

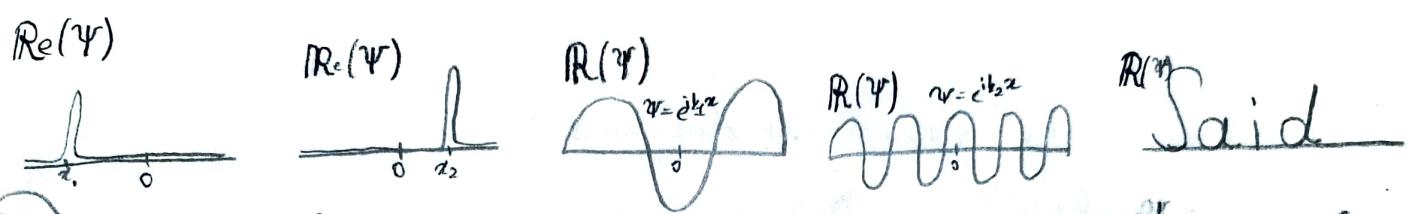
# Quantum Physics 1

How do we configure a system or a quantum particle, we need to know its position and momentum.

$$\{\vec{x}, \vec{p}\}, \vec{E}(\vec{x}, \vec{p}), \vec{L}(\vec{x}, \vec{p})$$

In Real World, uncertainty of position and momentum,  $\Delta x \Delta p \gtrsim \hbar/2$

I Specifying a state by  $(x, p)$  clearly will not work. The configuration of a quantum object is specified by a "wavefunction" denoted as  $\Psi(x) = \psi$  function

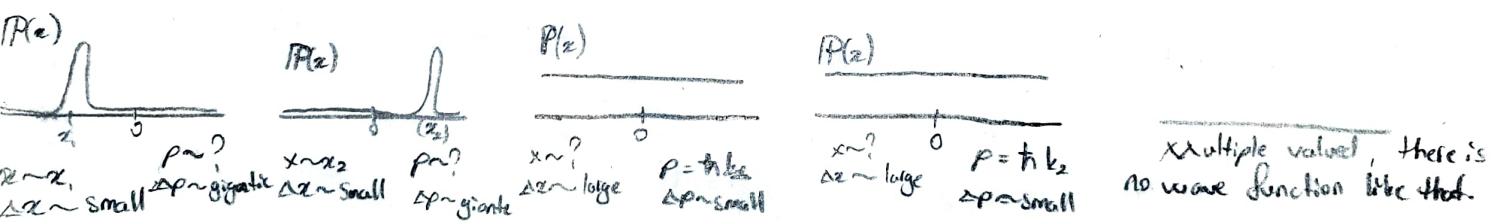


II  $P(x) = |\Psi(x)|^2$  determines probability density that the object is state  $\Psi(x)$  will be found at  $x$ .

$$P(x, x_1, x_2) = P(x) dx = |\Psi(x)|^2 dx, \int_{\text{All}} P(x) = 1 = \int_{\text{All}} |\Psi(x)|^2 dx$$

Dim of wavefunction =  $1/\sqrt{L}$  since  $\dim(dx) = L$ , so  $|\Psi(x)| = 1/\sqrt{L}$

$$|e^{i\alpha}|^2 = 1, |B|^2 = B \cdot B$$



de Broglie Relation:  $E \sim \hbar \omega$ ,  $P = \hbar k = h \nu \Rightarrow \omega = 2\pi\nu \Rightarrow k = 2\pi/L$

III Given Two Possible States of Quantum System Corresponding to Two Wavefunctions  $\Psi_1(x)$  and  $\Psi_2(x)$ , the system can also be in a superposition of these,

$$\Psi(x) = \alpha \Psi_1(x) + \beta \Psi_2(x) \quad \alpha, \beta \in \mathbb{C}, \text{ Subject to normalization.}$$

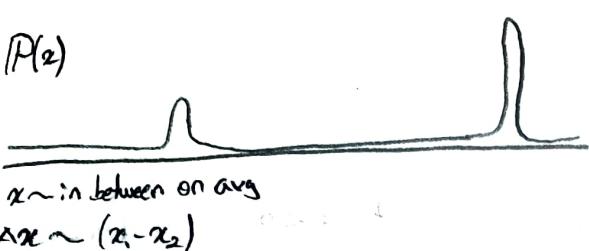
$$P(x) = \frac{|\Psi(x)|^2}{\int_{\text{All}} |\Psi(x)|^2}, \text{ another way to think about probability distribution.}$$

(1)

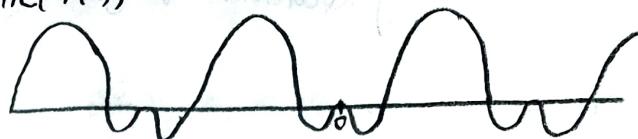
$R(\Psi(x))$



$P(x)$



$R(\Psi(x))$   $\Psi(x) = e^{ik_1 x} + e^{ik_2 x}$



$P(x)$



$$|P(x)|^2 = |\alpha|^2 |\Psi_1|^2 + |\beta|^2 |\Psi_2|^2 + \alpha^* \Psi_1^* \beta \Psi_2 + \alpha \Psi_1 \beta^* \Psi_2^* = P_1 + P_2 + \text{interference terms}$$

Thm: Any  $f(x)$  can be built by superposing enough plane-waves  $e^{ikx}$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{f}(k) e^{ikx}, \quad \lambda = 2\pi c/k$$

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{-ikx}$$

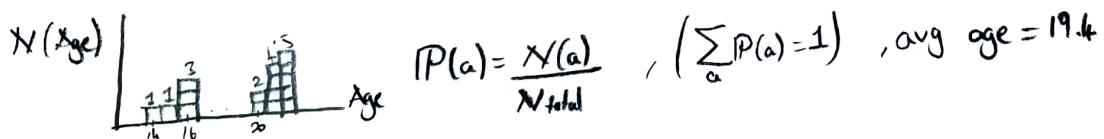
Any  $\Psi(x)$  can be expressed as a superposition

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{\Psi}(k) e^{ikx} \text{ of state with definite momentum, } p = \hbar k.$$

Reasonable  $\Psi(x)$  can be expressed as superposition of more easily interpretable WFs.

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int dk \hat{\Psi}(k) e^{ikx} \quad e^{ikx} = \cos(kx) + i \sin(kx)$$

$$\Psi(x) = \int dx_a \Psi_{(a)} \delta(x-x_a)$$



$$\langle a \rangle = \frac{\sum a N(a) \cdot a}{N_{\text{total}}} = \text{avg age.} = \sum_a a P(a) , \text{avg } a^2 , \langle a^2 \rangle = \sum_a a^2 P(a)$$

$\langle a^2 \rangle = \sum_a a^2 P(a) , \langle a^2 \rangle \neq a^2 , \text{ always.}$

$\text{dev} \Rightarrow (a - \langle a \rangle) , \text{ Note } \langle a - \langle a \rangle \rangle = \langle a \rangle - \langle a \rangle = 0$

$$\text{std. dev } \langle (a - \langle a \rangle)^2 \rangle = \langle a^2 - 2a \langle a \rangle + \langle a \rangle^2 \rangle = \langle a^2 \rangle - 2 \langle a \rangle^2 + \langle a \rangle^2 = \langle a^2 \rangle - \langle a \rangle^2 = \Delta a^2$$

$\Delta a = \text{uncertainty in a given } P(a)$

$P(a)$

Now for continuous variables

$$\langle x \rangle = \int_{-\infty}^{\infty} dx P(x)x, \langle f(x) \rangle = \int_{-\infty}^{\infty} dx P(x)f(x), \Delta x = \langle x^2 \rangle - \langle x \rangle^2$$

$$\langle x \rangle = \int_{-\infty}^{\infty} dx |\psi(x)|^2 x, f(x) = \int_{-\infty}^{\infty} dx |\psi(x)|^2 f(x), \langle x \rangle = \langle x \rangle_{\psi} = \langle \psi | x | \psi \rangle$$

Well, we should do with momentum too.

$$\langle p \rangle = \int_{-\infty}^{\infty} dp P(p)p \stackrel{?}{=} \int_{-\infty}^{\infty} dp |\tilde{\psi}(p)|^2 p, \text{ is it true?}$$

$\langle p \rangle = \int_{-\infty}^{\infty} dx |\psi(x)|^2 \cancel{p}$ , we can't say that we're in a definite position and definite momentum

$\delta(x-x_0) = \frac{1}{\sqrt{2\pi}} \int dk e^{ikx} e^{ikx}$ , Being in a state with definite position means that being  $\delta(x)$

Superposition with arbitrary momentum.

So we want some good def'n of  $p$  given that  $\psi(x)$ .

$$\text{Hint 1-} k = 2\pi/\lambda \Leftrightarrow p = \hbar k, e^{ikx} \Leftrightarrow p = \hbar k$$

Note:  $\partial x e^{ikx} = ike^{ikx}$   
 $\hbar \partial x e^{ikx} = \hbar k e^{ikx} = p e^{ikx}$ , check the units.  $\frac{\hbar}{2} \pi \partial x \Delta p [k] = \frac{1}{L}$ , good.

$$\frac{\hbar}{i} \partial x \stackrel{?}{=} p$$

Noether's Theorem:

To every symmetry is associated a conserved quantity transition

|                 |                       |               |
|-----------------|-----------------------|---------------|
| Transition      | $x \rightarrow x + L$ | $\dot{p} = 0$ |
| Time Transition | $t \rightarrow t + T$ | $\dot{E} = 0$ |
| Rotational      | $x \rightarrow Rx$    | $\dot{I} = 0$ |

Say that I have a particle which moving in some potential

$$u(x) \quad \left| \begin{array}{l} \dot{p} = -\nabla u \end{array} \right.$$

Constant potential has translation in Symmetry, so Force = 0,  $\dot{p} = 0$

$$T_L f(x) = f(x-L) \quad \int_0^L \rightarrow \int_L^0$$

$$\begin{aligned} T_L f(x) &= f(x-L) = f(x) - L \partial_x f(x) + \frac{L^2}{2} \partial_x^2 f(x) - \frac{L^3}{6} \partial_x^3 f(x) \dots \\ &= (1 - L \partial_x + \frac{L^2}{2} \partial_x^2 - \frac{L^3}{6} \partial_x^3 + \dots) \cdot f(x) \\ &= e^{-L \partial_x} f(x) \end{aligned}$$

(2)

- Translation in  $x$  are generated by  $\hat{p}_x$   
- Noether's Thm: Translation in  $x \leftrightarrow$  momentum  
 $\Rightarrow$  Not totally shocking that, in QM:  
 $\hat{p}_x \sim P$ ,  $\hat{p}_t \sim E$ ,  $\hat{p}_\theta \sim L_x$

$$\Psi(x) = e^{ikx} \quad ik = \hat{p}$$

$$\hat{p}\Psi(x) = ik\Psi(x), \quad \Psi_s = \frac{1}{\sqrt{2}}e^{ikx} + \frac{1}{\sqrt{2}}e^{-ikx}$$

$$P \leftrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \langle P \rangle = \int_{-\infty}^{\infty} \Psi^*(x)\Psi(x) \frac{\hbar}{i} \frac{\partial}{\partial x} dx$$

$$\Psi(x) = N e^{ikx} \Rightarrow \text{as } p = \hbar k$$

$$\hat{p}\Psi = \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi = ik\Psi$$

Operators and Measurable Quantities:

Operators act on objects. Vectors are objects and ops. are matrices or example.

Ex:  $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$  object,  $M = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ ,  $Mv$  is an object.

In quantum mechanics:

Objects: Complex functions of  $x$ .

Ops: Act on functions:  $\hat{f}: f(x) \rightarrow$  another function of  $x$ .

Some operators:

$$1: f(x) \rightarrow f(x), \quad \frac{\partial}{\partial x}: f(x) \rightarrow \frac{\partial f(x)}{\partial x}, \quad \hat{x}: f(x) \rightarrow xf(x), \quad \hat{S}_x: f(x) \rightarrow (f(x))^2$$

$$\hat{P}_{42}: f(x) \rightarrow 42, \quad \hat{\delta}_a: f(x) \rightarrow \delta(x-a)f(x); \quad \hat{\delta}_0: f(x) \rightarrow \delta(x)f(x), \quad \hat{\theta}_h(x): f(x) \rightarrow h(x)f(x)$$

$$\text{Linear Op: } \hat{\Theta}(af(x) + bg(x)) \rightarrow a\hat{f}(x) + b\hat{g}(x)$$

Linear Operators can have "eigenfunctions":

$$\hat{A}f(x) = af(x) \quad \begin{matrix} \downarrow \\ \text{Eigen value} \end{matrix} \quad \begin{matrix} \downarrow \\ \text{Eigenfunction} \end{matrix} \quad a \in \mathbb{C}, \text{ may take infinite values.}$$

$\hat{A} = \hat{p}$  has eigenfunction  $e^{ikx}$  and eigen value  $ik$ ;  $\hat{p}e^{ikx} = ik e^{ikx}$

$$\hat{p}, \hat{x}, \text{Energy Operator} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = \hat{E} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(\hat{x})$$

$$\hat{E}\Psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) + V(x)\Psi(x)$$

Thing that  $\hat{p} = \frac{\hbar}{i} \hat{x}$ , is the "fact" of Quantum Mechanics.

**IV** For each observable, we have an associated operator:

momentum  $\rightarrow \hat{p}$       position  $\rightarrow \hat{x}$       energy  $\rightarrow \hat{E}$ ,  $\hat{A} = \hat{p}, \hat{x}, \hat{E}, \dots$

$$\langle \hat{A} \rangle = \int \Psi^*(x) \Psi(x) \hat{A} dx \quad \text{uncertainty of } (\Delta A)_y = \sqrt{\langle \hat{A}^2 \rangle - \langle A \rangle^2}$$

Commutation?

$$(\hat{p}\hat{x})f(x) = \hat{p}(\hat{x}f(x)) = \hat{p}(xf(x)) = \frac{i}{\hbar} \frac{\partial}{\partial x}(xf(x)) = (\frac{i}{\hbar})f(x) + \frac{i}{\hbar} x \frac{\partial f}{\partial x}$$

$$(\hat{x}\hat{p})f(x) = \hat{x}(\hat{p}f(x)) = \hat{x}(pf(x)) = (\hbar/i)x \frac{\partial f}{\partial x}$$

$$(\hat{x}\hat{p} - \hat{p}\hat{x})f(x) = -\frac{i}{\hbar} df(x) = i\hbar f(x)$$

$$[\hat{x}, \hat{p}]f(x) = i\hbar f(x), [\hat{x}, \hat{p}] = i\hbar \mathbf{1}$$

**V** Upon measuring an observable  $A$  associated with  $\hat{A}$

1-) The measured values must be one of the eigenvalues of  $\hat{A}$ .

2-) After measurement, system collapses into  $\Psi_a$ ,  $\hat{A}\Psi_a = a\Psi_a$

Position of  $\Psi(x)$  at  $x_0$ :

$$\Psi \sim \delta(x-x_0), \hat{x} \delta(x-x_0) = x_0 \delta(x-x_0) = x_0 \delta(x-x_0)$$

**VI** Given an observable  $\hat{A}$  and its eigenfunctions  $\phi_a(x)$ , normalize them by

$$\int \Psi_a^*(x) \Psi_b(x) dx = \delta_{ab}$$

1-) Can expand  $\Psi(x)$  as

$$\Psi(x) = \sum_a c_a \Psi_a(x)$$

2-) Probability of measuring  $\hat{A}$  and getting  $a$  is

$$|c_a|^2 = P_\Psi(a_0)$$

Ex:  $\hat{x}, \left\{ \delta(x-x_0), \forall x_0 \right\}$

$$\Psi(x) = \underbrace{\int \Psi(x_0)}_{\text{"C}_a\text{"}} \underbrace{\delta(x-x_0)}_{\Psi_a} \underbrace{\sum}_{\Sigma}$$

## Schrodinger Equation:

$E = \hbar\omega$ ,  $\vec{p} = \hbar\vec{k}$  ( $p = \hbar k$ ) ; Planck, Einstein, Compton.

$$(E, \vec{p}) = \hbar(\omega, \vec{k}), \rho^{\mu} = (E, \vec{p}), x^{\mu} = (t, \vec{x})$$

$$\Psi(x, t) = e^{i(kx - \omega t)}, \rho = \hbar k$$

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \leftrightarrow p = \hbar k, \hat{E} = i\hbar \frac{\partial}{\partial t} \leftrightarrow E = \hbar\omega$$

$$i\hbar \frac{\partial}{\partial t} \Psi = i\hbar(-i\omega)\Psi = \hbar\omega\Psi$$

For this  $\Psi$   $\frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x, t) = p \Psi(x, t)$ ,  $i\hbar \frac{\partial}{\partial t} \Psi(x, t) = E \Psi(x, t)$

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \hat{E} \Psi(x, t), \hat{E} = \frac{\hat{p}^2}{2m} + v(\vec{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + v(x)$$

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + v(x) \Psi \quad \left. \right\} \text{Schrodinger's Equation.}$$

We know that any wavefunction can be expressed as the superposition of two wavefunctions. We also know that Schrodinger's Equation is linear. So we can say: If we know the state of a system at any time, we can also know all of the states of the system at any time.

So we can say that the system is deterministic.

$\hat{A} \Psi_a(x) = a \Psi_a(x)$  But if we measure the system at some point, the superposition of states will collapse to some specific state  $a$ ,  $\hat{A} = a \Rightarrow \Psi(x, t) = \Psi_a(x)$ .

System starts to evolve according to Schrodinger Equation but with new initial condition  $\Psi_a(x)$ .

So we say that in Quantum mechanics, we have "2" different definitions of time Evolution.

1-) Schrodinger Equation, "Deterministic"

2-) Collapse, Probabilities collapse to some non-deterministic state.

And the probability distribution determined by the which wavefunction you have

$$P(A=a) = |c_a|^2, c_a = (\Psi_a | \Psi)$$

$$(\Psi_a | \Psi) = \int_{-\infty}^{\infty} \Psi_a^*(x) \Psi(x) dx$$

How is that possible?

A. Said Tengel

Copenhagen Interpretation says that; "as long as the math fits the data just shut up and calculate". That is not acceptable so let us find an explanation.

### Theory of Decoherence:

It basically says that, that the reason you have this problem between Schrödinger's deterministic time and collapse is caused by measuring the quantum objects with macroscopic systems when you try to measure quantum "objects" with a system made by classical dynamics, quantum effects get dominated (gets washed out) by the interaction with laws of classical physics. You get rid of the interference effects. Dealing with that is hard because if you want to treat the system according to Schrödinger Evolution you have to work trajectories and motion of dynamics of every single particle in the whole system. So here is the question;

If you take a system where you have just one quantum object and other enormously high numbered particles act with classical dynamics, If you take whole system does Schrödinger Evolution collapses for this single quantum microsystem?

And the answer is yes, we're gonna see that later on.

### Solving Schrödinger's Equation

For solving Schrödinger's equation we need a specific energy operator  $\hat{E}$ .

$$\hat{E} = \frac{p^2}{2m} + \frac{m\omega^2}{2} \hat{x}^2, \quad \hat{p} = \frac{\hbar}{i} \partial_x$$

So

$$i\hbar \partial_t \Psi(x,t) = -\frac{\hbar^2}{2m} \partial_x^2 \Psi(x,t) + \frac{m\omega^2}{2} x^2 \Psi(x,t)$$

For a given specific  $\hat{E}$ , there are many ways to solve equation.

a-) Brute Force: Solving roughly.

b-) Extreme Cleverness: Elegant use of math, use structures of differential eq.

c-) Numerically, by computer.

1.) Start with Eigenfunctions:

$$[\hat{h}] = [\hat{E}] [\hat{t}] = [\hat{p}] [\hat{x}]$$

$$\Psi_E(x_0) = \Psi_E(x), \quad \hat{E} \Psi_E(x) = E \Psi_E(x)$$

$$i\hbar \partial_t \Psi(x_0) = E \Psi(x_0) \Rightarrow \partial_t \Psi(x_0) = -\frac{iE}{\hbar} \Psi(x_0) = -\frac{iE}{\hbar} \Psi_E(x) \Rightarrow \Psi(x,t) = e^{i\frac{Et}{\hbar}} \Psi_E(x), \quad \omega = E/\hbar$$

$$\Psi(x,t) = e^{i\omega t} \Psi_E(x) \equiv \text{"Stationary State"}$$

$$|\Psi(x,t)|^2 = |\Psi_E(x)|^2 \cdot \text{"means Independent in Time"}$$

$$\langle x >_t = \int |\Psi(x,t)|^2 x dx = \int |\Psi_E(x)|^2 x dx, \quad \text{if } \Psi(x_0) = \sum_n c_n \Psi_n(x)$$

$$\Rightarrow \Psi(x,t) = \sum_n c_n e^{i\omega t} \Psi_n(x)$$

Linearity of Schrodinger Equation:  $\frac{\partial}{\partial t} \Psi(x,t) = \frac{\hat{E}}{\hbar} \Psi(x,t)$

Suppose,

$$\Psi(x,t) = e^{-i\omega t} \Psi_E(x); \quad \hbar(\Delta\omega)t \geq \hbar \Rightarrow \Delta E \Delta t \geq \hbar$$

Then;

$\Rightarrow \Psi(x,t) = \sum_n c_n \Psi_n(x), \quad \Delta\omega \Delta t \geq 1, \quad \hbar(\Delta\omega)t \geq \hbar \Rightarrow \Delta E \Delta t \geq \hbar$   
we can't make measurement with zero error, there is always some accuracy level on the measurements.

For a given  $\hat{E} \rightarrow \{ \Psi_E(x) \}$  with eigenvalue "E".

Any wavefunction  $\Psi(x,t) = \sum_n c_n \Psi_n(x)$ , can be expanded as the superposition of eigenfunctions. So we can take an arbitrary condition and solve Schrodinger Equation.

$$\hat{p} \rightarrow \left\{ \frac{1}{i\hbar} e^{ikx} \right\} \rightarrow p = \hbar k, \quad f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ikx} f(k) dk$$

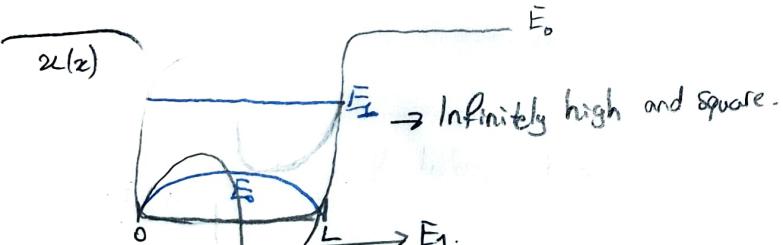
$$\hat{x} \rightarrow \{ x \delta(x-y) = y \delta(x-y), \quad f(x) = \int \delta(x-y) f(y) dy \}$$

Example:

$$\hat{E} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2, \quad \hat{E} \Psi_E(x) = E \Psi_E(x) \Leftrightarrow -\frac{\hbar^2}{2m} \nabla^2 \Psi_E(x) = E \Psi_E(x)$$

$$\Psi''_E(x) + \frac{2mE}{\hbar^2} \Psi_E(x) = 0, \quad \frac{2mE}{\hbar^2} = k^2 \Rightarrow \Psi_E(x) = A e^{ikx} + B e^{-ikx}, \quad E = \frac{\hbar^2 k^2}{2m}$$

Example:



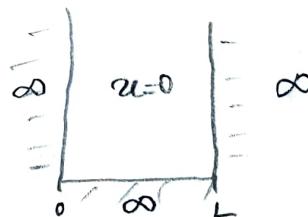
$\Psi(x) = 0$ , outside the box, and boundaries:  $x=0, L$ .

$$\text{Inside } \Psi_E = A \cos(k_x x) + B \sin(k_x x)$$

$$x=0 \Rightarrow A=0$$

$$x=L \Rightarrow k_x L = (n+1)\pi \sim k_n = \frac{(n+1)\pi}{L}$$

$$\Rightarrow \Psi_E = A_n \sin(k_n x)$$



The allowed energy levels are always bigger than zero, you can't have zero energy.

