think "box normalization" ⇒

Get ready for Quantum theory of Solid States [conduction when an $\vec{\mathcal{E}}$ field is applied]



$\sim e^{-ikx}$

$\sim e^{ikx}$

for an allowed k

Key Points

- We need traveling waves for some problems in QM
- Allowed energies form continuum spectrum: Wavefunctions cannot be normalized in usual way
- There are ways out
  - change normalization condition [δ-function]
  - form wave packets
  - Box normalization
- Need to be careful in treating traveling waves in QM, but there are ways out