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 (n+1)^2}{2m} \Rightarrow E_1 = 4E_0$$

$$(f | g) = \int_{-\infty}^{\infty} f(x) g(x) dx, \quad (1)$$

$$\begin{aligned} \hat{x} \varphi_{x_0}(x) &= x_0 \varphi_{x_0}(x), (\varphi_{x_0}(x) | \varphi_{x_1}(x)) = \delta(x_0 - x_1) \\ \hat{p} \varphi_k(x) &= \pm k \varphi_k(x), (\varphi_k(x) | \varphi_{k'}(x)) = \delta(k - k') \\ \hat{E} \varphi_n &= E_n \varphi_n, (\varphi_n | \varphi_m) = \varphi_{nm}. \end{aligned}$$

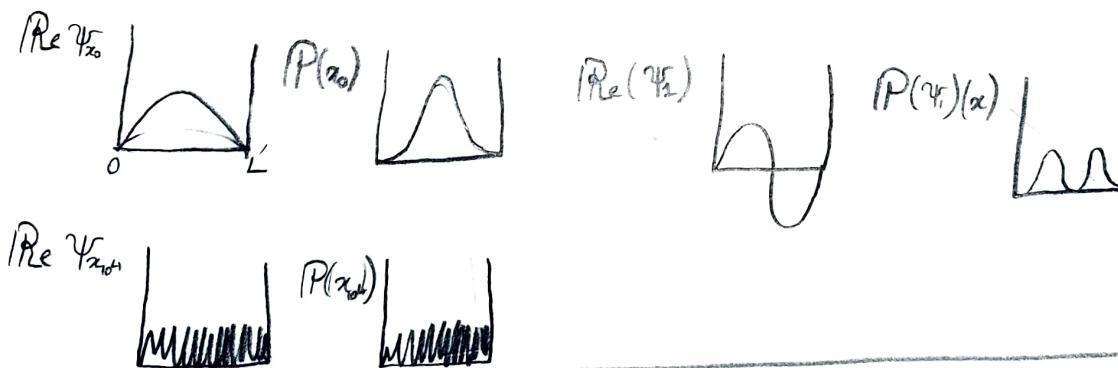
(2)  $i\hbar \partial_t \Psi(x,t) = \hat{E} \Psi(x,t)$   
 $\Psi(x,0) = \psi_n(x) \Rightarrow \Psi(x,t) = \psi_n(x) e^{-\frac{E_n t}{\hbar}}$   
 $\omega_n = E_n / \hbar$ .

$$\begin{aligned} \Psi(x) &= \int_{-\infty}^{\infty} \delta(x-x_0) \Psi(x_0) dx_0 \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{\Psi}(k) dk \\ &= \sum_n \psi_n(x) c_n \end{aligned}$$

(3)

Energy lvl's can be discrete or continuous.

$$\begin{aligned} \hat{E} &= \frac{\hat{p}^2}{2m} + u(x), \quad \Psi(x,t) = \sum_n c_n e^{i \frac{\hbar k_n^2 t}{2m}}. \\ \psi_n(x) &= \sqrt{\frac{2}{L}} \sin(k_n x), \quad k_n = \frac{(n-1)\pi}{L} \\ E_n &= \frac{\hbar^2 k_n^2}{2m} \end{aligned}$$



Qualitative Behaviour:

$u(x)$

Classically Allowed

$E > u(x)$

Curv.  $< 0$

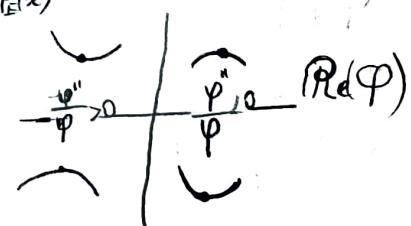
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$E < u(x)$

curv.  $> 0$

$$-\frac{\hbar^2}{2m} \Psi''_E(x) + u(x) \Psi_E(x) = E \Psi_E(x)$$

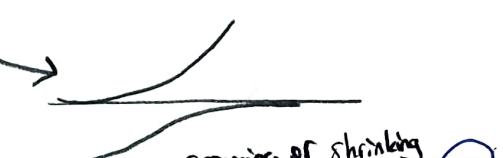
$$\frac{\Psi''_E(x)}{\Psi_E(x)} = -\frac{2m}{\hbar^2} (E - u(x))$$



$$\text{If } \frac{\Psi''}{\Psi} = x^2 \Rightarrow \text{Sol'n: } A e^{ix} + B e^{-ix}$$

$$\text{If } \frac{\Psi''}{\Psi} = -x^2 \Rightarrow \text{Sol'n: } A e^{ix} - B e^{-ix}$$

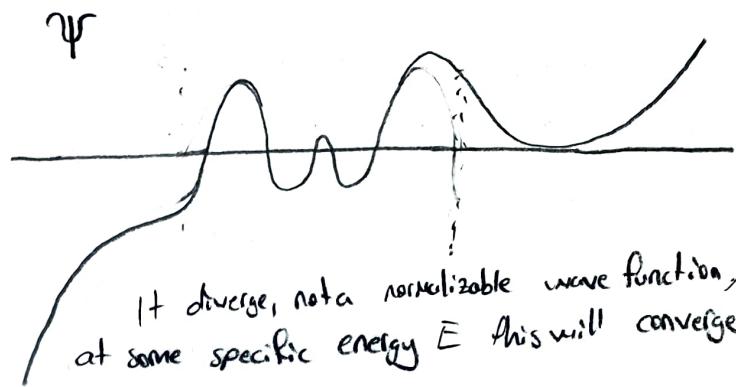
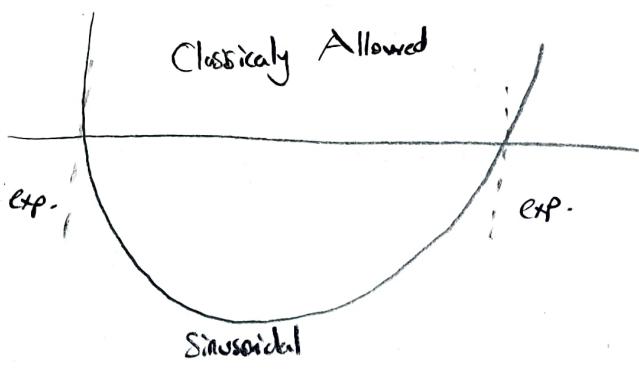
classically allowed  
region, sinusoidal



growing or shrinking  
exponentials on  
classically forbidden region

(5)

Exp.



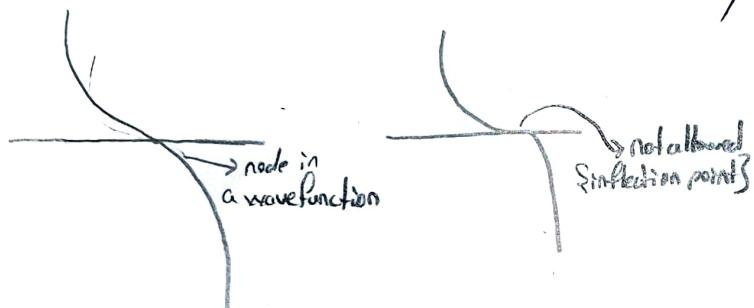
Schrodinger eqn. energy eigenstate

$$\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + V(x) \Psi(x) = E \Psi(x)$$

, if  $V(x)$  is a smooth potential then

$$\begin{cases} \Psi(x_0) = 0 \\ \Psi'(x_0) = 0 \end{cases} \Rightarrow \Psi(x) \equiv 0.$$

Bound State  $\Psi(x) \rightarrow 0$  as  $|x| \rightarrow \infty$



For bound states in 1-d, no degeneracy  
is possible.

Screened Potential

$\epsilon/\epsilon'$

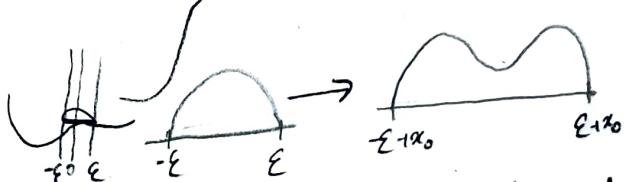
lowest  
energy state

$$V(x) \quad x(x) > 0 \quad \text{infinite # of nodes}$$

$$V(x) = \begin{cases} V(x), & |x| < a \\ \infty, & |x| > a \end{cases}$$

Let's take  $a = \epsilon \rightarrow 0$ .

If we scratch this interval, the wave function will start oscillating.



but from property of  $V(x)$ , wave function  
can't cross and pass through the axis since  
wave function can't vanish,

We say that ground state has "no nodes".

Now look excited states;  $\Psi_1, \Psi_2, \Psi_3, \dots$

Since we're working on 1 dimensional space, degeneracy is not possible.  
which means  $\Psi_i$  can not have same or lower energy compared to ground state  $\Psi_0$ .

So we say, for  $\Psi_0, \Psi_1, \Psi_2, \dots, \Psi_n$ ;  $\Psi_n$  has  $n$  nodes

$E_n > E_{n'}$  for  $n > n'$ .

### Harmonic Oscillator:

$$\hat{E} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2; [\omega] = 1/T, \frac{1}{2}m\omega^2x^2 = \omega(x).$$

Energy quantity  $[E] = [\hbar\omega]$ , Lengths "a"  $\frac{\hbar^2}{m\omega^2} = E = m\omega^2a^2 \Rightarrow a^2 = \hbar/m\omega$

$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) + \frac{1}{2}m\omega^2x^2 \Psi(x) = E \Psi(x)$ , we need to make it dimensionless so we can solve.

Multiply by  $2/\hbar\omega$ .

$$-\frac{\hbar}{2m\omega} \boxed{\frac{\partial^2}{\partial x^2}} \Psi(x) + \frac{m\omega \cdot x^2}{\hbar \frac{1}{L^2}} \Psi(x) = \frac{2E}{\hbar\omega} \Psi(x), \text{ apply } x=0 \text{ at } \text{dimensionless.}$$

$\boxed{\frac{1}{L^2}}$  unitless

$$\frac{d}{dx} = \frac{1}{a} \frac{d}{du}, \frac{d^2}{dx^2} = \frac{1}{a^2} \frac{d^2}{du^2} \Rightarrow \frac{\hbar}{2m\omega} \frac{1}{a^2} \frac{d^2}{du^2} + \frac{m\omega}{\hbar} u^2 \Psi = E \Psi$$

$$\Rightarrow \boxed{-\frac{d^2\Psi}{du^2} + u^2\Psi = E\Psi} \Rightarrow \frac{d^2\Psi}{du^2} + u^2\Psi - E\Psi = 0$$

when  $u \rightarrow \infty$ ,  $\Psi'' = +u^2\Psi$ . Try  $\Psi = u^k e^{u^2/2}$

$$\Psi' = \alpha u^k e^{u^2/2} + k u^{k-1} e^{u^2/2}$$

$$\Psi'' = (\alpha u)^2 u^k e^{u^2/2} + 2(\alpha u)(k) u^{k-1} e^{u^2/2} + k(k-1) u^{k-2} e^{u^2/2}$$

$$= \alpha^2 u^2 u^k e^{u^2/2} \left[ 1 + \frac{2k+1}{\alpha} \frac{1}{u^2} + \frac{k(k-1)}{\alpha^2} \frac{1}{u^4} \right] = \alpha^2 u^2 \Psi K. \text{ if } \alpha^2 = 1.$$

So as  $|u| \rightarrow \infty$

$$\Psi(u) \rightarrow A u^k e^{-u^2/2} + \underbrace{B u^k e^{u^2/2}}_{\text{we'll want this part to vanish.}}$$

(Write  $\Psi(u) = h(u)e^{-u^2/2}$ ,  $\Psi(u) = \frac{\Psi(u)}{e^{-u^2/2}} e^{-u^2/2} \Rightarrow$  we're hoping to get a simpler differential equation.)

$\boxed{h(u)} \Rightarrow$  Plug into I.

$$\frac{-d^2\Psi}{du^2} + u^2\Psi = \varepsilon\Psi \Rightarrow \frac{-d^2h(u)e^{-u^2/2}}{du^2} + u^2h(u)e^{-u^2/2} = \varepsilon h(u)e^{-u^2/2}$$

$$\Rightarrow \boxed{\frac{d^2h(u)}{du^2} 2u \frac{dh(u)}{du} + (\varepsilon - 1)h(u) = 0. \quad \text{II}}$$

Let's take power series.

$h(u) = a_0 + a_1 u + a_2 u^2 + a_3 u^3$ , see the behaviour of it.

$$h(u) = \sum_{j=0}^{\infty} a_j u^j \Rightarrow \frac{dh}{du} = \sum_{j=0}^{\infty} j a_j u^{j-1}$$

$$\Rightarrow \frac{d^2h}{du^2} - 2u \frac{dh}{du} + (\varepsilon - 1)h(u) = 0 = \sum_{j=0}^{\infty} [(j+2)(j+1)a_{j+2} - 2ja_j + (\varepsilon - 1)a_j] u^j$$

$$= \sum_{j=0}^{\infty} [(j+2)(j+1)a_{j+2} - 2(2j+1-\varepsilon)a_j] u^j = 0, \quad a_{j+2} = \frac{(2j+1-\varepsilon)}{(j+0)(j+1)} a_j$$

$a_0, a_1$  determines the whole function since its 2nd order ODE.

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Solutions fixed by given  $a_0, a_1$  ( $h(0), h'(0)$ )

From  $a_0$  is given; from  $a_1$  get odd solutions.

For  $j \gg$ ,  $a_{j+2} \approx \frac{2}{j} a_j$ , this behaviour is bad.

Let's see how  $e^{u^2} = \sum_{n=0}^{\infty} \frac{1}{n!} (u^2)^n = \sum_{j=0,2,4, \dots}^{\infty} \frac{1}{(j/2)!} u^j$ ;  $c_j = \frac{1}{0!(2)_1}, \frac{c_{j+2}}{c_j} = \frac{(j/2)!}{((j+2)/2)!} = \frac{1}{\frac{j}{2} + 1} \approx \frac{2}{j}$

Our series will diverge like  $e^{u^2}$ , if we want it to terminate

$2j+1 = \varepsilon$ , means  $\varepsilon$  must be an odd integer, makes  $a_{j+2} = 0$ .

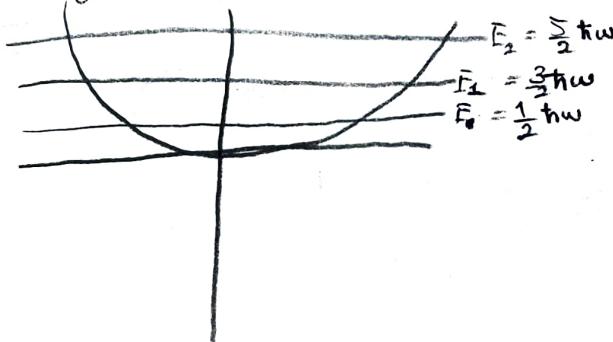
$h(u) = a_0 u + a_1 u^3 + \dots$ , call  $j=n$ ,  $2n+1 = \varepsilon = 0$ ,  $h(u) = a_0 u + a_{n-2} u^{2n-2} + \dots$

$$\varepsilon_n = \frac{E_n}{(\hbar\omega/2)} = 2n+1, \quad E_n = \hbar\omega(2n+1) = \hbar\omega(n+\frac{1}{2})$$

$$h_n(u) = H_n(u) = 2^n n! + \Theta(\varepsilon^{-2}), \quad \frac{d^2H_n}{du^2} - 2u \frac{dH_n}{du} + 2nH_n = 0.$$

$$e^{-u^2/2} + 2uH_n = \sum_{n=0}^{\infty} \frac{2^n}{n!} H_n(u)$$

$n$ -th degree polynomial means  $n$  nodes exists.



$$\hat{\Psi}_n = H_n(u) e^{-u^2/2}$$

$$\Psi_n(x) = H_n(\frac{x}{\sqrt{2\omega}}) e^{-x^2/2\omega^2}$$

## Operator Methods for Harmonic Oscillators

$$\hat{E} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 ; [\hat{t}, m\omega] = [\hat{p}]^2 \left[ \frac{\hat{t}}{m\omega} \right] = [\hat{x}]^2 ; x_0 = \sqrt{\frac{2\hbar}{m\omega}} , p_0 = \sqrt{2\hbar m\omega}$$

$$\hat{E} = \hbar\omega \left[ \frac{\hat{p}^2}{p_0^2} + \frac{\hat{x}^2}{x_0^2} \right] , x_0 p_0 = 2\hbar \cdot \left( \frac{\hat{x}}{x_0} - i\frac{\hat{p}}{p_0} \right) \left( \frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0} \right) = \frac{\hat{x}^2}{x_0^2} + \frac{\hat{p}^2}{p_0^2} + \frac{i}{2\hbar} [\hat{x}, \hat{p}]$$

$$\Rightarrow \frac{\hat{x}^2}{x_0^2} + \frac{\hat{p}^2}{p_0^2} - \frac{1}{2} \cdot \Rightarrow \hat{E} = \hbar\omega \left[ \frac{\hat{p}^2}{p_0^2} + \frac{\hat{x}^2}{x_0^2} \right] = \hbar\omega \left( \left( \frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0} \right) \left( \frac{\hat{x}}{x_0} - i\frac{\hat{p}}{p_0} \right) + \frac{1}{2} \right)$$

Def:  $\hat{a} = \left( \frac{\hat{x}}{x_0} - i\frac{\hat{p}}{p_0} \right)$ ,  $\hat{a}^\dagger = \left( \frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0} \right)$ ,  $\hat{E} = \hbar\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2})$

Given any  $\hat{\theta}$ , a Linear Operator, we can build  $\hat{\theta}^+$

$$\int f^*(\hat{\theta}g) dx \equiv \int (\hat{\theta}f)^* g dx , \hat{\theta}^+ = \begin{matrix} \text{Hermitian} \\ \text{Adjoint} \\ \text{of } \hat{\theta} \end{matrix}$$

Ex.1:  $c \in \mathbb{C}$ ,  $c^*$ :  $\int f^*(c^*g) dx = \int (cf)^* g dx = \int f^*(c^*g) dx$ . true for all f.g.

$$So \Rightarrow c^* = c^* .$$

Ex.2: What is  $\partial_x^+$

$$\int f^*(\partial_x^+ g) dx = \int (\partial_x f)^* g dx = \int (\partial_x f^*) g dx = - \underbrace{\int f^* \partial_x g dx}_{\text{From integration by parts.}} = \int f^* (-\partial_x g) dx$$

$$\partial_x^+ = -\partial_x$$

" we assumed that surface terms vanish."

Ex.3:  $\hat{x}^+ = \hat{x}f(x) = xf(x)$

$$\int f^*(\hat{x}^+ g) dx = \int (\hat{x}f)^* g dx = \int xf^* g dx = \int f^*(xg) dx , \hat{x}^+ = \hat{x} .$$

Def:  $\hat{\theta}^+ = \hat{\theta}$  called Hermitian.

Fact: Any operator which equals to its adjoint has Real eigenvalues only.

Ex.4:  $\hat{p}^+ = \hat{p}$  since  $\hat{p} = \frac{\hbar}{i} \partial_x$

Physical Fact: If all Observables are Real

Then in Quantum mechanics  $\Rightarrow$  All Operators  $\leftrightarrow$  Observables must be Real.

So we can say, the operator we defined as  $\hat{a}$  is not Hermitian and

NOT associated with an observable.

$$\hat{E} = \hat{E}^+, \quad [\hat{a}, \hat{a}^\dagger] = \left[ \frac{\hat{x}}{\hat{x}_0} + i \frac{\hat{p}}{\hat{p}_0}, \left( \frac{\hat{x}}{\hat{x}_0} - i \frac{\hat{p}}{\hat{p}_0} \right) \right] = \frac{i}{\hat{x}_0 \hat{p}_0} [\hat{x}, \hat{p}] + \frac{i}{\hat{x}_0 \hat{p}_0} [\hat{p}, \hat{x}]$$

$$\Rightarrow \frac{-i}{2\hbar} [\hat{x}, \hat{p}] + \frac{i}{2\hbar} [\hat{p}, \hat{x}] = \frac{-i}{2\hbar} i\hbar + \frac{i}{2\hbar} -i\hbar = \frac{1}{2} + \frac{1}{2} = 1.$$

Therefore  $[\hat{a}, \hat{a}^\dagger] = 1, [\hat{a}^\dagger, \hat{a}] = -1$ .

$$[\hat{E}, \hat{a}] = \hbar\omega [\hat{a}^\dagger \hat{a}, \hat{a}] = \hbar\omega (\hat{a}^\dagger \hat{a} \hat{a} - \hat{a} \hat{a}^\dagger \hat{a}) = \hbar\omega (\hat{a}^\dagger \hat{a} - \hat{a} \hat{a}^\dagger) \hat{a} = -\hbar\omega \hat{a}$$

$$\Rightarrow [\hat{E}, \hat{a}] = -\hbar\omega \hat{a} \Rightarrow [\hat{E}, \hat{a}^\dagger] = \hbar\omega \hat{a}^\dagger$$

Suppose  $\hat{E} \varphi_E = E \varphi_E$ , consider  $\Psi = \hat{a} \varphi_E \quad \left\{ AB f(x) = ([A, B] + BA) f(x) \right\}$

$$\hat{E} \Psi = \hat{E} \hat{a} \varphi_E = (\hat{E} \hat{a} - \hat{a} \hat{E} + \hat{a} \hat{E}) \varphi_E = ([\hat{E}, \hat{a}] + \hat{a} \hat{E}) \varphi_E = (-\hbar\omega \hat{a} + E \hat{a}) \varphi_E.$$

$= (E - \hbar\omega) \hat{a} \varphi_E = (E - \hbar\omega) \Psi \Rightarrow$  eigenvalue decreased by  $\hbar\omega$ .

And, consider  $\Psi = \hat{a}^\dagger \varphi_E$

$$\hat{E} \Psi = \hat{E} \hat{a}^\dagger \varphi_E = [\hat{E} \hat{a}^\dagger - \hat{a}^\dagger \hat{E} + \hat{a}^\dagger \hat{E}] \varphi_E = ([\hat{E}, \hat{a}^\dagger] + \hat{a}^\dagger \hat{E}) \varphi_E = (\hbar\omega \hat{a}^\dagger + E \hat{a}^\dagger) \varphi_E$$

$$= (E + \hbar\omega) \hat{a}^\dagger \varphi_E = (E + \hbar\omega) \Psi.$$

$\hat{E} \varphi_E = E \varphi_E \Rightarrow \begin{cases} \hat{a} \varphi_E \text{ has energy value } E - \hbar\omega, \Psi \propto \varphi_{E-\hbar\omega} \Rightarrow \text{called Lowering Operator} \\ \hat{a}^\dagger \varphi_E \text{ has energy value } E + \hbar\omega, \Psi \propto \varphi_{E+\hbar\omega} \Rightarrow \text{called Raising Operator} \end{cases}$

$$\hat{a} \varphi_E = \varphi_{E-\hbar\omega}, \hat{a}^\dagger \varphi_E = \varphi_{E+\hbar\omega}$$

The energy states evenly spaced because of the commutator, when we first computed the commutator of  $E$  with  $\hat{a}, \hat{a}^\dagger$  it was determined that it will leave a pattern like that.

They're called Landau Levels.

This ladder extends to infinitely up.

Let's show the min. value

$$\langle E \rangle = \int \varphi_E^* \hat{E} \varphi_E dx = \int \underbrace{|\tilde{\Psi}(p)|^2 \frac{p^2}{2m}}_{\text{positive}} dp + \int \underbrace{|\Psi(x)|^2 \frac{m\omega^2 x^2}{2}}_{\text{positive}} dx$$

So  $E$  must have a "ground state".

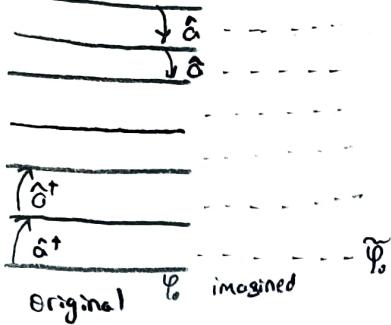
minimum  $E$ ,  $\hat{a} \varphi_E = 0 \Rightarrow$  non-normalizable

$\left\{ \text{But, can't we create different intersection ladders?} \right\}$

Imagine it is not all of them, if there is another state there must be a states of ladder.

Can there be two states with two different energies  $\phi_0$

Can there be two different states with annihilated by  $a_0$



$\hat{E} \phi_0 = \hbar\omega(a^\dagger a + \frac{1}{2}) \phi_0$ ,  $a$  also called annihilation operator  
 $= \frac{1}{2} \hbar\omega \phi_0$  so any annihilated ground state must have  
 "Some" energy, means the imagined ladder is degenerate.

Last time we showed the Node theorem and said we can not have degeneracies in 1-D.  
 which means we missed no states and that is the all states must exists.

$$\hat{a} \phi_0(x) = 0 = \left( \frac{\hat{x}}{x_0} + i \frac{\hat{p}}{p_0} \right) \phi_0(x) = \left( \frac{\hat{x}}{x_0} + i \frac{\hbar}{\ell} \partial_x - \frac{1}{p_0} x \right) \phi_0 = \left( \partial_x + \frac{p_0}{\hbar x_0} x \right) \phi_0(x)$$

$\hookrightarrow 0$  Function, not zero energy.

$$\Rightarrow \text{Its solution is Gaussian} \Rightarrow \left( \partial_x + \frac{2}{x_0^2} x \right) \phi_0(x) = 0 \Rightarrow \phi_0 = C e^{-x^2/x_0^2}, \phi_1 = N \left( \partial_x - \frac{2}{x_0^2} x \right) \phi_0$$

$$\phi_1 = N \left( \partial_x - \frac{2}{x_0^2} x \right)^k \phi_0$$

$\hat{A}, \hat{B}$ ; is it possible for these to be function  $\phi_{ab}$  simultaneously.

$$\hat{A} \phi_{ab} = a \phi_{ab}, \hat{B} \phi_{ab} = b \phi_{ab}$$

$$\text{Take } [\hat{A}, \hat{B}] \phi_{ab} = (\hat{A}\hat{B} - \hat{B}\hat{A}) \phi_{ab} = \hat{A}\hat{B} \phi_{ab} - \hat{B}\hat{A} \phi_{ab} = ab \phi_{ab} - ba \phi_{ab} = (ab - ba) \phi_{ab} = 0.$$

$[\hat{A}, \hat{B}]$  must be zero.

Let's say.

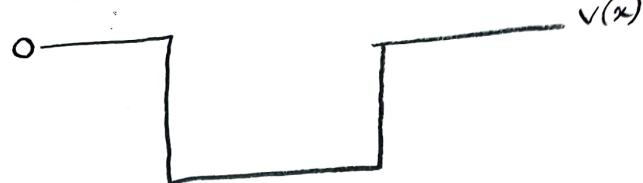
$[\hat{A}, \hat{B}] = c \cdot \mathbf{1}$ . The state of being in a definite value of  $ab$  simultaneously does not exist.  
 Because being in a state with definite value of  $ba$  would be an eigenfunction of  $a$ , and its also true  
 for the  $b$  case but there are no common states or common eigenfunctions because  
 commutator never kills the state

$$[x, p] = i\hbar \mathbf{1} \rightarrow \Delta x \Delta p \geq \frac{\hbar}{2} |\langle \psi | [\hat{A}, \hat{B}] | \psi \rangle|$$

$$\langle \psi | i\hbar \mathbf{1} | \psi \rangle = i\hbar$$

$\Delta x \Delta p \geq \frac{\hbar}{2}$ , uncertainty does not depends on wave function.

## Finite Potential Well



$$\hat{E} \varphi_E(x) = -\frac{\hbar^2}{2m} \varphi''_E(x) + V(x) \varphi_E(x)$$

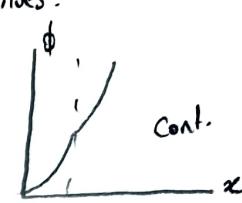
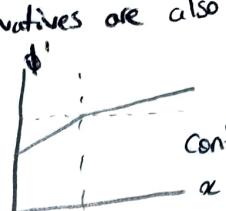
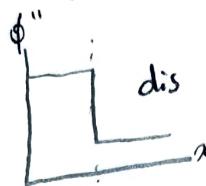
$\varphi''_E(x) = \frac{2m}{\hbar^2} (V(x) - E) \varphi_E(x)$ , there should be discrete energy levels.

### Continuity of $\varphi_E(x)$

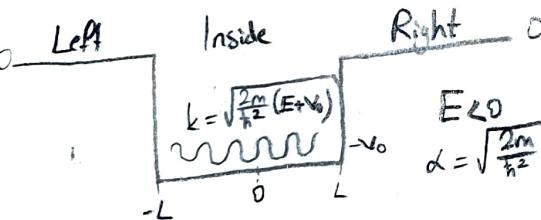
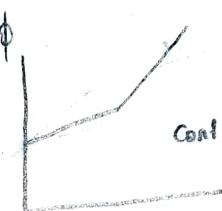
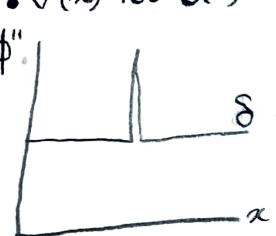
•  $v(x)$  continuous, means function itself and first two derivatives are also continuous.

•  $v(x)$  has step-discontinuity

- $\varphi(x)$ ,  $\varphi'(x)$  continues but  $\varphi''(x)$  is discontinuous



•  $v(x)$  has  $\delta(x)$



General Solution

$$\varphi_E(x) = \begin{cases} A \cos(kx) + B \sin(kx) & \Rightarrow \text{Inside} \\ C e^{ax} + D e^{-ax} & \Rightarrow \text{Left} \\ G e^{ax} + F e^{-ax} & \Rightarrow \text{Right} \end{cases}$$

$$\left. \begin{array}{l} \text{If } E > V(x) \\ \varphi'' = -k^2 \varphi \Rightarrow \text{osc.} \end{array} \right\} k^2 = \frac{2m}{\hbar^2} (E - V(x))$$

$$\left. \begin{array}{l} \text{If } E < V(x) \\ \varphi'' = \alpha^2 \varphi \Rightarrow \text{exp.} \end{array} \right\} \alpha^2 = \frac{2m}{\hbar^2} (V(x) - E)$$

Normalizable:

$$\varphi(2\pi \rightarrow \infty) = 0 \Leftrightarrow D = 0$$

$$\varphi(\infty \rightarrow \infty) = 0 \Leftrightarrow G = 0$$

|                     |                    |
|---------------------|--------------------|
| parity, sym. (even) | $B = 0$ , $C = F$  |
| anti-sym (odd)      | $A = 0$ , $C = -F$ |

For Even:

$$\text{Right B.C. } \varphi(x=L) = 0$$

$$\varphi = C e^{-\alpha L} = A \cos(kL) \Rightarrow C = A \cos(kL) e^{-\alpha L}$$

$$\varphi' = -\alpha C e^{-\alpha L} = -k A \sin(kL) \Rightarrow C = +A \frac{k}{\alpha} \sin(kL) e^{-\alpha L}$$

$$-\frac{\varphi'}{\varphi} = k \tan(kL) = \alpha \Rightarrow kL \tan(kL) = L\alpha = \text{Condition on } E.$$

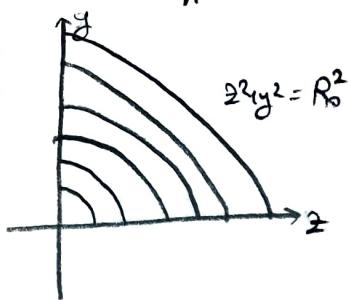
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$$k^2 = \frac{2m}{\hbar^2} (V_0 + E), \quad \alpha^2 = \frac{2m}{\hbar^2} (-E)$$

Graphical Solution:

$$kL = \frac{y}{\hbar}, \alpha L = y$$

$$\frac{y^2}{\hbar^2} = \frac{2mL^2}{t^2} V_0 \equiv R_0^2$$

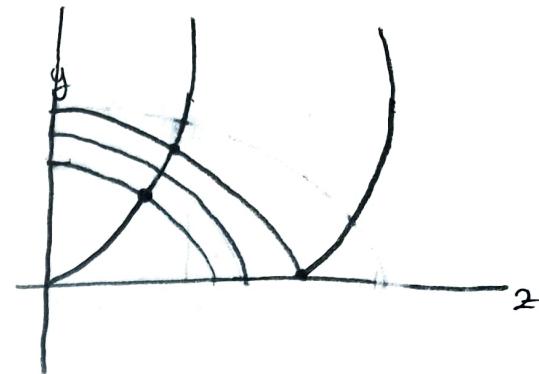


$$2 \tan z = y, \frac{y^2}{R_0^2} = \frac{\sin^2 z}{\cos^2 z}$$

We want solutions simultaneously for these equations.

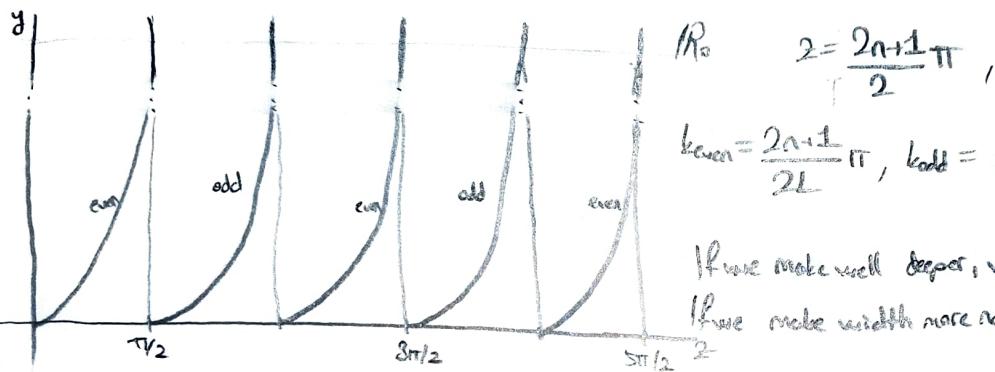
$$2 \tan z = y$$

$\Rightarrow$



In 1-D we always have at least 1 bound state.

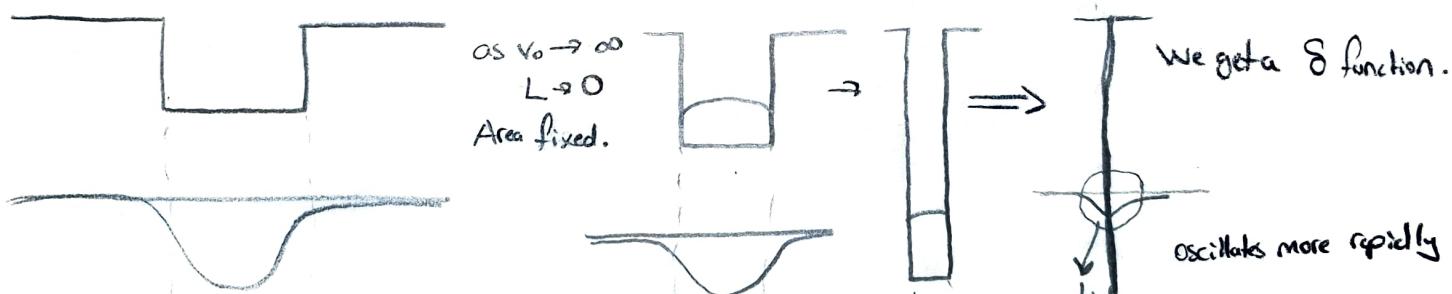
If we take "well" arbitrarily deep.



$$R_0 = \frac{2n+1}{2}\pi,$$

$$k_{\text{even}} = \frac{2n+1}{2L}\pi, k_{\text{odd}} = \frac{n+1}{L}\pi$$

If we make well deeper, we get more states and if we make width more narrow we get less states.



$$\text{Ex: } V = -V_0 \delta(x) \quad \begin{array}{c} L \\ \diagdown \\ R \end{array}$$

$$\delta(x) = \frac{1}{|\Delta|} \delta(x)$$

$$\frac{V_0}{\epsilon}, \epsilon \text{ is width.}$$

$$\phi_E(x) = \begin{cases} Ae^{ix} + Be^{-ix} & x < 0 \\ Ce^{ix} + De^{-ix} & x > 0 \\ A=0 \text{ since sym.} \end{cases}$$

$$\phi'' = -\frac{2m}{\hbar^2} (V_0 \delta(x) + E) \phi$$

- $\phi'' = \delta$
- $\phi' = \text{step}$
- $\phi = \text{cont.}$

$$\int_{-\epsilon}^{\epsilon} \phi'' dx = \phi'(E) - \phi'(\epsilon) = -\frac{2m}{\hbar^2} V_0 \phi(0) + \delta(\epsilon)$$

$$\lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \phi'' dx \Rightarrow \Delta \phi'(0) = -\frac{2m}{\hbar^2} V_0 \phi(0) \Rightarrow \text{This is only solvable if}$$

$$\epsilon = \frac{m V_0}{\hbar^2}$$

$$E = -\frac{\hbar^2 \alpha^2}{2m}, \text{ Delta function has "1" even bound state}$$

"Every isolated Delta function has 1 bound state".

For odd ones,  $A=-D$  and wavefunction  $\phi(0)=0$ . This becomes zero for it and discontinuity is also zero. Means there is no potential.

(9)

# Scattering in 1-D Space:

$$\phi_E = A e^{i(kx - \omega t)} + B e^{-i(kx + \omega t)} \quad \text{to solve Schrodinger Eq.} \quad \omega = \frac{\hbar k^2}{2m}$$

$\underbrace{x = \omega t}_{E}$   $\underbrace{x = \omega t}_{k}$   $\phi_E$  is not normalizable  
 along  $+x$  direction along  $-x$  direction

$$\phi_k = \frac{1}{\sqrt{2\pi}} e^{ikx} \quad \text{such that } (\phi_k | \phi_{k'}) = \delta(k - k')$$

Evolution in time of a well localized wavepacket.

Ex: Consider a free particle in a min. uncertainty  $\mathcal{W}$ .

$$\Psi(x, 0) = \frac{1}{\sqrt{a\pi}} e^{-x^2/2a^2} \rightarrow \text{what is } \Psi(x, t)?$$

$$\Psi(x, 0) = \sum_n c_n \Psi_n(x) \Rightarrow \Psi(x, t) = \sum_n c_n \Psi_n(x) e^{-i \frac{E_n t}{\hbar}}, \quad \hat{E} \Psi_n = E_n \Psi_n$$

$$\Rightarrow \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (e^{ikx}) \tilde{\Psi}(k) dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \frac{1}{\sqrt{\pi}} e^{-k^2 a^2/2} dk.$$

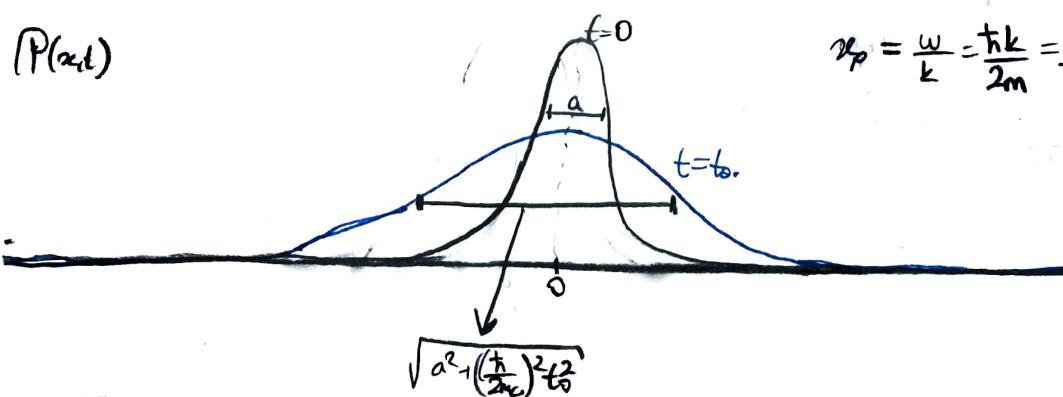
$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} e^{i(kx - \omega_k t)} e^{-k^2 a^2/2} dk = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} e^{i(kx - \frac{\hbar k^2}{2m} t)} e^{-k^2 a^2/2} dk$$

$$= \sqrt{\frac{a}{\pi}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} e^{-k^2/2(1 + \frac{i\hbar}{2ma} t)^2} dk$$

$$\Psi(x, t) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{a^2 + (\frac{\hbar}{2ma} t)^2}} e^{-x^2/2(a^2 + (\frac{\hbar}{2ma} t)^2)}$$

Probability at any point as time goes on is decreasing.  
 Width is getting increased.  $\Delta x = \frac{\hbar}{2ma}$

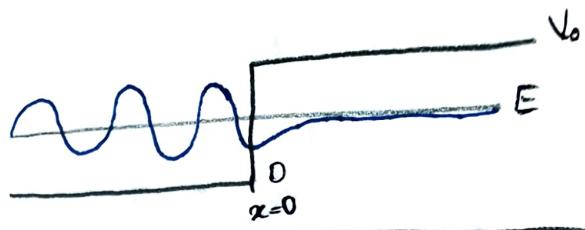
$$\nu_p = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{\omega_c}{2}; \nu_g = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m} = \omega_c$$



Ex: Potential Step:

$$\phi_E(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ C e^{\alpha x} + D e^{-\alpha x} & x > 0 \end{cases}$$

L  
R



$\phi, \phi'$  must be continuous at  $x=0$ .

$$\phi: A+B=D, \phi': i(A-B)=\alpha D.$$

$$\Rightarrow D = \frac{2k}{k+\alpha}, B = \frac{k-\alpha}{k+\alpha} = e^{i\phi} \quad \omega = E/\hbar$$

$$\phi_E(x,t) = \begin{cases} Ae^{i(kx-\omega t)} + Be^{-i(kx-\omega t)} & x < 0 \\ De^{\alpha x - \omega t} & x > 0 \end{cases}$$

$Ae^{i(kx-\omega t)}$  Right Moving Contribution

$Be^{-i(kx-\omega t)}$  Left Moving Contribution

$De^{\alpha x - \omega t}$  Exponentially falling, rotating phase

Suppose we have a wavefunction such

$$\int |\psi|^2 dx = N \neq 1. \quad (1)$$

$$(2) \int dP = \frac{1}{N} \int |\psi|^2 dx \quad \text{Since } \int dP = \frac{1}{N} \int |\psi|^2 dx = \frac{1}{N} \cdot N = 1 \quad (3)$$

$N$  is called normalization factor as long as  $\int |\psi|^2 dx < \infty$  we can find a  $N$  and normalize the wavefunction. This functions called

normalizable or square integrable functions.

By adjusting the coeff. of  $\psi$  we can make it normalized. Assuming (1) we define  $\psi'$  as

$$\psi' = \frac{1}{\sqrt{N}} \psi \quad (4) \quad \text{is properly normalized. So}$$

$$\int |\psi'|^2 dx = \frac{1}{N} \int |\psi|^2 dx = 1. \quad (5)$$

Now let's look at  $\psi'$  as a probability amplitude. Suppose  $\psi'$  is a normalized wavefunction

at initial time  $t_0$ .

$$\int_{-\infty}^{\infty} \psi'^*(x, t_0) \psi'(x, t_0) dx = 1. \quad (6)$$

Since Schrodinger Equation determine  $\psi'$  for all times, Do we have

$$\int_{-\infty}^{\infty} \psi'^*(x, t) \psi'(x, t) dx = 1 ? \quad (7)$$

First Define the Probability Density,  $\rho(x,t)$

$$\rho(x,t) = \Psi^*(x,t) \Psi(x,t) = |\Psi(x,t)|^2 \quad (8)$$

Define also  $N(t)$  as the integral of probability density throughout space

$$N(t) \equiv \int \rho(x,t) dx \quad (9)$$

Since wavefunction initially normalized,  $N(t_0)=1$ .

To say that  $N(t)=1$ , we should show that

$$\frac{dN(t)}{dt} = 0 \quad (10)$$

We call this conservation of probability. Let's check on Schrodinger Equation

$$\frac{dN(t)}{dt} = \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t} dx = \int_{-\infty}^{\infty} \left( \frac{\partial \Psi^*}{\partial t} M(x,t) + \Psi^*(x,t) \frac{\partial M(x,t)}{\partial t} \right) dx \quad (11)$$

Take its complex conjugate,

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi \Rightarrow \frac{\partial \Psi^*}{\partial t} = -\frac{i}{\hbar} \hat{H} \Psi^* \quad (12)$$

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = (\hat{H} \Psi)^* \Rightarrow \frac{\partial \Psi^*}{\partial t} = \frac{i}{\hbar} (\hat{H} \Psi)^* \quad (13)$$

Now use (12) and (13) in (11),

$$\begin{aligned} \frac{dN(t)}{dt} &= \int_{-\infty}^{\infty} \left( \frac{i}{\hbar} (\hat{H} \Psi)^* \Psi - \frac{i}{\hbar} \Psi^* (\hat{H} \Psi) \right) dx \\ &= \frac{i}{\hbar} \left[ \int_{-\infty}^{\infty} (\hat{H} \Psi)^* \Psi dx - \int_{-\infty}^{\infty} \Psi^* (\hat{H} \Psi) dx \right] \end{aligned} \quad (14)$$

To show that time derivative of  $N(t)$  vanishes

$$\int_{-\infty}^{\infty} (\hat{H} \Psi)^* \Psi dx = \int_{-\infty}^{\infty} \Psi^* (\hat{H} \Psi) dx \quad (15)$$

must be equal. If  $\hat{H}$  is a Hermitian operator the condition will be satisfied.  $\hat{H}$  is Hermitian if

$$\int_{-\infty}^{\infty} (\hat{H} \Psi_1)^* \Psi_2 dx = \int_{-\infty}^{\infty} \Psi_1^* (\hat{H} \Psi_2) dx \quad (16)$$

By defining Hermitian conjugate  $\hat{H}^\dagger$

$$\int_{-\infty}^{\infty} \Psi_1^* (\hat{H} \Psi_2) dx = \int_{-\infty}^{\infty} (\hat{H}^\dagger \Psi_1)^* \Psi_2 dx \quad (17)$$

$\hat{A}$  is Hermitian if  $\hat{A} = \hat{A}^\dagger$ .

A. Said Tongel

Now take a look to the integrand of equation (14).

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar} \left[ (\hat{H}\psi)^* \psi - \psi^* (\hat{H}\psi) \right] \\ = \frac{i}{\hbar} \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \psi^*}{\partial x^2} \psi - \frac{\partial^2 \psi}{\partial x^2} \psi^* \right) + V(x,t) \psi^* \psi - \psi^* V(x,t) \psi \right] \quad (18)$$

$$= \frac{\hbar}{2im} \left( \frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) \quad (19)$$

To show that the integral is zero if must be a total derivative.

$$\Rightarrow \frac{\partial}{\partial x} \left[ \frac{\hbar}{2im} \left( \frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right) \right] \quad (20)$$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} J(x,t) \quad \text{where } J(x,t) = \frac{\hbar}{2im} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x} J(x,t)$ .  $J(x,t)$  is called current associated probability P.  
Conservation equation.

Now if we come back to our Potential Step Problem;

$$\psi = \begin{cases} \psi_I & L \\ \psi_R & R \end{cases} \quad T = \left| \frac{J_T}{J_I} \right|^2 = 0 \\ R = \left| \frac{J_R}{J_I} \right|^2 = 1 \quad \left. \right\}$$

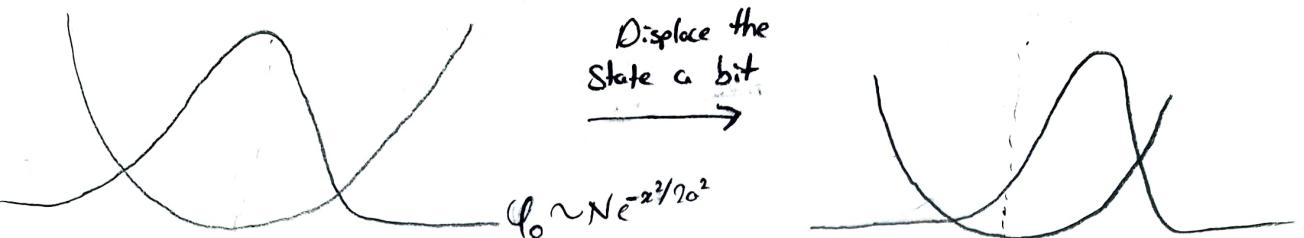
$$J_I = \frac{\hbar k}{m} |A|^2 \quad J_R = \frac{\hbar k}{m} |B|^2$$

$$J_T = 0.$$

Def:

$$T \equiv \left| \frac{J_T}{J_I} \right|^2 \Rightarrow \text{Transmission Probability} \\ R \equiv \left| \frac{J_R}{J_I} \right|^2 \Rightarrow \text{Reflection Probability} \quad \left. \right\}$$

Coherent States: The ground state of a Harmonic Oscillator, Gaussian.



If we take a state  $\psi_0$  and translate it by  $x_0$  and act with annihilation operator  
- Normally if we act on  $\psi_0$  with  $\hat{a}$  -

$\hat{a}\psi_0(a)=0$ , since  $\psi_0$  is ground state but

$\hat{a}\psi_0(x-x_0)=C\psi_0(x)$  it turns out that displaced Gaussian states are eigenstates of the annihilation operator

which are "Coherent States".

Coherent States mostly behaves classically even created by quantum mechanical wavefunction.

Ex. Scattering:

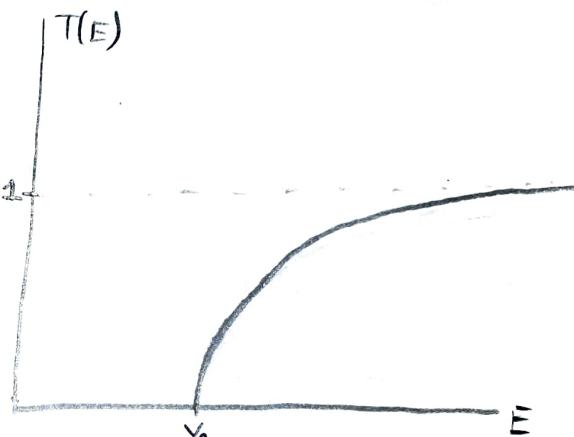


$$E > V_0$$

$$\frac{\hbar^2 k_1^2}{2m} = E, \quad \frac{\hbar^2 k_2^2}{2m} = E - V_0$$

$$\phi_E = \begin{cases} \text{In} \\ A e^{ik_1 x} + B e^{-ik_1 x} \\ \text{Out} \\ C e^{ik_2 x} + D e^{-ik_2 x} \end{cases}$$

$$\left. \begin{array}{l} L \\ R \end{array} \right\} e^{\pm i k x}$$



Incident From L  $\Rightarrow D=0, A \neq 0$   
" " R  $\Rightarrow A=0, D \neq 0$

$$D=0 \quad C = \frac{2k_1}{k_1+k_2} A, \quad B = \frac{k_1-k_2}{k_1+k_2} A$$

$$A=0 \quad C = \frac{k_1-k_2}{k_1+k_2} D, \quad B = \frac{2k_2}{k_1+k_2} D$$

$$\Rightarrow R = \left| \frac{k_1-k_2}{k_1+k_2} \right|^2 = \left| \frac{1-\sqrt{1-V_0/E}}{1+\sqrt{1-V_0/E}} \right|^2$$

$$T = \frac{4k_1 k_2}{(k_1+k_2)^2} = \frac{4\sqrt{1-V_0/E}}{(1+\sqrt{1-V_0/E})^2}$$

$$R+T=1$$

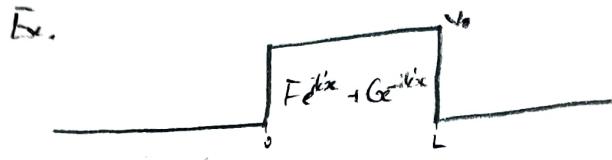
But transmission was also this.  
So we can say transmission and reflection amplitude are the same.

In classical mechanics when an object travels from low to high potential it would slow down and when traveling from high to low it gets faster.

But in Quantum Mechanics this thing is symmetric whether its moving from high to low or low to high.

From the detailed shape of the graph of transmission as a function of Energy, we can deduce what the potential and using phase shift.

A. Said Tengel



$$\frac{\hbar^2 k^2}{2m_e} = E, \quad \frac{\hbar^2 k'^2}{2m_e} = E - V_0$$

$$g_0^2 = \frac{2m_e L^2 V_0}{\hbar^2}, \quad \varepsilon = \frac{E}{V_0}.$$

$$D=0, E > V_0$$

$$T = \left| \frac{C}{A} \right|^2 = \frac{4k^2 k'^2}{4k^2 k'^2 \cos^2(k'L) + (k^2 k'^2) \sin^2(k'L)}$$

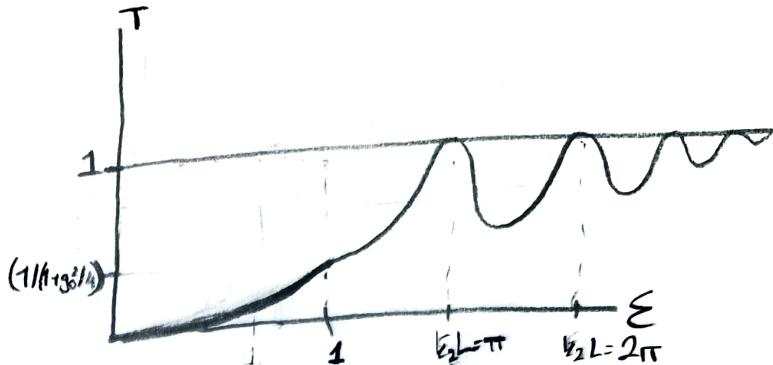
$$T_{E > V_0} = \frac{1}{1 + \frac{1}{4\varepsilon(\varepsilon-1)} \sin^2(g_0 \sqrt{\varepsilon-1})}$$

$$\Rightarrow \sim \frac{1}{1 + \frac{g_0^2}{4}} \text{ as } \varepsilon \rightarrow 1.$$

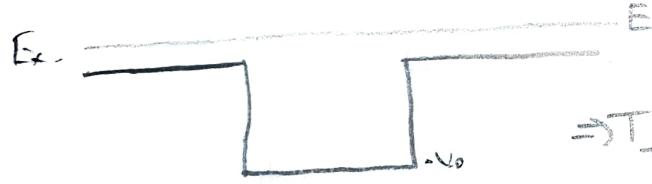
$$T_{E < V_0} = \frac{1}{1 + \frac{1}{4\varepsilon(1-\varepsilon)} \sinh^2(g_0 \sqrt{1-\varepsilon})}$$

For  $L \gg 1$ ,  $T \sim e^{-2kL}$

$\alpha$  is proportional with  $E$ .

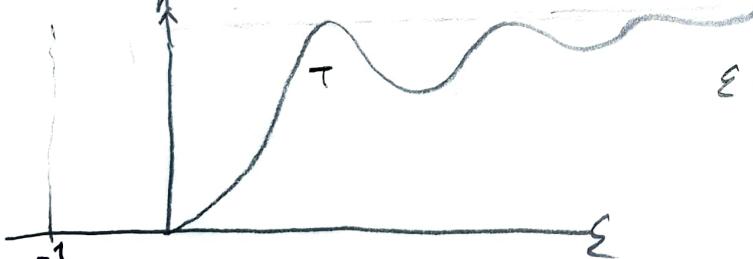


This transmission across classically disallowed barrier is called "Quantum Tunneling".

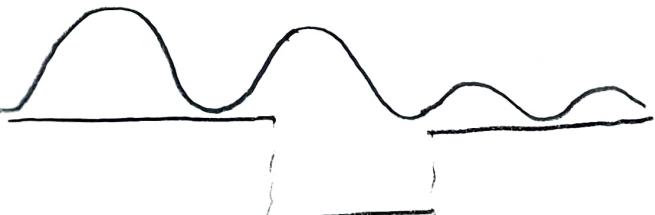


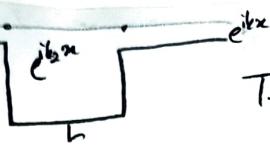
$$\Rightarrow T = \frac{1}{1 + \frac{1}{4\varepsilon(\varepsilon+1)} \sin^2(g_0 \sqrt{\varepsilon+1})}$$

$$g_0^2 = \frac{2m_e L^2}{\hbar^2} V_0, \quad \varepsilon = \frac{E}{V_0}$$



$\varepsilon$  must be greater than -1.

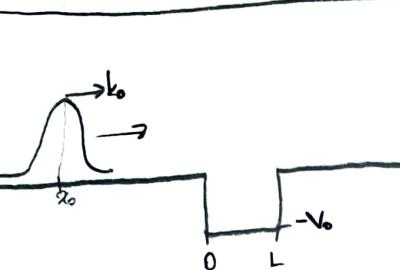




$T_{ur} \neq T_u T_r$ , probabilities don't add up wavefunctions do.

$$t_{ur} = t_u e^{ik_0 L} t_r + t_r e^{ik_1 L} r e^{ik_0 L} e^{ik_1 L} + \dots$$

$$\Rightarrow t_{ur} = t_u e^{ik_0 L} t_r \left( \frac{1}{1 - (r)^2 e^{2ik_0 L}} \right) = \frac{1}{e^{ik_0 L} - \frac{2i}{T_r} \sin(k_0 L)} \Rightarrow T_{ur} = \frac{1}{1 + \frac{1}{4\epsilon(E-\epsilon)} \sin^2(g_0 \sqrt{E-\epsilon})}$$



$$\Psi(x_0) = N e^{-(x-x_0)^2/2\sigma^2} e^{ik_0 x}, \quad \tilde{f}(k) = \sqrt{\epsilon} e^{-\epsilon^2 (k-k_0)^2/2} e^{-ik_0 x}$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int e^{ikx} \tilde{f}(k) dk, \quad \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \tilde{f}(k) e^{ikx - wt} dk$$

$$\frac{k^2 L^2}{2m} = \hbar w$$

$$E = \frac{k^2 L^2}{2m} \quad \phi_L = \frac{1}{\sqrt{2\pi}} \left[ e^{ikx} \delta(-x) + r e^{-ikx} \delta(-x) + t e^{ikx} \delta(x) \right], \quad r = \text{reflection amplitude}, \quad t = \text{transmission amplitude}$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int \tilde{f}(k) \phi_L dk = \frac{1}{\sqrt{2\pi}} \int [\tilde{f}(k) e^{ikx} \delta(-x) + \tilde{f}(k) (e^{-ikx} \delta(-x) + \tilde{f}(k) \cdot t e^{ikx} \delta(x))] dk. \quad \delta(x) = \begin{cases} 1, & x=0 \\ 0, & x \neq 0 \end{cases}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int [\tilde{f}(k) e^{i(kx-wt)} \delta(-x) + \tilde{f}(k) (e^{-i(kx-wt)} \delta(-x) + \tilde{f}(k) (e^{i(kx-wt)} \delta(x))] dk$$

at  $t=0$ :

$$\int (\tilde{f}(k) e^{ikx} \delta(x)) dk \Rightarrow G(x_0, k_0, 0) \delta(x). \text{ That gives us our Gaussian back.}$$

$$\frac{d}{dk} (kx - w(k)t) \Big|_{k_0} = x - \frac{\hbar k}{m} t = 0 \Rightarrow x = \frac{\hbar k}{m} t = v_0 t, \text{ where } v_0 \text{ is classical velocity}$$

$$\tilde{f}(kx-wt) \delta(-x) \equiv \text{Term 1}, \quad e^{-i(kx-wt)} \delta(-x) \equiv \text{Term 2}, \quad (e^{i(kx-wt)} \delta(x) \equiv \text{Term 3}).$$

As time goes forward Term 1 will gone and get replaced by term 2 and 3.

Focus on 3rd term.

$$t = \sqrt{T} e^{-i\varphi}, \quad \delta(x) \frac{1}{\sqrt{2\pi}} \int \tilde{f}(k) e^{i(kx-wt-\varphi)} \sqrt{T} dk$$

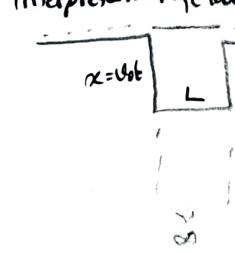
$$\Rightarrow \frac{d}{dk} (kx - wt - \varphi) \Big|_{k_0} = 0 \quad , \quad \frac{d\varphi}{dk} = \frac{dw}{dk} \frac{d\varphi}{dw} = v_0 \frac{\hbar}{m} \frac{d\varphi}{dE}$$

$$= x - v_0 t - \frac{d\varphi}{dk}$$

$$= x - v_0 \left( t + \hbar \frac{\partial \varphi}{\partial E} \right) = 0$$

$$x = v_0 \left( t + \hbar \frac{\partial \varphi}{\partial E} \right)$$

Interpretation [classically]



$$x = v_0 (t + \frac{L}{v_0})$$

$$\Delta t = \frac{L}{v_0}$$

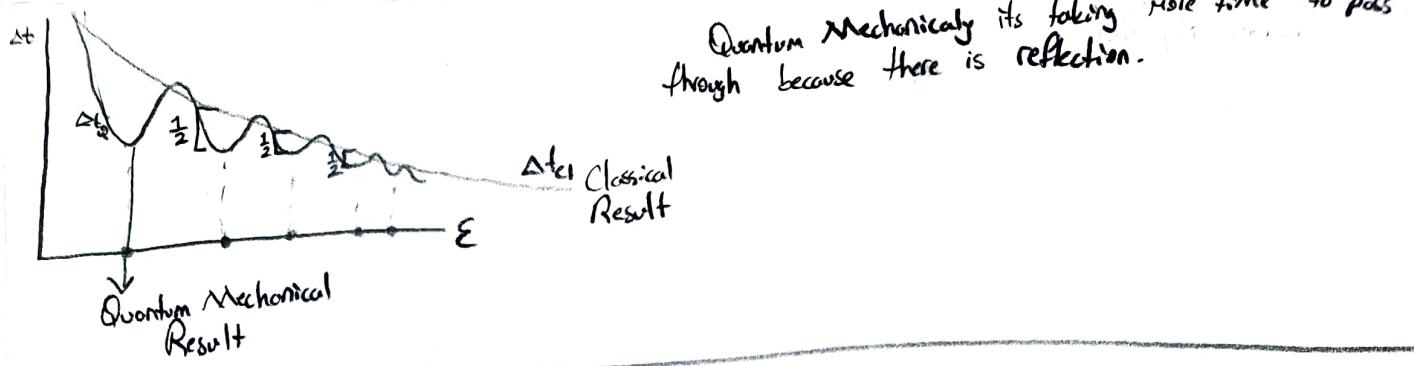
$\Rightarrow$   
Compare with Q.R.

$$\Delta_{cl} = \frac{L}{v_0} \stackrel{?}{=} \hbar \frac{\partial \varphi}{\partial E}$$

$$\varphi = k_2 L - \arctan \left( \frac{k_1^2 + k_2^2}{2k_1 k_2} \tan(k_2 L) \right)$$

Near resonance  $k_2 L \approx \pi$

$$\Rightarrow \hbar \frac{\partial \varphi}{\partial E} = \frac{L}{2v_0} \left( 1 - \frac{E}{v_0} \right)$$



$$\left( \begin{matrix} B \\ C \end{matrix} \right) = \left( \begin{matrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{matrix} \right) \left( \begin{matrix} A \\ 0 \end{matrix} \right)$$

The "S-scattering-"  
Matrix

1-) Stuff does not disappear

$$|A|^2 + |D|^2 = |B|^2 + |C|^2, \quad \left( \begin{matrix} A^* & D^* \end{matrix} \right) \left( \begin{matrix} A \\ 0 \end{matrix} \right) = \left( \begin{matrix} B^* & C^* \end{matrix} \right) \left( \begin{matrix} B \\ C \end{matrix} \right) = \left( \begin{matrix} A^* & D^* \end{matrix} \right) S^* S \left( \begin{matrix} A \\ 0 \end{matrix} \right)$$

$S^* S = \mathbf{1}$ ,  $S$  is unitary matrix.

(Consequence of that, eigenvalues of  $S$  are pure phases;  $S_{11} = e^{i\theta_1}$ ,  $S_{22} = e^{i\theta_2}$

$$|S_{21}| = |S_{22}|, \quad |S_{12}| = |S_{21}|, \quad |S_{12}|^2 + |S_{21}|^2 = 1, \quad S_{11} S_{22}^* + S_{21} S_{22}^* = 0$$

Case,  $\boxed{D=0}$        $\left\{ \begin{array}{l} \frac{B}{A} = S_{12} = T \leftarrow \\ \frac{C}{A} = S_{21} = R \rightarrow \end{array} \right. \quad |T| = |R|, \quad |S_{12}|^2 + |S_{21}|^2 = T^2 + R^2 = 1.$

$A=1$ , for normalization. =

Suppose our system is time reversal invariant  $t \rightarrow -t$ ,  $\Psi$  is a sol'n then  $\Psi^*$  is also sol'n.  
 $\Psi = \begin{cases} Ae^{ikx} + Be^{-ikx} \\ Ce^{ikx} + De^{-ikx} \end{cases}, \quad \Psi^* = \begin{cases} A^*e^{-ikx} + B^*e^{ikx} \\ C^*e^{-ikx} + D^*e^{ikx} \end{cases}, \quad \left( \begin{matrix} A^* & D^* \end{matrix} \right) = \left( \begin{matrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{matrix} \right) \left( \begin{matrix} B^* \\ C^* \end{matrix} \right) \Rightarrow S^* S = \mathbf{1}$

$$\Rightarrow S = S^T \Rightarrow S_{21} = S_{12}$$

We can determine the bound states from the information gathered from scattering.

$$(B) = S_E (A), \quad \text{Take ELO, } k \approx \infty. \quad S_E (B) \neq 0 \text{ unless } S_E \text{ is divergence.} \quad S \sim \frac{c}{\Theta}.$$

$$\Psi = \begin{cases} Ae^{ikx} + Be^{-ikx} \\ Ce^{ikx} + De^{-ikx} \end{cases}, \quad A, D \text{ must } \Rightarrow (A) = (B), \quad \text{For finite square well: } S_{21} = t_{21} = \frac{2k_1 k_2 e^{j k_2 L}}{2k_1 k_2 \cos(k_2 L) - i(k_1^2 - k_2^2) \sin(k_2 L)}$$

$$\text{When } S_{21} \text{ has a pole, } \frac{k_2 L - \tan(\frac{k_2 L}{2})}{2} = \frac{k_2 L}{2} \Rightarrow \text{condition for the bound states of a square well.}$$

Node Theorem {Rephrased}:

If  $\psi_1, \psi_2, \psi_3, \dots$  are energy eigenstates of a 1-D potential where  $E_1 < E_2 < E_3 < \dots$ , then  $\psi_n(x)$  has exactly  $n-1$  nodes.

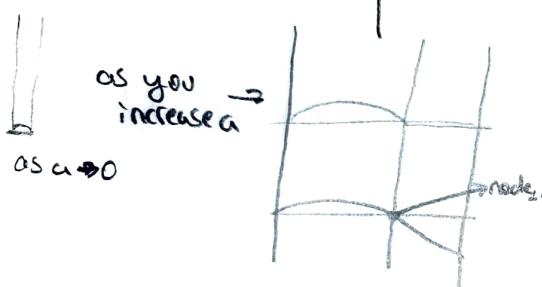


Consider that  
 $\psi(x_0) = \psi'(x_0) = 0$   
 Not possible.

Screened potential  $v_a(x)$

$$v_a(x) = \begin{cases} v(x) & \text{if } |x| < a \\ \infty & \text{if } |x| > a \end{cases}$$

Bound states of  $v_a(x)$  as  $a \rightarrow \infty$   
 are the bound states of  $v(x)$



$$[\hat{E}, \hat{A}] = i\hbar\omega\hat{A} \Rightarrow E_n \text{ evenly spaced by } \hbar\omega \quad \hat{A}\phi_E = \phi_{E+\hbar\omega}$$

$$[\hat{E}, \hat{B}] = 0 \Rightarrow \begin{aligned} 1-) \phi_{E,B} &\text{ are simultaneous eigenfunctions} \\ 2-) \hat{B}\phi_E &= \tilde{\phi}_E \end{aligned}$$

$$[\hat{E}, \hat{u}] = 0, \hat{u}^\dagger \hat{u} = \mathbf{1} \Rightarrow \begin{aligned} 1-) &\text{ Both simultaneous eigenfunctions} \\ 2-) u\phi_E &= \tilde{\phi}_E \\ 3-) u &= e^{i\hat{A}} \end{aligned}$$

$$\hat{T}_L = e^{-i\hat{L}\hat{x}} \Rightarrow \text{Translation by } L.$$

$$\hat{B}_q = e^{-i\hat{q}\hat{x}} \Rightarrow \text{Boost by } q$$

$$\hat{U}_t = e^{-i\frac{t}{\hbar}\hat{E}} \Rightarrow \text{Time translation.}$$

Quantum Mechanics in 3-D:

$$\hat{x}, \hat{y}, \hat{z}, \hat{p}_x, \hat{p}_y, \hat{p}_z \quad | \quad [\hat{x}, \hat{p}_x] = i\hbar, \quad [\hat{x}, \hat{y}] = 0, \quad [\hat{p}_x, \hat{p}_y] = 0, \quad [\hat{p}_x, \hat{y}] = -i\hbar$$

$\Delta x \Delta p \geq \frac{\hbar}{2}$

no sim.  
eq. bnc.

$$\hat{E} = \frac{\hat{p}^2}{2m} + u(\hat{x}, \hat{y}, \hat{z}) \quad , \quad \hat{p} = -i\hbar \vec{\nabla}$$

SE.

$$i\hbar \partial_t \Psi(x, y, z, t) = i\hbar \partial_t \Psi(\vec{r}, t) = \left[ \frac{\hbar^2}{2m} \vec{\nabla}^2 + u(r) \right] \Psi(\vec{r}, t)$$

$$\dim(\Psi(\vec{r}, t)) = 1 / L^3$$

Ex. 1: Free particle in 3-D \* Cartesian coords.

$$E \psi_E = \frac{\hbar^2}{2m} (\partial_x^2 + \partial_y^2 + \partial_z^2) \psi_E$$

$$\psi_E(x, y, z) = \phi_x(x) \phi_y(y) \phi_z(z)$$

$$E \psi_E = \frac{\hbar^2}{2m} (\phi_x''(x) \phi_y(y) \phi_z(z) + \phi_x(x) \phi_y''(y) \phi_z(z) + \phi_x(x) \phi_y(y) \phi_z''(z)), \text{ divide both sides by } \psi_E.$$

$$E = \frac{\hbar^2}{2m} \left( \frac{\phi_x''(x)}{\phi_x(x)} + \frac{\phi_y''(y)}{\phi_y(y)} + \frac{\phi_z''(z)}{\phi_z(z)} \right) \Rightarrow \frac{2m}{\hbar^2} E = f(x) + g(y) + h(z)$$

$\Rightarrow$  This implies that

$$\frac{\phi_x''(x)}{\phi_x(x)} = -\varepsilon_x, \quad \frac{\phi_y''(y)}{\phi_y(y)} = -\varepsilon_y, \quad \frac{\phi_z''(z)}{\phi_z(z)} = -\varepsilon_z \Rightarrow \frac{2m}{\hbar^2} E = \varepsilon_x + \varepsilon_y + \varepsilon_z$$

$$\phi_x''(x) + \varepsilon_x \phi_x(x) = 0$$

$\Rightarrow \phi_x = A e^{i k_x x} + B e^{-i k_x x} \Rightarrow \lambda_x^2 = \varepsilon_x$  shows that  $\varepsilon$ 's are positive.

$$E = \frac{\hbar^2}{2m} (\lambda_x^2 + \lambda_y^2 + \lambda_z^2) = \frac{\hbar^2}{2m} \vec{\lambda}^2$$

$$\psi_E = N \underbrace{e^{i k_x x} e^{i k_y y} e^{i k_z z}}_{\text{Some good basis.}} = N e^{i \vec{k} \cdot \vec{r}}, \quad E = \frac{\hbar^2 \vec{k}^2}{2m}$$

Gen. Sol'n is

$$\psi_E = A e^{i k_x x} \phi_y \phi_z + B e^{-i k_x x} \phi_y \phi_z$$

Suppose we take  $X_1$  such that  $\frac{\hbar^2 X_1^2}{2m} = E = \frac{\hbar^2 X_2^2}{2m}$  where  $X_1 \neq X_2$

In 1-D  $(X, -X)$  had some energy.

In 3-D  $X_1, X_2$  /some magnitude  $\rightarrow$  same energy means degenerate

System is symmetric so degeneracy occurs

Symmetry  $\Leftrightarrow$  degeneracy

### 3-D Harmonic Oscillator

$$V(\vec{r}) = \frac{m\omega^2}{2} (x^2 + y^2 + z^2) = \frac{m\omega^2}{2} |\vec{r}|^2$$

$$\begin{aligned} E\phi_E &= \left[ -\frac{\hbar^2}{2m} [d_x^2 + d_y^2 + d_z^2] + \frac{m\omega^2(x^2 + y^2 + z^2)}{2} \right] \phi_E \\ &= \left[ \left( -\frac{\hbar^2}{2m} d_x^2 + \frac{m\omega^2}{2} d_x^2 \right) + (|''y|) + (|''z|) \right] \phi_E \end{aligned}$$

$$\sum d_x \phi_x = \left( -\frac{\hbar^2}{2m} d_x^2 + \frac{m\omega^2}{2} d_x^2 \right) \phi_x, \quad \phi_E = \phi_x(x) \phi_y(y) \phi_z(z), \quad E = E_{dx} + E_{dy} + E_{dz}$$

$\phi_E = \phi_x(x) \phi_y(y) \phi_z(z)$  } Basis of solutions of

$E = \hbar\omega_x (l+1+m+n+\frac{3}{2})$  } the energy eigenfunctions for 3-D Harmonic Oscillator

Degeneracy

|                     |  |
|---------------------|--|
| $\frac{3}{2}$       | $(2,0,0)(0,2,0)(0,0,2)(1,1,0)(0,1,1)(1,0,1)$ |
| $\frac{5}{2}$       | $(1,0,0)(0,1,0)(0,0,1)$                      |
| $\frac{3}{2}$ total | $(0,0,0)$                                    |

$$\left. \begin{array}{l} d_1 = 15 \\ d_2 = 10 \\ d_3 = 6 \\ d_4 = 3 \\ d_5 = 1 \end{array} \right\} d_n = \frac{(n+1)(n+2)}{2}$$

\* There can be degeneracies among bound states.

Imagine that potential was not symmetric.

Ex.

$$(|''w_0|_x) + (|''w_0|_y) + (|''w_0|_z) \rightarrow (|''w_0|_x) + (|''w_1|_y) + (|''w_2|_z) \text{ where } w_0 \neq w_1 \neq w_2 \text{ or } w_0 \neq 1 \text{ or } w_0 \neq w_2$$

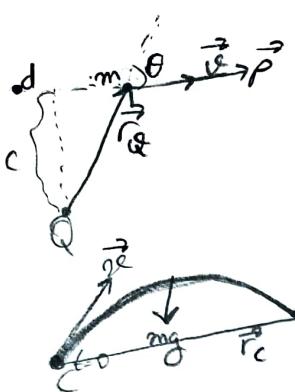
$$E = \hbar\omega_0(l+\frac{1}{2}) + \hbar\omega_1(m+\frac{1}{2}) + \hbar\omega_2(n+\frac{1}{2})$$

We don't get degeneracy, so this implies that

"when you have symmetry there is degeneracy, where you don't have symmetry you don't get degeneracy"

Note: Getting a degenerate case without symmetry may happen with rational  $l, m, n$  but it's unlikely to face. Generally getting a case like that is impossible but could happen

# Classical Angular Momentum:

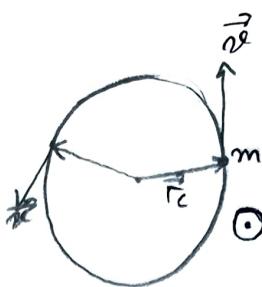


$$\vec{L}_Q = \vec{r}_Q \times \vec{p} = (\vec{r}_Q \times \vec{\omega}) m. \quad |L_Q| = m r_Q^2 \omega_Q \sin\theta$$

$$\vec{L}_d = 0.$$

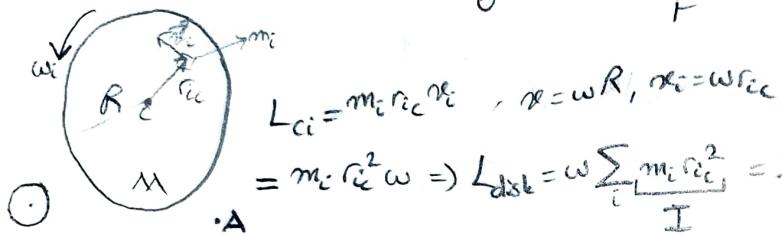
$$t=0, \vec{L}_S = 0$$

$$t=t, \vec{L}_c \neq 0$$



$$|\vec{L}_c| = m |\vec{r}_c \times \vec{\omega}| = m r_c \omega_c$$

$$\vec{L}_Q = \vec{r}_Q \times \vec{p} \quad \frac{d\vec{L}_Q}{dt} = \frac{d\vec{r}_Q}{dt} \times \vec{p} + \vec{r}_Q \times \frac{d\vec{p}}{dt} = \vec{r}_Q \times \vec{F} = \tau \Rightarrow \text{Torque.}$$



$$L_{ci} = m_i r_{ci} \omega_i, \quad \omega = \omega R, \quad \omega_i = \omega r_{ci}$$

$$= m_i r_{ci}^2 \omega \Rightarrow L_{disk} = \omega \sum_i \frac{m_i r_{ci}^2}{I} = I_c \omega, \quad I_c = \text{moment of inertia respect to } C.$$

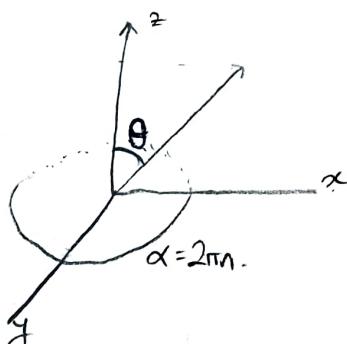
what about respect to a point A?

Even if you calculate the angular momentum respect to any point, as long as there is a rotation about center of mass - the angular momentum will be conserved. This is called "Spin Angular Momentum"

$$\vec{L} = \vec{r} \times \vec{p} = (x, y, z) \times (p_x, p_y, p_z) = i(y p_z - z p_y) + j(z p_x - x p_z) + k(x p_y - y p_x) \quad \text{Classically}$$

In QM.

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \hat{p}_x & \hat{p}_y & \hat{p}_z \\ x & y & z \end{vmatrix} = \begin{pmatrix} \hat{L}_x \\ \hat{L}_y \\ \hat{L}_z \end{pmatrix}, \quad \hat{L}_z = -i\hbar \partial_\alpha$$



$$\hat{L}^2 = -\hbar^2 \left( \frac{1}{\sin\theta} \partial_\theta \sin\theta \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi \right)$$

$$L_z \phi_m = -i\hbar \partial_\phi \phi_m = \hbar m \phi_m \Rightarrow \phi_m = C e^{im\phi} : m \in \mathbb{Z}$$

$$[L_x, L_y] = [yP_x - zP_y, zP_x - xP_z] = [yP_x, zP_x] - [yP_z, xP_z] + [zP_y, zP_x] + [zP_y, xP_z]$$

$$= yP_x [P_x, z] - \underbrace{yz[P_x, P_z]}_0 + \underbrace{P_y P_z [z, z]}_0 + xP_z [z, P_x] = -i\hbar y P_x + i\hbar x P_y = i\hbar (xP_y - yP_x) = i\hbar L_z$$

$$\Rightarrow [L_x, L_y] = i\hbar L_z \quad \left\{ \begin{array}{l} [L^2, L_x] = 0 \\ [L^2, L_y] = 0 \end{array} \right\}$$

$$[L_y, L_z] = i\hbar L_x \quad \left\{ \begin{array}{l} [L^2, L_y] = 0 \\ [L^2, L_z] = 0 \end{array} \right\}$$

$$[L_z, L_x] = i\hbar L_y \quad \left\{ \begin{array}{l} [L^2, L_z] = 0 \\ [L^2, L_x] = 0 \end{array} \right\}$$

we can find simultaneous eigenfunctions of  $L^2$  with  $L_x, L_y, L_z$ .

So we can say;

$[L^2, L_x]$  or  $[L^2, L_y]$  or  $[L^2, L_z]$  gives complete set of commuting observables for angular momentum.

We want to find eigenfunctions of  $\{L^2, L_z\}$

$$L_+ \equiv L_x + iL_y \quad \left| \begin{array}{l} [L^2, L_+] = 0, \quad [L_z, L_+] = \hbar L_+ \\ [L^2, L_-] = ? \quad [L_z, L_-] = -\hbar L_- \end{array} \right.$$

$$L_- \equiv L_x - iL_y \quad \left| \begin{array}{l} [L^2, L_-] = ? \quad [L_z, L_-] = -\hbar L_- \end{array} \right.$$

$\overbrace{\hspace{10em}}$

Definition.

Let  $\psi_{lm}$  be eigenfunctions of  $L^2, L_z$ .

$$L^2 \psi_{lm} = \hbar^2 l(l+1) \psi_{lm}, \quad L_z \psi_{lm} = \hbar m \psi_{lm}$$

①  $L_+$  leave  $l$  alone

$$L^2 L_+ \psi_{lm} = L_+ L^2 \psi_{lm} = \hbar^2 l(l+1) L_+ \psi_{lm}$$

②  $L_+$  raise/lower  $m$  by 1.

$$L_+ L_+ \psi_{lm} = ([L_z, L_+] + L_+ L_z) \psi_{lm} = (\hbar L_+ + \hbar m L_+) \psi_{lm} = \hbar(m+1) L_+ \psi_{lm}.$$

$\Rightarrow$  ladder of states

$$\begin{array}{c} \vdots \\ \hline m+1 & \nearrow L_+ \\ \hline m & \nearrow L_+ \\ \hline m-1 & \searrow L_- \\ \vdots & \searrow L_- \end{array} \quad \left| \begin{array}{l} \text{Is this tower infinite?} \Rightarrow \text{No.} \\ L^2 = L_x^2 + L_y^2 + L_z^2 \\ \langle \psi_{lm} | \Rightarrow \hbar^2 l(l+1) = \langle L_z^2 \rangle + \langle L_y^2 \rangle + \hbar^2 m^2 \\ \Rightarrow \hbar^2 m^2 = m_+, m_-. \end{array} \right.$$

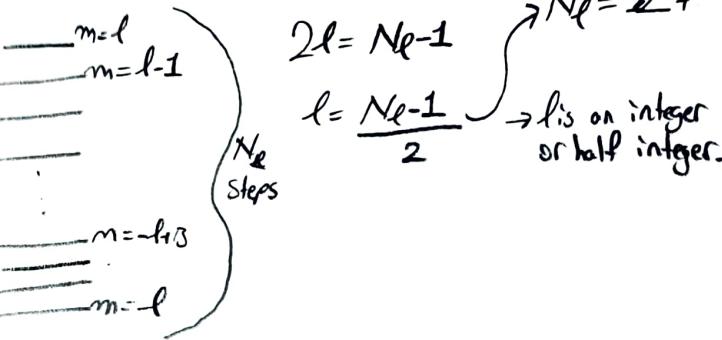
$$\begin{aligned} \text{Suppose } L_+ \psi_{lm} = 0 \Rightarrow (L_+ \psi_{lm}) L_+ \psi_{lm} = 0 = (\psi_{lm} | L_+ L_+ \psi_{lm}) = (\psi_{lm} | [L_x^2 + L_y^2 + i[L_x, L_y]] \psi_{lm}) \\ = (\psi_{lm} | [L^2 - L_z^2 - \hbar L_z] \psi_{lm}) = (\hbar^2 l(l+1) - m^2 \hbar^2 - m \hbar^2) = 0. \end{aligned}$$

$$\Rightarrow \hbar^2 (l(l+1) - m_+ (m_+ + 1)) = 0$$

$$\Rightarrow m_+ = +l \Rightarrow m_- = -l.$$

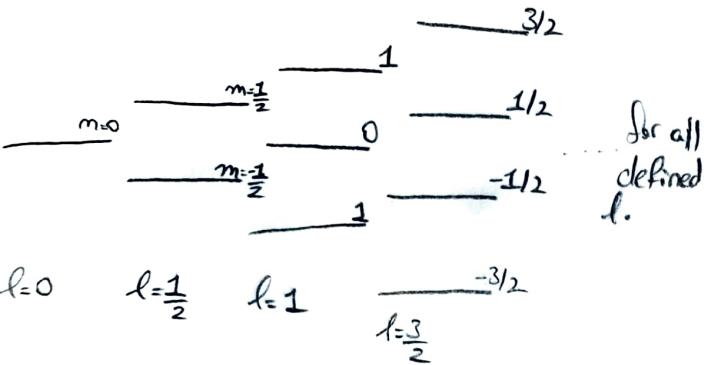
A  $\leq -1$  Target

Which means  $m$  spans values from  $-l$  to  $l$  in unit steps.



$$2l = N_l - 1 \quad \rightarrow N_l = \mathbb{Z}^+$$

$$l = \frac{N_l - 1}{2} \quad \rightarrow l \text{ is an integer or half integer.}$$



For the state  $l, m=l$

$$\langle L^2 \rangle = \hbar^2 l(l+1)$$

$$\langle L_x^2 \rangle = \hbar^2 l^2$$

$$\Rightarrow \langle L_x^2 \rangle + \langle L_y^2 \rangle = \hbar^2 l, \langle L_{x,y}^2 \rangle = \frac{1}{2} \hbar^2 l$$

$$\psi_{lm}(\theta, \alpha); L_z = \frac{\hbar}{i} \partial_\alpha, L_\pm = \hbar e^{\pm i\alpha} (\partial_\theta \pm i \cot \theta \partial_\phi)$$

$$im \partial_m = \frac{i\hbar}{c} \partial_\alpha \partial_m \rightarrow im \partial_m = \partial_\alpha \partial_m \Rightarrow \partial_m(\theta, \alpha) = e^{im\alpha} P_{lm}(\theta)$$

$$\partial_m(\theta, 2\pi) = e^{im2\pi} P_{lm}(\theta) = \begin{cases} \partial_m(\theta, 0), & m \Rightarrow \text{integer} \\ -\partial_m(\theta, 0), & m \Rightarrow \text{half-integer} \end{cases}$$

$$m \text{ int}, \partial_m(\theta, 0) = \partial_m(\theta, 2\pi)$$

$m$  half-int,  $\partial_m(\theta, 0) = -\partial_m(\theta, 2\pi) = 0 \Rightarrow \partial_m(\theta, 0) = 0$  if  $m$  is half integer.

which means half integers cannot describe a ~~atom~~ particle state.

$$L \perp \partial_\theta = 0.$$

$$\Rightarrow \hbar e^{i\alpha} (\partial_\theta + i \cot \theta \partial_\phi) e^{il\alpha} P_l(\theta) = 0 = (\partial_\theta - l \cot \theta) P_l(\theta)$$

$$\Rightarrow P_{ll}(\theta) \propto \sin^l(\theta) \Rightarrow \partial_\theta = N_{ll} e^{il\alpha} \sin^l(\theta)$$

$$\partial_{\theta,1} \perp L \cdot \partial_\theta$$

$$\text{Ex: } l=0$$

$$\partial_\theta = \frac{1}{4\pi}$$

$$l=1$$

$$\partial_{\theta,1} = c e^{i\alpha} \sin(\theta)$$

$$\partial_{\theta,0} = b \cos(\theta)$$

$$\partial_{\theta,-1} = a e^{-i\alpha} \sin(\theta)$$

$$l=2$$

$$\partial_{\theta,2} = c e^{i2\alpha} \sin^2(\theta)$$

$$\vdots$$

$$\partial_{\theta,0} = a \cdot (3 \cos^2(\theta) - 1)$$

$$\partial_{\theta,-2} = b \cdot e^{-i2\alpha} \sin^2(\theta)$$

# Laplacian in 3D {Spherical Coordinates}

$$\vec{\nabla}^2 = \partial_r^2 + \frac{2}{r} \partial_r + \frac{1}{r^2} \left[ \partial_\theta^2 + \cot\theta \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi^2 \right] \stackrel{\downarrow}{=} \left( \frac{1}{r} \partial_r r \right)^2 + \frac{1}{r^2} \left( -\frac{1}{r^2} L^2 \right)$$

From product rule.

$$\hat{E} = \frac{p^2}{2m} + U(r), \quad \hat{p}^2 = -\hbar^2 \nabla^2 = -\frac{\hbar^2}{r} \partial_r^2 r + \frac{L^2}{r^2}$$

$$\hat{E} = -\frac{\hbar^2}{2mr^2} \partial_r^2 r + \frac{1}{2mr^2} L^2 + U(r)$$

$[\hat{E}, \hat{L}^2] = 0$ . So we can find common eigenbasis of functions which are both  $\hat{E}$ 's and  $\hat{L}^2$ 's.

Separation of Variables:

$$\hat{E}\phi_E = E\phi_E \quad \phi_E(\vec{r}) = \varphi(r) Y_{lm}(\theta, \phi), \quad l \text{ must be integer - we're talking about rotational angular momentum -}$$

$$\hat{E}\phi_E = \left( -\frac{\hbar^2}{2mr^2} \partial_r^2 r + \frac{\hbar^2 l(l+1)}{2mr^2} + U(r) \right) \phi_E, \quad \frac{\hbar^2 l(l+1)}{2mr^2} + U(r) = V_{\text{effective}}(r)$$

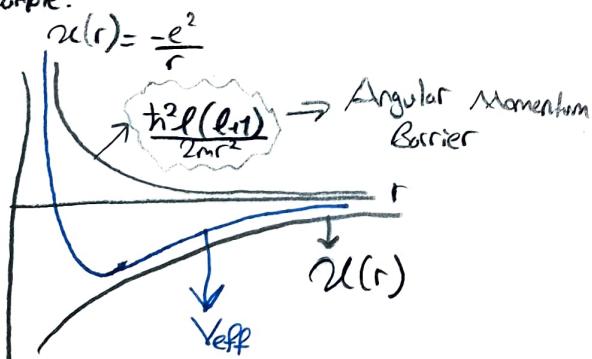
We reduced angular dependence so  $\phi_E = \varphi(r)$

$$E\varphi(r) = \left( -\frac{\hbar^2}{2m} \frac{1}{r} \partial_r^2 r + V_{\text{eff}}(r) \right) \varphi(r)$$

$$\varphi(r) = \frac{1}{r} u(r); \quad \frac{1}{r} \partial_r^2 r \varphi(r) = \frac{1}{r} \partial_r^2 u(r), \quad V_{\text{eff}} \varphi = \frac{1}{r} V_{\text{eff}} u(r)$$

$$\Rightarrow E u(r) = \left( -\frac{\hbar^2}{2m} \partial_r^2 + V_{\text{eff}}(r) \right) u(r)$$

Example:



## General Facts for Central Potentials.

As  $r \rightarrow 0$ , what must be true for  $u(r)$ ?  
 if  $u(r) \rightarrow c$  as  $r \rightarrow 0 \Rightarrow \phi = \frac{c}{r}$ ,  $\nabla^2 \frac{1}{r} \sim \frac{1}{4} \partial r^2$  is not possible since it diverges and  
 become  $\nabla^2 \frac{1}{r} = \delta(r)$ .

So  $u(r) \rightarrow 0$  as  $r \rightarrow 0 \Rightarrow \phi$  becomes constant

$\bullet E$  only depends on  $l$ , but not on  $m$

for each  $m \in \{l, l-1, \dots, -l\}$

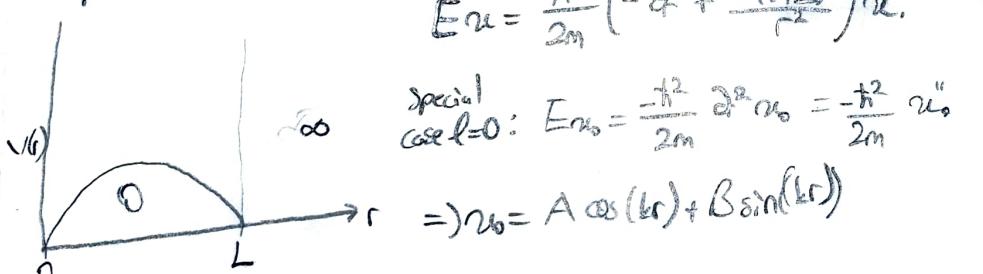
For each  $m$ 's energy is the same  $\bar{E}_l$ .

$d(\bar{E}_l) = 2l+1 \equiv$  Degeneracy of  $E_l$ . Because of Rotational Symmetry

$$[\hat{E}, L_x] = 0, [\hat{E}, L_y] = 0, [\hat{E}, L_z] = 0$$

So we can find a common eigenbasis of  $E$  with  $L_{x,y,z}$ .  $[E, L_{\pm}] = 0$ .

Example:



$$\hat{E}u = \frac{\hbar^2}{2m} \left( -\partial_r^2 + \frac{l(l+1)}{r^2} \right) u, \quad E_0 = \frac{\hbar^2 k^2}{2m}$$

$$\text{special case } l=0: E_{k_0} = \frac{-\hbar^2}{2m} \partial_r^2 u_0 = -\frac{\hbar^2}{2m} u_0''$$

$$\Rightarrow u_0 = A \cos(kr) + B \sin(kr)$$

$$\text{Boundary: } u(0) = 0 \Rightarrow A = 0$$

$$u(L) = 0 \Rightarrow kL = n\pi$$

$$\Rightarrow \phi_{E_0} = \propto_0 \frac{1}{r} \sin\left(\frac{n\pi}{L} r\right) = N \frac{1}{r} \sin\left(\frac{n\pi}{L} r\right)$$

$$\text{Coulomb Potential: } V(r) = \frac{-e^2}{r}$$



$$\frac{-\hbar^2}{2m} u''(r) + \left( \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} - \frac{e^2}{r} \right) u(r) = E_\ell u(r)$$

$$\textcircled{1} [e^2] = E \cdot L = \frac{p^2 L}{2m}, [p] = p \cdot L, [m] = m$$

$$\Rightarrow r_0 = \frac{\hbar^2}{2me^2} \Rightarrow E_0 = \frac{e^2}{r_0} = \frac{2me^4}{\hbar^2} = 4R \quad |_{13.6 \text{ eV}} \rightarrow R = \text{Rydberg's Constant.}$$

$$\textcircled{2} r = r_0 \rho \quad E = E_0 \varepsilon$$

$$\left( -\frac{\partial^2}{\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{1}{\rho} + \varepsilon \right) u = 0$$

\textcircled{3} Asymptotic Analysis

$$\left. \begin{array}{l} \cdot \rho \rightarrow \infty \rightarrow u \sim e^{-\sqrt{\varepsilon} \rho} \\ \cdot \rho \rightarrow 0 \rightarrow u \sim \rho^{(\ell+1)} \end{array} \right\} \rightarrow u = \rho^{(\ell+1)} e^{-\sqrt{\varepsilon} \rho} \propto (\rho) = e^{-r/2r_0m} \left( \frac{r}{r_0} \right)^{\ell+1} u_{\text{re}} \left( \frac{r}{r_0} \right)$$

$$\Rightarrow \rho u'' + 2(1+\ell - \sqrt{\varepsilon} \rho) u' + (1 - 2\sqrt{\varepsilon}(\ell+1)) u = 0$$

$$\Rightarrow u = \sum_{j=0}^{\infty} a_j \rho^j \rightarrow a_{j+1} = \frac{2\sqrt{\varepsilon}(j+\ell+1-1)}{(j+1)(j+2\ell+2)} a_j, \text{ To terminate;}$$

$$a_{j_{\max}+1} = 0 \text{ must be}$$

$$\Rightarrow \varepsilon = \frac{1}{4n^2}, n = j_{\max} + \ell + 1.$$

$$\Rightarrow E_{n,\ell,m} = \frac{-E_0}{4n^2}, \text{ independent of } n, \ell, m$$

$$\text{Spectrum of Light of Hydrogen} \sim \frac{E_0}{4n^2} \rightarrow \text{Rydberg Relation}$$

When  $j \gg$ ,

$$a_{j+1} \approx a_j \frac{2\sqrt{\varepsilon}}{(j+1)} \Rightarrow a_j = a_0 \frac{(2\sqrt{\varepsilon})^j}{j!} = \text{Exponent coeffs. of exponential}$$

Then  $u$  becomes  $e^{2\sqrt{\varepsilon} r / r_0} \Rightarrow$  This destroys our asymptotic analysis so at some point it must terminate if

$$2\sqrt{\varepsilon} (j_{\max} + \ell + 1) = 1. \Rightarrow \varepsilon = \frac{1}{4(j_{\max} + \ell + 1)^2}$$

$$\text{For } l, m, j_m, \text{, } E_{l,m,j_m} = \underbrace{\frac{-E_0}{4(j_m + l + 1)^2}}_{\propto} ; n > l, n \text{ is an integer}$$

$$d(E_n) = \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} 1 = \sum_{\ell=0}^{n-1} 2\ell + 1 = n^2, \text{ there is a high degeneracy.}$$

$\Rightarrow$  Symmetric Conserved Quantity  $[\hat{E}, \hat{A}] = 0$ .

This quantity  $\hat{A} = \vec{p} \times \vec{r} - mc^2 \vec{r}$   $\Rightarrow$  This showed that there is some conserved quantity but about sym?

There are two explanations.

- $\frac{\delta x}{\delta t} = f(\vec{x}, \vec{p})$

- If you work with Coulomb problem in 3D = free particle in 4D, constrained to  $S^3$ .

There is a  $SO(4) =$  special orthogonal transformation in 4D.

\* Arg. Momentum in 3D =  $SO(3) = 3 = L_x, L_y, L_z$   
" " " 4D =  $SO(4) = 6 \Rightarrow$  if you map this in 3D Coulomb problem, becomes.

$\Rightarrow SO(4) = L_x, L_y, L_z, 3 \hat{A}$ 's.  $\hat{A}$  is symmetric.

There is an enhanced symmetry group and there is a conserved quantity which related to operator  $\hat{A}$  which commutes with  $\hat{E}$ .

$$i\hbar \frac{d}{dt} \langle \hat{B} \rangle_{\text{rel}} = \langle [\hat{E}, \hat{B}] \rangle, [\hat{E}, \hat{B}] = 0 \Rightarrow \frac{d}{dt} \langle \hat{B} \rangle = 0$$

Classically to being a conserved quantity means its time independent.

Quantum mechanically it means that commutes with energy  $\hat{E}$ .  
 $L_x, L_y, L_z \Rightarrow [\hat{E}, \hat{L}_{x,y,z}] = 0$ , so their time der. of their expectation values are both zero.

Let's try to break / split degeneracy  $\Leftrightarrow$  Break Symmetry.

$\hat{L}_z$ : Relativistic corrections to kinetic energy, change  $\hat{E}$ , preserve  $[\hat{E}, \hat{L}] = 0$ .

$KE = \sqrt{m_e c^4 + p^2 c^2} - m_e c^2 = m_e c^2 (\sqrt{1 + \frac{p^2}{m_e c^2}} - 1) \Rightarrow$  if we Taylor expand this.

$$\Rightarrow \frac{p^2}{2m_e} - \frac{p^4}{8m_e^3 c^2} \approx \text{it is an approximation, } \Rightarrow E_{\tilde{n}_g} = E_c - \frac{p^4}{8m_e^3 c^2}, \quad \tilde{E}_{nlm} = \frac{-\tilde{E}_0}{n^2}$$

We have to solve the eigenvalue eq. again, also energy eigenvalue has a 4-th derivative.

So let's see what we can do.

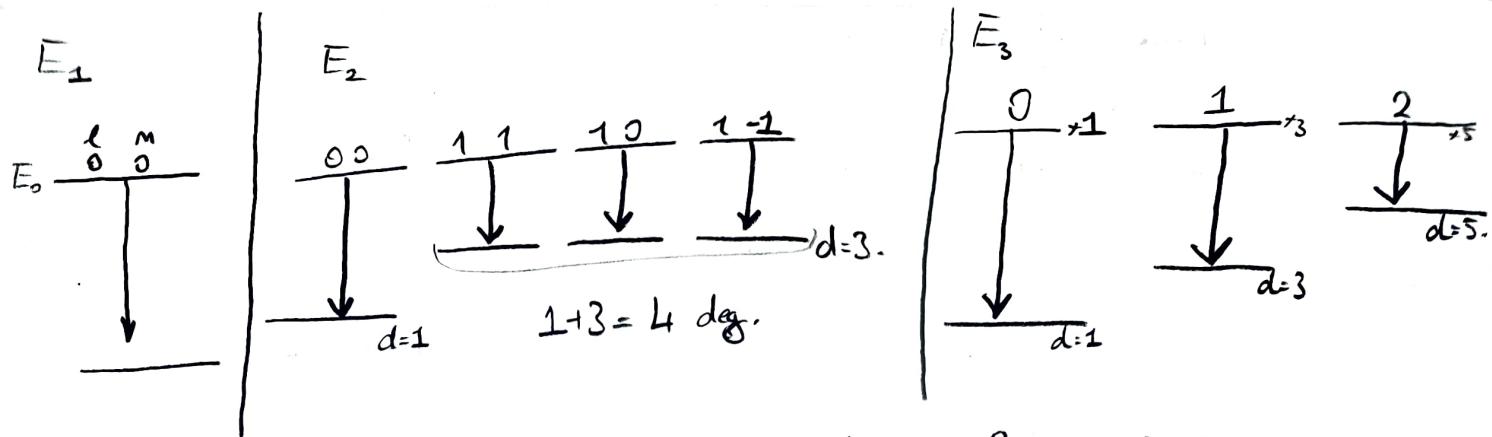
- Dimensional analysis, try to break degeneracy.

- Use the expectation value of  $\hat{p}^4$

$$\Rightarrow E_{nlm}^{\tilde{n}_g} = \frac{-\tilde{E}_0}{n^2} - \frac{\tilde{E}_0^2}{m^4 m_e^2} \left( \frac{4n}{l + \frac{1}{2}} - 3 \right) \rightarrow \tilde{E} \text{ depends on } l \text{ and } n, \text{ yay.}$$

$$\Rightarrow [\tilde{E}_{nlm}, \hat{A}] \neq 0, [\tilde{E}, \hat{L}] = 0 \text{ still.}$$

Let's see degeneracy explicitly.



What must be done to break deg. caused by ang. momentum  $\Leftrightarrow$  Break rotational sym.

Zeeman: using magnetic field, tried to get a spectrum.

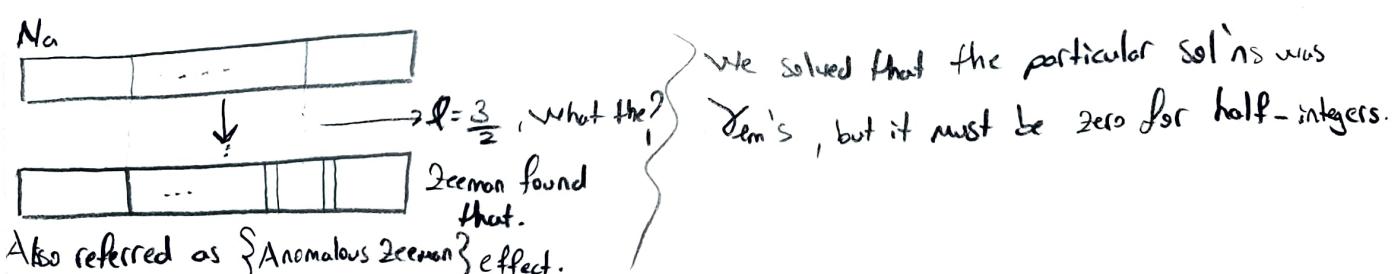
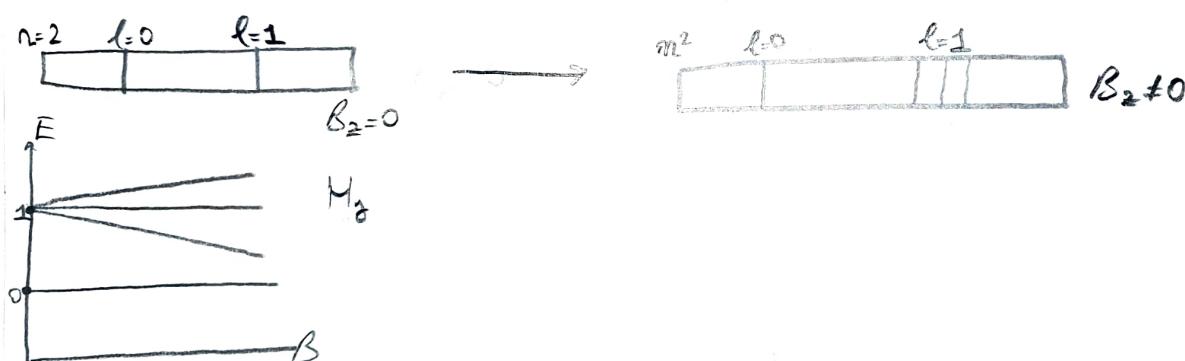
$$E = E_c - \vec{p} \cdot \vec{B}$$

$$\vec{p} = \frac{I A}{c} = \frac{-e}{2m_e c} \vec{L}$$

$$\Rightarrow E_c - \mu_2 B_z = E_c - \frac{e \hbar}{2m_e} L_z \Rightarrow \text{Since } L_z \text{ is dep. of } m$$

Our  $E$  is dep. of  $m$

$$E_{\text{nem}}^2 = \frac{E_0}{n^2} + \frac{e \hbar}{2m_e} B_{z m} \Rightarrow E_{\text{nem}} = E_{\text{nem}}^{l=0} + \frac{e \hbar}{2m_e} B_{z m}$$



Coulomb:  $d(E) = m^2$  | But they observed that  $d(n) = 2n^2$

If you have 4e you can put them in different or sometimes right.

But there are twice as many groupings.

Pauli said: ① No two e<sup>-</sup> can live in the same quantum state

② There are twice as many states as you think in H.

{ I post the existence of an additional quantum number which the e can have which takes one of two values }

A. Said Tammel

Goudsmid and Uhlenbeck tried to explain this.

- 1-) There is Zeeman effect.
- 2-) There is also some wrong total angular momentum, there are twice as many states for one in Coulomb potential.

They supposed that the total angular momentum was not right  
They " " e can have some intrinsic angular momentum

e:  $\vec{J} = \vec{L} + \vec{S}$ , which has the property  $S = \frac{1}{2}$ ,  $m_s = \pm 1/2$ .

If you have some integer ratio, ang. mom. and S, what is the total ang. mom.?

Some half-int number, this can explain anomalous Zeeman effect.

[Q]

if  $\hat{E}$  is not Hermitian, energy eigenvalues are no longer real and probability would no longer be conserved.

Assume that  $\hat{E}$  is t independent.

Suppose we have a stationary state with  $\hat{E} \in \mathbb{C}$ ,  $\hat{E} = E_R + i\Gamma$

[Q]

$$\psi(t) = e^{-\frac{i}{\hbar} \hat{E} t} \psi(0) = e^{-i \frac{E_R t}{\hbar}} e^{-i \Gamma t} \psi(0)$$

When we take norm square of it shows that,

Having loss of probability is having a complex eigenvalue

$$\Psi_{\text{hem}} = N \frac{1}{r} \underbrace{R_{nl}(r)}_{\propto(r)} \sum_m (\theta, \alpha) = N \frac{1}{r} R_{nl}(r) P_l(\cos\theta) e^{im\alpha}, \Rightarrow \text{Stationary State.}$$

$$\frac{d}{dt} \langle \vec{r} \rangle = 0, \quad \rho(\vec{r}) = |\Psi_{\text{hem}}(\vec{r})|^2$$

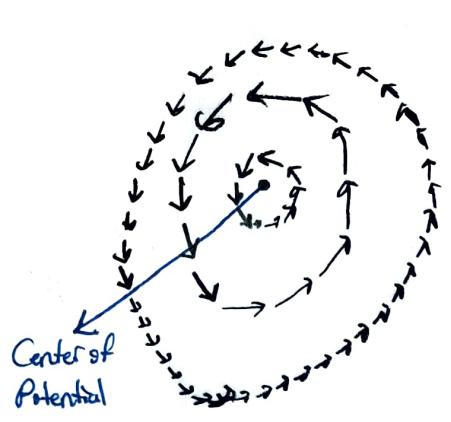
$$\partial_t \rho(\vec{r}) = -\vec{\nabla} \cdot \vec{j}, \quad \vec{j} = \frac{\hbar}{mc} \text{Im}(\Psi^* \vec{\nabla} \cdot \Psi)$$

$$\text{In St. State } \Psi_{\text{hem}}, \quad \partial_t \rho(\vec{r}) = 0 \Rightarrow \vec{\nabla} \cdot \vec{j} = 0$$

$$\text{What's current? } (\nabla_r = \partial_r, \quad \nabla_\theta = \frac{1}{r} \partial_\theta, \quad \nabla_\alpha = \frac{1}{r \sin\theta} \partial_\alpha)$$

$$J_r = 0, \quad J_\theta = 0, \quad J_\alpha = \frac{\hbar}{mc} \text{Im} \left( \Psi^* \frac{1}{r \sin\theta} \text{Im} \Psi \right) = \frac{1}{mc} |\Psi|^2 \frac{1}{r \sin\theta} \text{ with}$$

$$\Rightarrow \vec{j} = \frac{1}{mc \sin\theta} \text{Im} \vec{\nabla}_\alpha \cdot \Rightarrow \text{Probability Density Rotating.}$$



Center of Potential

$$\vec{I} = -e\vec{J} \Rightarrow \vec{p} = \vec{p}_0 m \hat{z} \text{ where } \vec{p}_0 = \frac{e\vec{t}}{2m_e}.$$

What happens when the state has a real eigenfunction?

$$(\Psi_{nlm} + \Psi_{nl-m}) = \Psi_{nl}, \text{ for a free particle.}$$

Current will be  $\equiv$  zero.

It's some arbitrary superposition of having opposite ang. mom.  
so expectation value of mom. is zero

If we're interested in to find states with def.  $E$  and def. momentum, it is not going to be a real function  
on some dir. -

"End of Coulomb Potential"

Multiple Particles:

1st p. 2nd p.

$$(M: (x_1, p_1, x_2, p_2), QM: \Psi(x_1, x_2), \hat{x}_1, \hat{x}_2, \hat{p}_1, \hat{p}_2)$$

$$P(x_1, x_2) = |\Psi(x_1, x_2)|^2; [x_1, x_2] = 0, [x_1, p_1] = i\hbar, [x_2, p_2] = 0.$$

Ex: Two free particles,  $V(a, b) = 0$

$$\hat{E} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2}, \quad \Psi(a, b) = K(a)\phi(b)$$

$$\frac{p_a^2}{2m} K(a) = E_a K(a) \Rightarrow K(a) = C e^{ik_a a}, \quad \frac{p_b^2}{2m_2} \phi(b) = e^{ik_b b}.$$

$$\Psi_E(a, b) = e^{i(k_a a + k_b b)}, \quad E = \frac{\hbar^2}{2m} (k_a^2 + k_b^2)$$

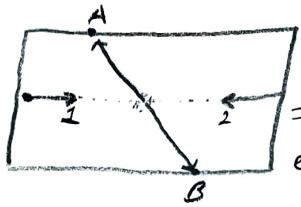
$$\text{Ex. } \hat{E} = \frac{p_a^2}{2m_1} + \frac{p_b^2}{2m_2} + V(|a-b|); \quad a = \text{proton}, b = \text{-electron}$$

$$R = \left( \frac{1}{m_a + m_b} \right) (m_a a + m_b b), \quad r = a-b$$

Center of mass position.

$$\hat{E} = \frac{\hbar^2}{2m} \nabla_R^2 - \frac{\hbar^2}{2\mu} \nabla_r^2 + V(r), \quad \mu = \frac{m_a m_b}{m_a + m_b} \approx m_b$$

## Identical Particles:



which particle ended up where?

$\Rightarrow \hat{P}(A, B) = \hat{P}(B, A)$ , because particles are identical. we can't know which ended up where.

$\hat{P}_{\text{sw}} : 1 \leftrightarrow 2 : \hat{P}(A, B) = \hat{P}(B, A), \hat{P} \Psi(A, B) = \Psi(B, A) \Rightarrow \text{it does not have to be invariant.}$

$$\Psi(B, A) = e^{i\theta_{BA}} \Psi(A, B)$$

$$\hat{P} \hat{P} \Psi(A, B) = e^{2i\theta_{AB}} \Psi(A, B) = (e^{i\theta_{AB}})^2 = 1 \Rightarrow e^{i\theta_{AB}} = \pm 1$$

$$\hat{P}(A, B) = \pm \Psi(A, B) \Rightarrow \hat{P}^2 \Psi = \Psi \Rightarrow \text{eigenvalues of } \hat{P} \text{ are } \pm 1$$

If our particles are distinguishable, then

$$\Psi_0(A, B) = \chi(A)\phi(B), \hat{P}_0(A, B) \neq \hat{P}_0(B, A), |\Psi_0(A, B)|^2 = |\chi(A)\phi(B)|^2$$

If we have indistinguishable particles;

$$|\Psi(A, B)|^2 = |\Psi(B, A)|^2 \Rightarrow \Psi = \frac{1}{\sqrt{2}} (\chi(A)\phi(B) \pm \chi(B)\phi(A))$$

$$\Rightarrow \hat{P} \Psi_{\pm}(A, B) = \pm \Psi(A, B) \xrightarrow{\text{+ means sym.}} - \text{means anti-sym.} \} \text{for combinations of states}$$

If you have identical particles, then

$$\hat{E} \hat{P} = \hat{P} \hat{E} \Rightarrow [\hat{E}, \hat{P}] = 0 \Rightarrow \hat{P} \Psi(t) \text{ doesn't change in time}$$

Initially

$$\hat{P} \Psi_A = +\Psi(0) \Rightarrow \hat{P} \Psi(t) = f \Psi(t)$$

① Distinguishable particles

$$\Psi_f(A, B) = -\Psi(B, A) \Rightarrow \Psi(A, A) = -\Psi(A, A) = 0 \} \text{Pauli}$$

② Identical,  $\hat{P} \Psi = +\Psi \Rightarrow$  Called Bosons

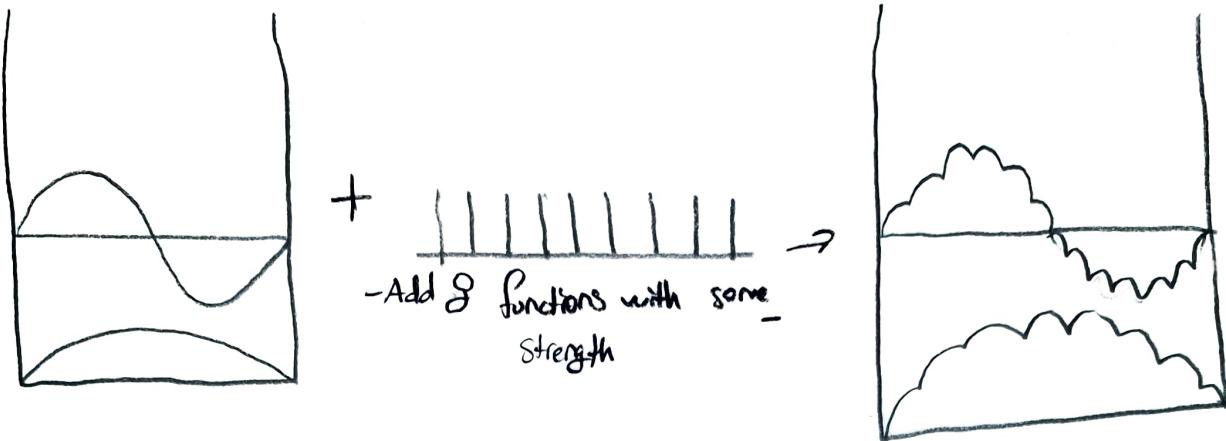
$$\Psi_B = \frac{1}{\sqrt{2}} (\chi(A)\phi(B) + \chi(B)\phi(A)) \} \text{Principle.}$$

③ " ,  $\hat{P} \Psi = -\Psi \Rightarrow$  Called Fermions

$$\Psi_F(A, A) = \sqrt{2} \chi(A)\phi(A)$$

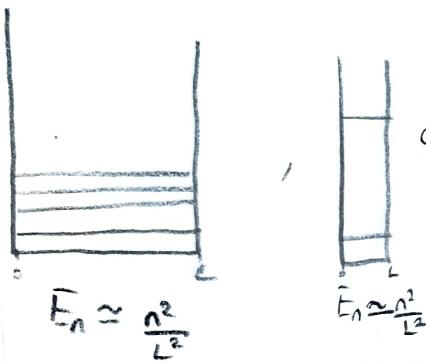
$$\Psi_{\pm}(A, B) = \pm \Psi(B, A) \xrightarrow{\text{Bosons}} \xrightarrow{\text{Fermions}}$$

(20)

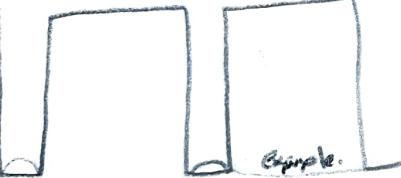


$\Rightarrow$  - Eventually will look like this

[Q]



whenever we have a narrow box the energy differences between states are gigantic compared to a wider box.

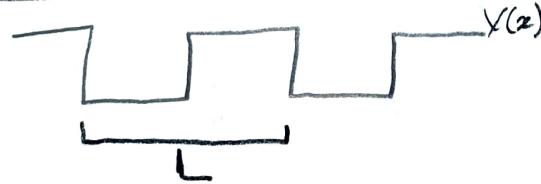


$\rightarrow$  If the height of the well is infinitely high then the states of each well is some linear combinations of  $\downarrow$ ,  $\uparrow$ ,  $-$ .

If the height of the barrier is large but finite, from the energy convention we can determine its specific energy

[Q]

Periodic Potentials:



$$V(x+L) = V(x)$$

$$\hat{T}_L V(x) = V(x)$$

$$= \left[ \hat{E}, \hat{T}_L \right] = 0, \quad \left[ \hat{E}, \hat{P} \right] \neq 0$$

Note:  $\hat{T}_L$  is unitary

$$\hat{T}_L \hat{T}_L^\dagger = \mathbb{1}$$

$$\hat{T}_L^\dagger = e^{-\frac{i\hat{P}L}{\hbar}}.$$

A. Sard Tengel

$$\begin{aligned} \hat{T}_L (\hat{V}(x) f(x)) &= \hat{V}(x) \hat{T}_L f(x) \quad \left[ \hat{L}, \hat{V}(x) \right] = 0 \\ V(x+L) f(x+L) &= \hat{V}(x) f(x+L) \quad \left[ \hat{L} = e^{i\hat{P}L/\hbar} \Rightarrow \left[ \hat{L}, \rho^2 \right] = 0 \right] \end{aligned}$$

$$\hat{E} \phi_{Ex} = E \phi_{Ex}, \quad \hat{T}_L \phi_{Ex} = e^{i\alpha} \phi_{Ex}$$

$$\text{Let } u(x) = e^{-iqx} \phi_{Ex}$$

$$\hat{T}_L u(x) = e^{i\alpha} (x+L) \phi_{Ex}$$

$$= e^{i\alpha L} e^{i\alpha} e^{-iqx} \phi_{Ex}(x)$$

$$= e^{i(\alpha - qL)} u(x) \quad \Rightarrow \alpha = \frac{qL}{\hbar} \Rightarrow u(x) \rightarrow u(x) \text{ "periodic"}$$

$\Rightarrow \phi_{E,q} = e^{iqx}\psi(x)$ ;  $e^{iqx} = e^{iql}$ ,  $\psi(x)$  is periodic.

$$q \approx q + \frac{2\pi}{L}, e^{iqx} \rightarrow e^{iqx}$$

①  $\phi_{E,q}(x)$  is not periodic by  $L$  unless  $q=0$ .

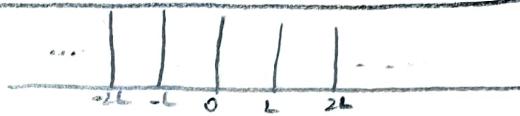
②  $P(x+L) = P(x) = |\psi(x)|^2$  is periodic

To normalize probability we need wave packets.  $\Rightarrow$  all  $\phi_{E,q}$  are extended, not localized.

③  $\phi_{E,q}(x)$  is not a momentum eigenstate ( $\Rightarrow q$  is not "the momentum"; crystal momentum).

Example:  $V(x) = \sum_{n=0}^{\infty} \frac{\hbar^2}{2mL} g_0 \delta(x-nL)$

$\underbrace{\dots}_{\text{dimensionless strength}}$   $\delta(x-nL)$



between  $0 < x < L$ ,  $\phi_{E,q} = A e^{ikx} + B e^{-ikx}$

"  $L < x < 2L$ ,  $\phi_{E,q} = e^{iql} (A e^{ikx} + B e^{-ikx})$ ,  $\frac{\hbar^2 k^2}{2m} = E$

B.C. at  $\delta$ 's.

- $\phi(0^+) = \phi(0^-) \equiv \phi(L) e^{-iqL}$

$$\Rightarrow A+B = A e^{i(k-q)L} + B e^{-i(k+q)L} \quad ①$$

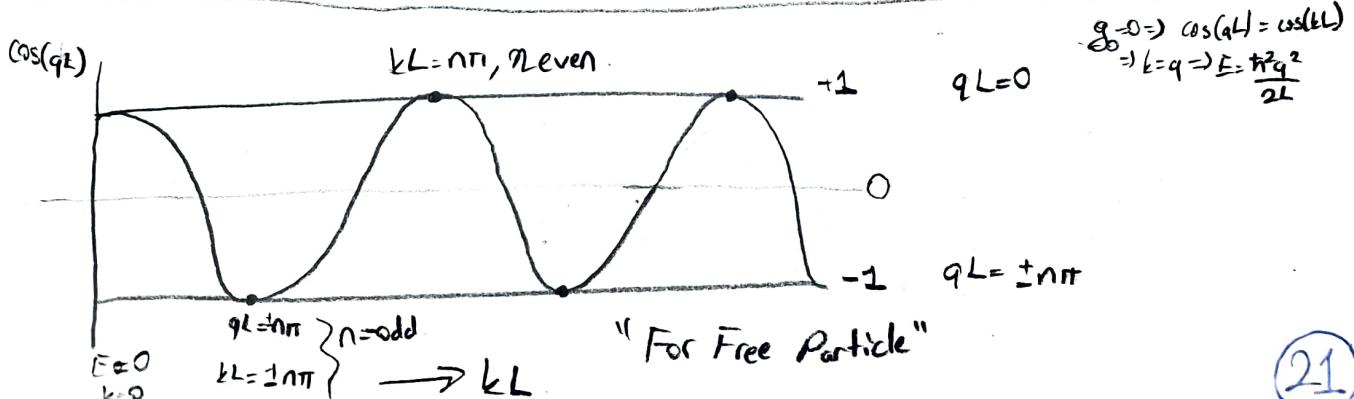
- $\phi(0^+) - \phi(0^-) = \frac{g_0}{L} \phi(0)$

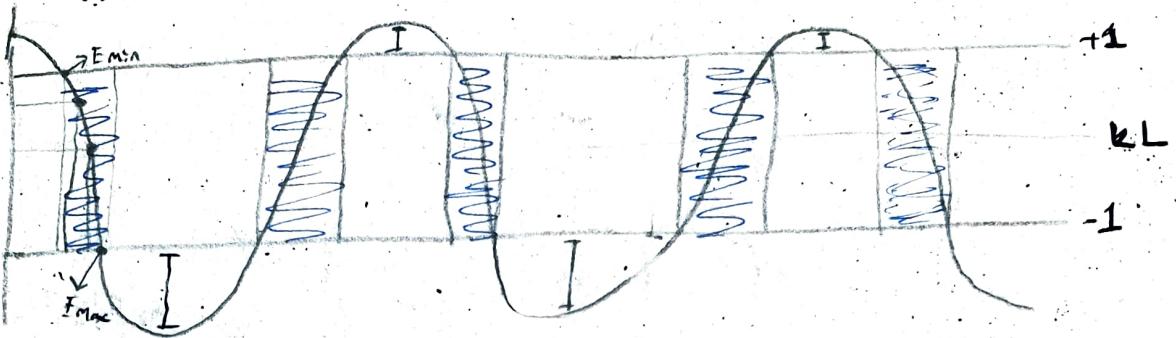
$$\Rightarrow ik(A-B) - ik(A e^{i(k-q)L} - B e^{-i(k+q)L}) = \frac{g_0}{L} (A+B) \quad ②$$

$$\Rightarrow A = B \cdot (kq)_2, \quad A = B(kq)_2. \quad \text{if you set this two equations equal to each other;}$$

$$\Rightarrow \cos(qL) = \cos(kL) + \frac{g_0}{2kL} \sin(kL), \quad k \text{ determines } E.$$

$\Rightarrow$  There exists states for any  $(q, E)$  satisfies the given last equation.





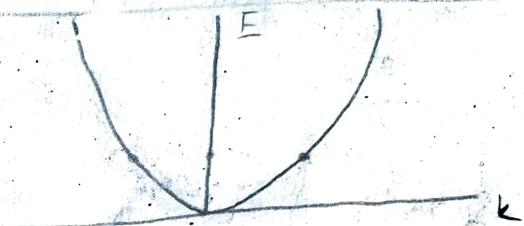
$\exists E, T_L$  energy eigenstate for any  $(E, q)$  such that there exists a solution.

$\forall E$  in the colored region corresponds to a state.

There are continuous bands of allowed and continuous bands of disallowed energies.

$$\text{Free Particle: } \hat{E} = \frac{\hat{p}^2}{2m} \Rightarrow [\hat{E}, \hat{p}] = 0$$

$$\exists \text{ basis } \hat{E} \phi_{Ek} = E \phi_{Ek}, \hat{p} \phi_{Ek} = i\hbar k \phi_{Ek}$$



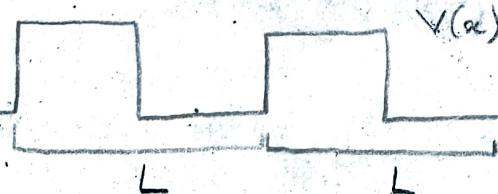
$$\Rightarrow \text{Solve } \phi_{Ek} = \frac{1}{\sqrt{2\pi}} e^{ikx}, E_k = \frac{\hbar^2 k^2}{2m} = \omega_k t$$

Note: all  $\phi_E = e^{i(kx - \omega_E t)}$  are extended

$\Rightarrow$  Build wavepacket  $\Psi = \int f(k) e^{i(kx - \omega_k t)} dk$   $\rightarrow$  peaked at  $k_0$ .

$$x_g = \frac{\partial \omega(k_0)}{\partial k} \stackrel{p}{=} \frac{\hbar k}{m} = \frac{\langle p \rangle}{m}$$

$$m_x = \frac{\langle p \rangle}{x_g}$$



$$\hat{E} = \frac{\hat{p}^2}{2m} + g_0 V(x)$$

$\Rightarrow [\hat{E}, \hat{p}] \neq 0$  but  $[\hat{E}, \hat{T}_L] = 0 \Rightarrow \exists$  common eigenbasis of  $\hat{E}, \hat{T}_L$ .

$$\phi_q(x) = e^{iqx} u(x), \hat{T}_L \phi_q(x) = e^{iqL} \phi_q(x) \rightarrow \text{periodic function, } u(x+L) = u(x)$$

$$\left\{ \hat{T}_L f(x) = f(x+L) \right\}$$

$\Rightarrow \hat{E}$  eigenfunctions can be organized as

$$\hat{E} \phi_{Eq} = E \phi_{Eq}, \hat{T}_L \phi_{Eq} = e^{i q L} \phi_{Eq}$$

$\Rightarrow$  Solve Equation  $\Rightarrow$  Relationships between  $E, q$ . For  $g_0 = 0, f_{qp}$ , we find

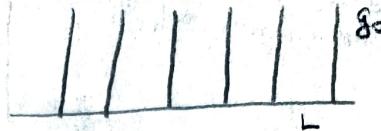
$$E_q = \frac{\hbar^2 q^2}{2m}, \quad \phi_{qE} = \frac{1}{\sqrt{2\pi}} e^{iqx} \cdot c.$$

$$\Psi = \int e^{iqx} u(q) f(q) dq.$$

$$\partial_q = \frac{\partial w(q_0)}{\partial q}, \quad m_* = \frac{c_p}{2q}$$

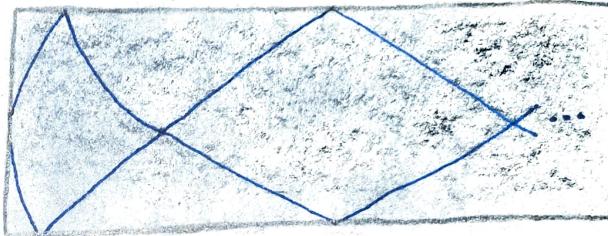
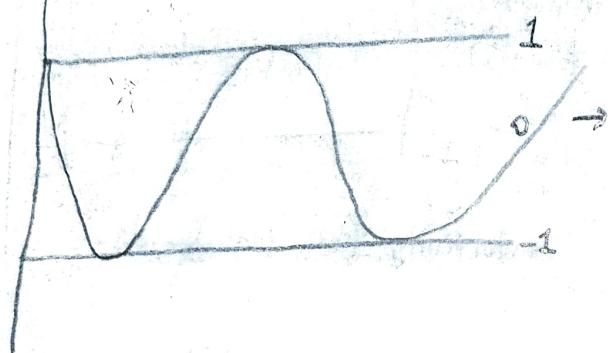
When  $g_0 \neq 0$ .

$$\phi_{qE} = e^{iq(x)} u(q) \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

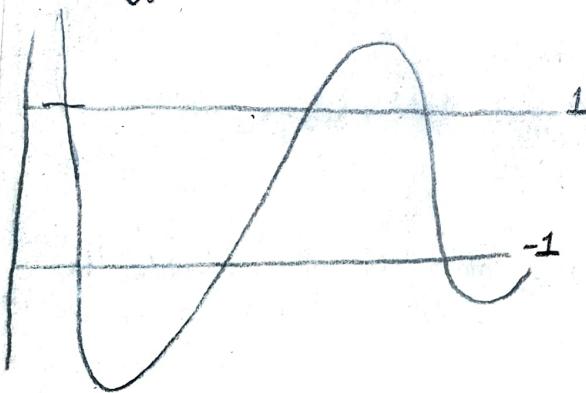


$$\cos(qL) = \cos(kL) + \frac{g_0}{2kL} \sin(kL)$$

When  $g_0 = 0$ ,



When  $g_0 \neq 0$ ,

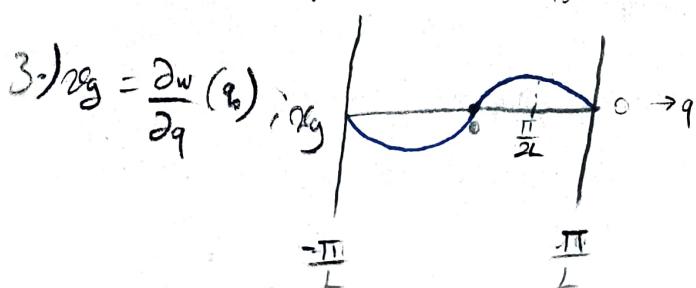


\* Lessons from  $g_0 \neq 0$ .

1-)  $E$  eigenvalues are restricted to lie within bands.

2-)  $E$  eigenstates are all extended.

$$\Rightarrow$$
 build wave packets  $\Psi = \int_{q_0}^q f(q) e^{i(qx - w_q t)} u_q(x) dq$



$$4-) \langle F \rangle = \frac{d}{dt} \langle \hat{p}_q \rangle$$

For a wavepacket localized around  $q_0$ .

- \* How does the direction of force and acceleration can be opposite?

It accelerates back and forth even the dir. of force is same - in a periodic lattice, like copper.

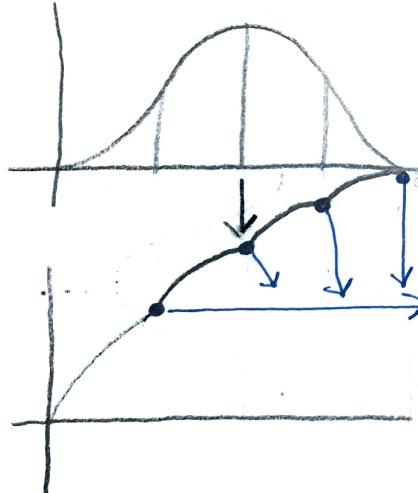
But copper conducts.  $e^-$  don't oscillate

back and forth. Let us explain

- The mass of ions are not infinite so they wiggle, as a consequence they're not perfectly periodic. That gives us bunch of things.
- The eigenfunctions we found are not exact eigenfunctions since we need to deal with wiggling of lattice
- $e^-$  can move along and kick one of these ions and scatter some of its momentum into ions. This changes the structure of lattice. We get a chain of momentum scattering and they move up.

\* Disorder is essential in conductivity for real solids.

- For direct currents -



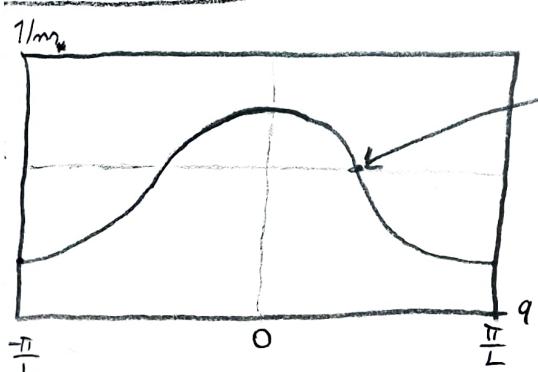
What about the force and dir of acc.?

Let's calculate the mass

$$\Rightarrow \frac{1}{m_x} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial q^2}$$

\* The effective mass is used to describe the motion particles in a medium. Instead of using actual mass we describe an adjusted mass that accounts for the interactions in the medium.

$m_x \rightarrow 0$  means the particle is localized at that point and has no motion.



Q

$\Psi(x)$  such that  $\langle \hat{x} \rangle = x_0$ ,  $\langle \hat{p} \rangle = p_0$

$$\tilde{\Psi}(x) = e^{ikx} \Psi(x) \Rightarrow \langle \hat{x} \rangle_{\tilde{\Psi}} = x_0, \langle \hat{p} \rangle_{\tilde{\Psi}} = p_0 + \hbar k.$$

$[\hat{x}, \hat{p}] = i\hbar$ ,  $T_L = e^{-i\hbar p L}$ ,  $\alpha$  governs the spatial variation of phase of  $\Psi$ .

$$\frac{d}{dt} \langle \hat{p} \rangle = \left\langle \frac{\partial V(x)}{\partial x} \right\rangle = \langle F \rangle$$

Crystal momentum:  $V(x+L) = V(x) \Rightarrow [\hat{E}, \hat{T}_L] = 0$

$$\Rightarrow \phi_{E,q} = e^{iqx} u(x), \text{ } q \text{ governs the phase as a function of } x.$$

$$\Rightarrow \frac{d}{dt} \langle \hat{p} \rangle = \langle \hat{F} \rangle \rightarrow \text{sharply peaked at } q_0, \nabla \cdot \left. \begin{array}{l} \text{S} \\ \phi_{E,q} \neq p_0 \phi_{E,q} \end{array} \right\} \text{ } q_0 \text{ is not eigenvalue of } \hat{p}.$$

eig. value of  $T_L$  on  $u(x) = e^{iqL}$ .

- Momentum is strictly conserved if there is no force and if there is a force that it is just constantly increase
- For crystal momentum it's not increasing constantly it's periodic, it increases then decrease to its initial case under some period even if you don't change the force.

How can we know that  $u(x)$  is Real?

Q

$$\textcircled{1} T_L \phi_{E,q} = e^{i\alpha} \phi_{E,q} \Rightarrow \phi_{E,q} \cdot e^{iqx} = u \equiv u_q(x), q_L = \alpha \Rightarrow T_L u_q(x) = u_q(x+L) = u_q(x)$$

$$\Rightarrow \phi_{E,q} = e^{iqx} u_q(x) \rightarrow \text{periodic.}$$

$$\textcircled{2} q \sim q + \frac{2\pi}{L}, \phi_{q, E} = e^{iqx} u(x) \equiv e^{ikx} \rightarrow \text{constant and } q = k \text{ however } q \text{ is periodic by } \frac{2\pi}{L}$$

but any  $k$  is allowed for a free particle

$$\Rightarrow e^{ikx} = e^{iqx} \cdot e^{\frac{i(k-q)x}{\hbar}} u(x) \text{ is not Real for free particle.}$$

If we want  $u(x)$  to be Real,  $q$  can not be periodic.

$$q = q_0 + \frac{n\pi}{L}$$

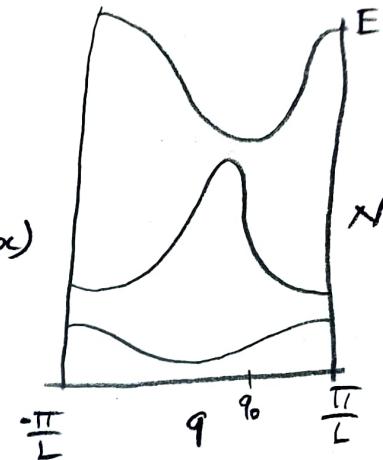
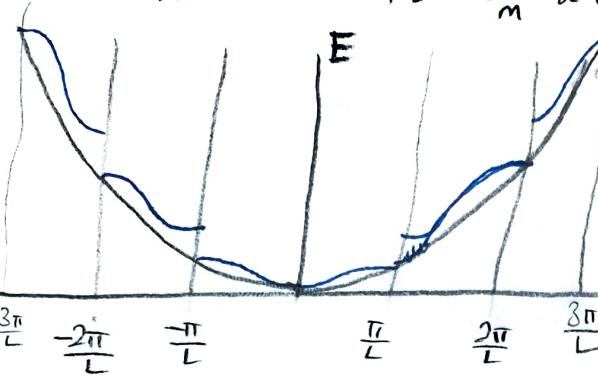
$$\phi_{q,u} = e^{iqx} e^{i\frac{n\pi x}{L}} u(x)$$

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Suppose  $x \in \mathbb{R}$ ,  $q \in \mathbb{R}$  (not periodic)

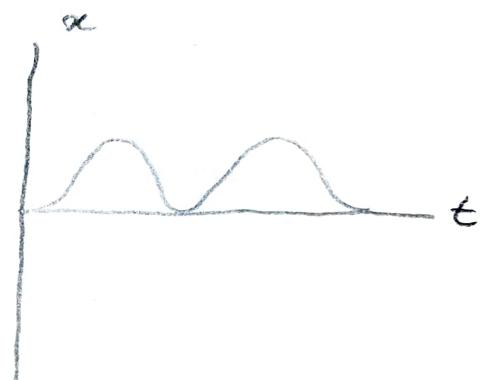
$$\phi_q = e^{iqx} \psi(x)$$

$$J_x = \frac{\hbar}{2m} \operatorname{Im}(\phi^* \partial_x \phi) = \frac{\hbar q}{m} \psi^2(x) = \left( \frac{\hbar q_0}{m} + \frac{n\pi\hbar}{mL} \right) \psi^2(x)$$

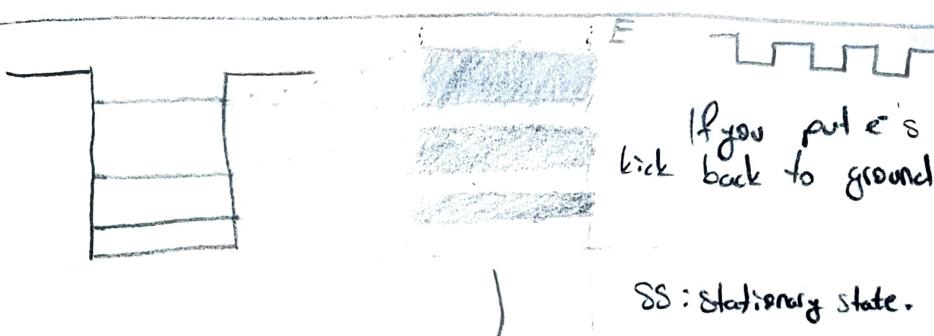


- Some values of  $E$  allowed,  $E$  gives inf. about  $k$ .
- $q$  gives inf. about  $E$ .

For our periodic lattice our particle oscillates back and forth, our materials - copper etc - are not perfect. We need a perfect crystal to build this system and test it.



Now try to understand our - real - materials.



If you put e's into a system it will eventually kick back to ground state

SS: Stationary state.

$\langle x \rangle_{ss} = 0$ , superposition states will correspond to different  $\langle x \rangle$ . In order to induce a current we must put e's into superposition of being into higher energy states.

• Think this square-wells as atoms - hydrogen -

(In order to system be neutral, there must e- for every well.)

There are  $n$  states for  $n$  wells and to neutralize our systems we must put e's into those states which are in the first band.

A. Said Tongel

If we want to induce a current, the next allowed state is in "next band".

In order to take an  $e^-$  from the first bond and put it in 2nd bond we have to put in a minimum energy  $\Delta E$ .

$$\text{So } \hbar\omega \geq \Delta E.$$

$\boxed{\Delta E}$  Crystals are transparent unless at sufficiently high frequencies.

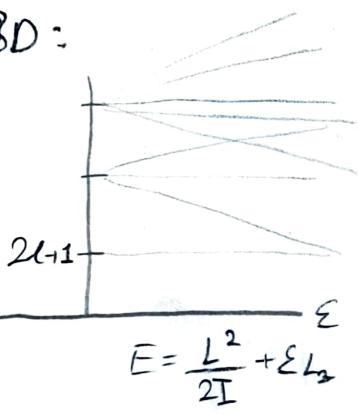
-Diamond and copper, they are both crystals.

Diamond is transparent for visible light - since copper is not transparent for visible light -

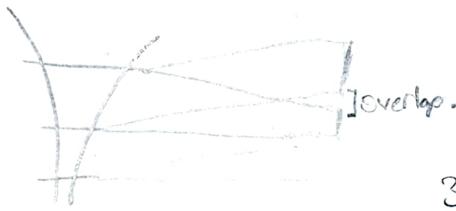
$$\Delta E_0 > \Delta E_c.$$

In 1-D crystal if you have each bond come from an allowed energy state, each well comes with integer number of  $e^-$ , you will always have filled bonds and then a gap, you're stuck. That property comes from "spin" which we'll talk later.

In 3D:



In 3D, there are crossed states



Let's say 1st band is filled. Now most of 2nd band and part of 3rd band available, then much of 3rd and bit of 2nd band.

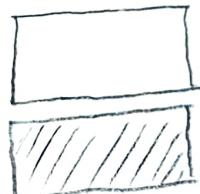
The  $E$  needed to excite will be so small, acting like a "classical conductor" because there is an unfilled band.

There were filled bonds which made them "Insulators".

IP (of electron to be excited through empty gap)

$$\sim e^{-\frac{\Delta E}{kT}}$$

if this gap  $\Delta E$  is small it makes us system a "semiconductor"



Spin:

$$S = \frac{\sqrt{2}}{2} \quad \frac{\sqrt{3}}{2} \quad \frac{\sqrt{5}}{2} \quad \dots$$

$$\left. \begin{array}{l} [S_x, S_y] = i\hbar S_z, [S_y, S_z] = i\hbar S_x \\ S_{\pm} = S_x \pm i S_y \\ S^2 = \hbar^2 s(s+1) , s \in \frac{2n+1}{2} \\ S_z = \hbar m_s , -s \leq m_s \leq s \end{array} \right\}$$

$S=1/2$

$$\Psi(x) = \Psi_{\frac{\uparrow}{2}}(x) + \Psi_{\frac{\downarrow}{2}}(x) \quad \left| P(x, \pm \hbar/2) = |\Psi_{\pm}(x)|^2 \right.$$

$$\Psi(x) = \begin{pmatrix} \Psi_{\uparrow}(x) \\ \Psi_{\downarrow}(x) \end{pmatrix} \quad \Psi^{\dagger} = (\Psi_{\uparrow}^*, \Psi_{\downarrow}^*)$$

$$\text{Norm: } (\Psi | \Psi) = 1 = \int (|\Psi_{\uparrow}|^2 + |\Psi_{\downarrow}|^2) dx$$

$$\Psi(x) = \Psi_{\uparrow}(x) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \Psi_{\downarrow}(x) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, |\Psi(x)\rangle = |\Psi_{\uparrow}(x)| \uparrow \rangle + |\Psi_{\downarrow}(x)| \downarrow \rangle$$

$$S_z |\uparrow\rangle = \frac{\hbar}{2} |\uparrow\rangle, S_z |\downarrow\rangle = -\frac{\hbar}{2} |\downarrow\rangle, S^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3\hbar^2}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \dots$$

$$S_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, S_z \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, S^2 |\uparrow\rangle = \frac{3\hbar^2}{4} |\uparrow\rangle$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad S^2 = \frac{3\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$S_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}, S_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0, S_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0, S_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\left. \begin{array}{l} S_z = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ S_x = \frac{S_+ + S_-}{2\hbar}, S_y = \frac{S_+ - S_-}{2i} \end{array} \right\} \Rightarrow \begin{array}{l} S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y = \frac{\hbar}{2i} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{array}$$

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[S_x, S_y] = ? \text{ ch } S_z = \left( \frac{\hbar}{2} \right)^2 \left[ \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right) \right] = \frac{\hbar^2}{4} \left( \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \right)$$

$$= \frac{\hbar^2}{4} \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = \frac{\hbar^2}{2} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = (\text{ch}) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \text{ch } S_z$$

$S_z$ : Eigen values?

$$S_z \left( \frac{1}{2} \right) = \frac{\hbar}{2} \left( \frac{1}{2} \right) = \uparrow_2 + \downarrow_2$$

$$\uparrow_2 = \frac{1}{\sqrt{2}} (\uparrow_1 + \downarrow_2) \quad S_z \left( \frac{-1}{2} \right) = \frac{\hbar}{2} \left( \frac{-1}{2} \right) = \downarrow_2$$

$$\downarrow_2 = \frac{1}{\sqrt{2}} (\uparrow_2 - \downarrow_2)$$

$$|P(\uparrow_2, \downarrow_2)| = |P(\uparrow_2)| \text{ given that we measured } \uparrow_2 \\ = \left| \frac{1}{\sqrt{2}} \right|^2 = 1/2$$

$$S_y : \uparrow_y = \frac{1}{\sqrt{2}} (\uparrow_2 + i \downarrow_2), \downarrow_y = \frac{1}{\sqrt{2}} (\uparrow_2 - i \downarrow_2)$$

$$\hat{S}_\theta \equiv \left. \begin{array}{c} \uparrow_2 \\ \downarrow_2 \\ \theta \end{array} \right\} \Rightarrow \begin{aligned} \uparrow_\theta &= \cos \left( \frac{\theta}{2} \right) \uparrow_2 + \sin \left( \frac{\theta}{2} \right) \downarrow_2 \\ \downarrow_\theta &= \sin \left( \frac{\theta}{2} \right) \uparrow_2 - \cos \left( \frac{\theta}{2} \right) \downarrow_2. \end{aligned}$$

$$\hat{\vec{z}} \quad \Psi_e = a \uparrow_2 + b \downarrow_2 \\ \beta_2 \approx \beta_0 + \beta^2$$

$$\vec{E} = \vec{n}_0 \cdot \vec{S} \cdot \vec{B}_2 - \left. \begin{array}{c} 0 \\ -n_0 \cdot S_z (\beta_0 + \beta \cdot z) \\ 0 \end{array} \right\} \text{ In Region } R$$

$$= \frac{\hbar}{2} n_0 B_2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} C(2) & 0 \\ 0 & -C(2) \end{pmatrix}$$

$$E \uparrow_2 = C(2) \uparrow_2, E \downarrow_2 = -C(2) \downarrow_2$$

$$E_{\uparrow_2} = -C(2), E_{\downarrow_2} = -C(2)$$

$$\Rightarrow \Psi(t) = a e^{i \frac{E_{\uparrow_2} t}{\hbar}} \uparrow_2 + b e^{-i \frac{E_{\downarrow_2} t}{\hbar}} \downarrow_2$$

$$= a e^{i \frac{n_0 B_0 t}{2}} e^{i \frac{\hbar \beta t}{2}} \uparrow_2 + b e^{-i \frac{n_0 B_0 t}{2}} e^{-i \frac{\hbar \beta t}{2}} \downarrow_2$$

Entanglement:

$$\downarrow_g = \cos\left(\frac{\theta}{2}\right)\downarrow_0 + i \sin\left(\frac{\theta}{2}\right)\uparrow_0$$

$$\Psi(0) = \frac{1}{\sqrt{2}} (\uparrow_2 + \downarrow_2) = \uparrow_2, E = -\mu_B B_2 S_2 \Rightarrow E_1 = \pm \hbar \omega, \omega = \frac{\mu_B B_2}{2}$$

$$\Rightarrow \Psi(t) = \frac{1}{\sqrt{2}} (e^{i\omega t} \uparrow_2 + e^{-i\omega t} \downarrow_2)$$

$$\omega t = \frac{\pi}{2} \Rightarrow \Psi_{\text{after}} = \frac{i}{\sqrt{2}} (\uparrow_2 - \downarrow_2) = i \downarrow_2$$

we have

1-) The system can be put in  $\uparrow_2, \downarrow_2$   
2-) Ability to evolve states from  $\Psi_0 \rightarrow \Psi_1$  w/  $B$  fields.

This will allow us to do Quantum Computing.

Quantum Computing:

$N$  bits  $\{0, 1\}$ ,  $2^N$  binary numbers

$N$  Qubits  $\{|\psi\rangle, |\bar{\psi}\rangle\}$ ,  $2^N$  complex numbers

$$\Psi = \alpha |000\dots0\rangle + \beta |1000\dots\rangle$$

$2^N$  possibility

Systems:  $N$  Qubits  $\begin{array}{c} \uparrow \\ \downarrow \end{array}$

In:  $\Psi_{\text{in}}^{(N)}$     Evolve w/  $E$   $\xrightarrow{\text{implement algorithm}}$   $\Psi_{\text{out}}^{(N)}$

- In/out are superposition of values we measure.
- Measure  $\rightarrow$  Interference
- $\Rightarrow$  Probabilistic outcomes
- Orchestrate the interference to get definite outcome
- Focus on checkable problems.

Qbit = a 2-state system  $|0\rangle |1\rangle$

$$\Psi = \alpha|0\rangle + \beta|1\rangle, P(0) = |\alpha|^2$$

2-Qbits =

$$\Psi = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$P(A=0) = \alpha^2 + \beta^2, P(A=0, B=1) = |\beta|^2$$

Separable States

$$|\Psi\rangle = |\Psi_1\rangle |\Psi_2\rangle$$

$$\text{eg} = (a|0\rangle + b|1\rangle)(c|0\rangle - d|1\rangle) = ac|00\rangle - ad|01\rangle - bc|10\rangle - bd|11\rangle$$

$$\text{measure } A=0 : |\Psi\rangle = |0\rangle \otimes (c|0\rangle - d|1\rangle)$$

Generic States are Not Separable.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \Rightarrow \boxed{\text{Entangled}}$$

$$\text{Suppose } B=1. \Rightarrow P(A=0)=0, P(A=1)=1$$

How to Compute:

Sch. Env w/our tuned  $E$ .

$$\rightarrow 2: \text{Gate NOT: } |0\rangle \xrightarrow{(1)} |1\rangle, |1\rangle \xrightarrow{(2)} |0\rangle.$$

$$U_{NOT} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = i e^{\frac{\pi i}{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -i \left( \cos(\pi/2) + i \sin(\pi/2) \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$U \text{ for } B_x \text{ for } t_w = \frac{\pi}{2}$$

Ex 2: Turn on  $\mathcal{U}_H$  for a time  $t$ .

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

$$\mathcal{U}_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$



CNOT: Apply NOT to the second qubit if and only if first qubit is 1.

$$\begin{aligned} 00 &\rightarrow 00 \\ 01 &\rightarrow 01 \\ 10 &\rightarrow 11 \\ 11 &\rightarrow 10 \end{aligned}$$



What can you do with these operations?

Sch. Eq.  $\Rightarrow$  Linear, Unitary

No cloning

Suppose that  $|x\rangle|y\rangle \rightarrow |x\rangle|x\rangle$ ,  $\forall |y\rangle$ ,

$$\mathcal{U}|x\rangle|y\rangle \rightarrow |x\rangle|x\rangle, \forall |y\rangle$$

$$\mathcal{U}|z\rangle|y\rangle \rightarrow |z\rangle|z\rangle, \forall |y\rangle$$

Because  $\mathcal{U}$  is unitary it preserves inner product

$$|x\rangle|z\rangle = (|x\rangle|z\rangle)^2 \text{ since inner product implies}$$

$$|x\rangle|z\rangle \times |y\rangle|y\rangle = |x\rangle|z\rangle \times |x\rangle|z\rangle$$

Assuming  $|y\rangle|y\rangle = 1$ , this reduces to

$$|x\rangle|z\rangle = (|x\rangle|z\rangle)^2$$

This is true if  $|x\rangle|z\rangle = 0$  or  $|x\rangle|z\rangle = 1$   
orthogonal same state

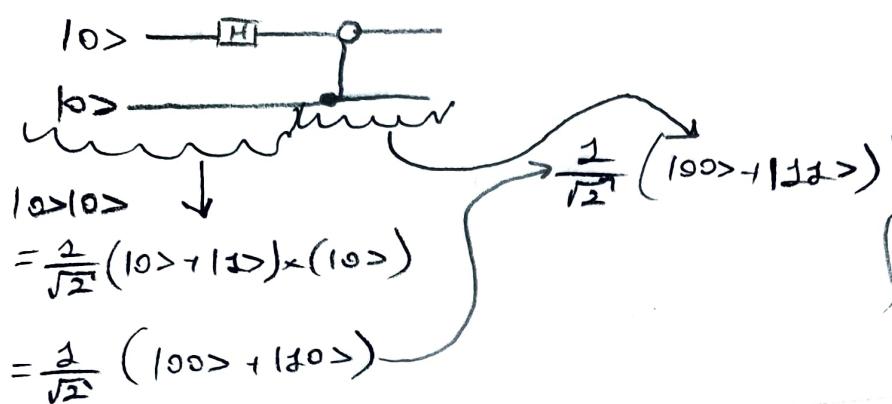
Cloning an arbitrary unknown quantum state is impossible

You also can't lose information since universe preserves info.

{ The information of state  $y$ , that we tried to copy into it is lost }

Now Let's see what we can do.

- You can entangle.



By using Hadamard and CNOT operations to a two state system, we entangled the states.

Deutsch-Jozsa Algorithm:

Suppose that I have a function which I want to evaluate but it cost \$2<sup>60</sup> and I want to know whether  $f(0) = f(1)$  which cost \$2 · 10<sup>9</sup>.

$f(0) = f(1) \Rightarrow$  Classically requires 2 evaluations which will require less resources.

We'll build a setup which will give us the answer.

$$f(0) \oplus f(1) = \begin{cases} 0 & \text{if } \text{even} \\ 1 & \text{if } \text{not} \end{cases}$$

Setup:  $\mathcal{U}_f: |x\rangle|y\rangle \rightarrow |x\rangle|f(x) \oplus y\rangle$ ,  $\oplus = \text{odd mod two. } |x\rangle \rightarrow |f(x)\rangle$

Algorithm In:  $\Psi = |0\rangle|0\rangle$ .

Apply Hadamard on both qubits.

1-) Apply Hadamard on both qubits.

$$\Psi \rightarrow \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) = \frac{1}{2} ((|0\rangle(|0\rangle - |1\rangle)) + (|1\rangle(|0\rangle - |1\rangle)))$$

2-) Apply  $\mathcal{U}_f$  operator.

$$\frac{1}{2} [ |0\rangle \times (|f(0) \oplus 0\rangle - |f(0) \oplus 1\rangle) + |1\rangle \times (|f(1) \oplus 0\rangle - |f(1) \oplus 1\rangle) ]$$

$$\begin{aligned} \Rightarrow f(0) = 0 &\Rightarrow (0 - 1) \\ \Rightarrow f(0) = 1 &\Rightarrow (1 - 0) = -(0 - 1) \end{aligned} \left\{ = (-2)^{f(0)} (|0\rangle - |1\rangle) \right\}$$

$$\Rightarrow \frac{1}{2} \left[ (-2)^{f(0)} |0\rangle \times (|0\rangle - |1\rangle) + (-2)^{f(1)} |1\rangle \times (|0\rangle - |1\rangle) \right] = \frac{1}{2} (-2)^{f(0)} \left[ |0\rangle + (-2)^{f(0)} |1\rangle \right] (|0\rangle - |1\rangle)$$

3-) Don't care about 2nd qubit for now

$$\text{If } f(0) = f(1) \Rightarrow |0\rangle + |1\rangle$$

$$\text{If } f(0) \neq f(1) \Rightarrow |0\rangle - |1\rangle$$

4-) Hadamard the first qubit.

$$|\psi_{\text{out}}\rangle = \frac{1}{2} \left( 1 + (-1)^{f(0)+f(1)} \right) |0\rangle + \frac{1}{2} \left( 1 - (-1)^{f(0)+f(1)} \right) |1\rangle$$

5-) Measure first qubit

$\Rightarrow 0 \Rightarrow \text{same}$

$\Rightarrow 1 \Rightarrow \text{different}$ .

But still it cost us  $\$10^6$ .

Let's see the part of Joza

N Bits DJ problem for every measurement,  $2^N$ , classically  
"1" Quantum operation  
N Qubits " " it requires

EPR:  
Let's say that I have an entangled state  $\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)$



when we measure  $\alpha$ , we know the state of  $\beta$ .

Now there are 2 possibilities

1-) It was already determined that both would be up or down

2-) xor there is some nonlocality in universe such that a distant measurement  
on  $\alpha$  has effects on the state of  $\beta$ .

There are some answers to this problem.

2-) The quantum mechanics is insufficient and there is some hidden variable that we haven't observed which makes role on determining the particles spin from the creation.

It looks probabilistic but actually there is some hidden fact which controlling the probability distribution.

2-) That is some upsetting fact but we're not going to throw it out just because there is some nasty problem that we need to face. QM models works like a champ in other problems.

Now let's look at the problem with a different aspect.

Let's measure the spin of  $\alpha$  along  $\vec{z}$  and measure  $\beta$  along  $\alpha$  direction. BUT know we have lost information about  $S_x$  and  $S_z$  on both particles. At the very beginning of  $S_x$  we said that  $S_x$  and  $S_z$  DO NOT COMMUTE, but know we know spin along  $x$  and  $z$  both COMPUTE. Einstein said "QM is incomplete" but Bell came with an idea.

Bell used classical statistics to show that argument 1 is trash.

$$N(A, \bar{B}) + N(B, \bar{C}) \geq N(A, \bar{C})$$

$$\rightarrow N(A, \bar{B}, C) + N(\bar{A}, B, \bar{C}) \geq 0$$

First, we will measure  $\alpha$  at  $\theta$  and  $\beta$  at  $\vartheta$ .

Then, we will measure  $\alpha$  at  $\theta$  and  $\beta$  at  $2\vartheta$ .

Finally, " " "  $\alpha$  at  $\theta$  and  $\beta$  at  $2\vartheta$

$$A: \uparrow_\theta, \bar{A}: \downarrow_\theta, B: \uparrow_\vartheta, \bar{B}: \downarrow_\vartheta, C: \uparrow_{2\vartheta}, \bar{C}: \downarrow_{2\vartheta} \quad \left. \right\} \quad j_\theta = \cos(\theta/2)\downarrow_\theta + \sin(\theta/2)\uparrow_\theta$$

$$IP(\uparrow_\theta, \downarrow_\vartheta) + IP(\uparrow_\vartheta, \downarrow_{2\vartheta}) \geq IP(\uparrow_\theta, \downarrow_{2\vartheta})$$

$$\sin^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\vartheta}{2}\right) \geq \sin^2(\theta), \text{ at small } \theta;$$

$$\Rightarrow \left(\frac{\theta}{2}\right)^2 + \left(\frac{\vartheta}{2}\right)^2 \neq \epsilon^2 \Rightarrow \text{Violation of the Bell's Inequality}$$

We observed this result which is an empirical proof that Arg. 1 is not possible.