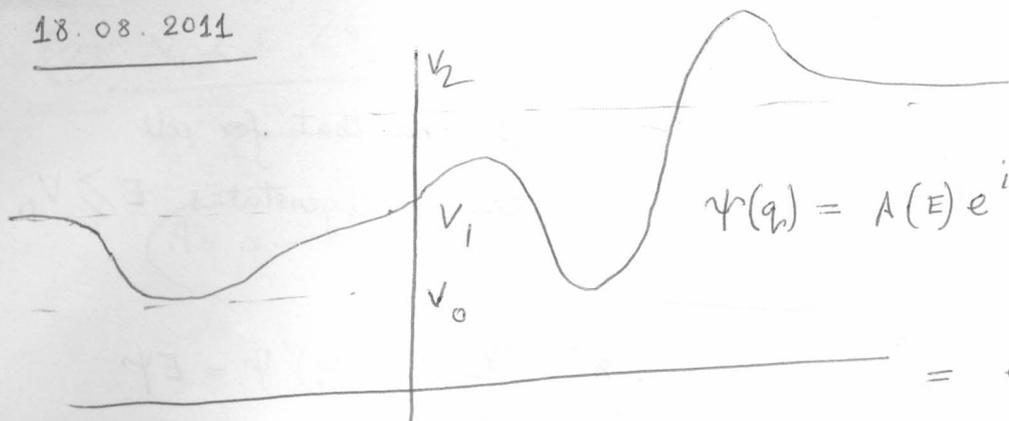


18.08.2011



$$\psi(q) = A(E) e^{ik_1 q} + B(E) e^{-ik_1 q} \quad \text{as } q \rightarrow -\infty$$

$$= e^{ik_2 q} \quad \text{as } q \rightarrow \infty$$

$A(E) e^{ik_1 q}$  : Incident wave  
 Density :  $|A(E)|^2$   
 $B(E) e^{-ik_1 q}$   
 ↓  
 reflected wave  
 Density :  $|B(E)|^2$

$e^{ik_2 q}$  → transmitted wave  
 (density 1) :  $|A(E)|^2 = |B(E)|^2 + 1$   
 $\left\{ \begin{array}{l} |\psi(q)|^2 \delta q \quad \checkmark \\ = \text{Prob. of finding a particle between } q \text{ and } q + \delta q \end{array} \right.$

For large -ve q, average number of particles / length

$$\frac{1}{L} \int_{-\pi/L}^{-\pi/L + L} |\psi(q)|^2 dq$$

$$= \frac{1}{L} \int_{-\pi/L}^{-\pi/L + L} (|A(E)|^2 + |B(E)|^2 + A^* B e^{-2ik_1 q} + B^* A e^{2ik_1 q}) dq$$

$$= |A(E)|^2 + |B(E)|^2$$

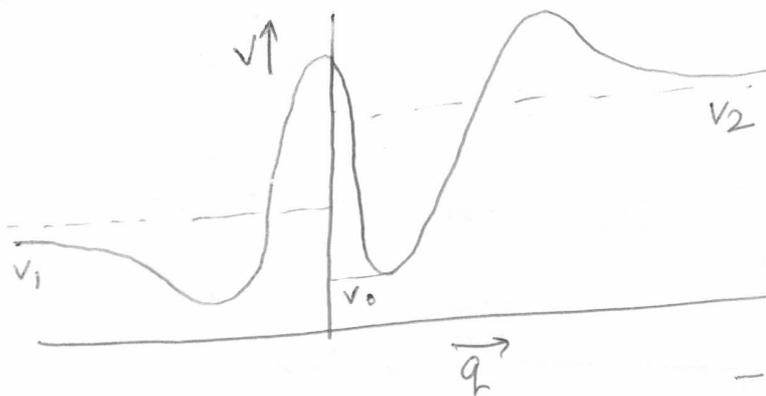
Average momentum

$$\frac{1}{L} \int_{-\pi/L}^{-\pi/L + L} dq \psi^*(q) \left( -i\hbar \frac{\partial \psi}{\partial q} \right)$$

$$= \hbar k_1 |A|^2 - \hbar k_1 |B|^2$$

Calculate avge. energy

get  $\hbar k_1 (|A|^2 + |B|^2)$   
 $|A|^2$  → density of incident wave  
 $|B|^2$  → density of reflected wave



① Show that for all energy eigenstates  $E \geq V_0$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dq^2} + V(q)\psi = E\psi$$

$$\textcircled{1} -\frac{\hbar^2}{2m} \frac{d^2\psi}{dq^2} = (E - V(q))\psi(q)$$

$$\times \int_{-\infty}^{\infty} \psi^*(q) dq$$

$$\text{LHS} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^*(q) \frac{d^2\psi}{dq^2} dq$$

$$= \frac{\hbar^2}{2m} \int dq \frac{d\psi^*}{dq} \frac{d\psi}{dq} - \frac{\hbar^2}{2m} \left[ \psi^* \frac{\partial\psi}{\partial q} \right]_{-\infty}^{\infty}$$

$$\geq 0$$

$$\text{RHS} = \int_{-\infty}^{\infty} dq \psi^*(q) (E - V(q))\psi(q)$$

$$\text{If } E < V_0, \quad \text{RHS} < 0 \quad (\text{for } E < V_0)$$

So, contradiction

$$-\frac{\hbar^2}{2m} \frac{d^2\psi^*}{dq^2} + V(q)\psi^* = E\psi^*$$

$$\text{Define } J = \left( \psi^* \frac{d\psi}{dq} - \frac{d\psi^*}{dq} \psi \right)$$

$$\frac{dJ}{dq} = \psi^* \frac{d^2\psi}{dq^2} - \frac{d^2\psi^*}{dq^2} \psi = 0$$

(Using Schrödinger eq<sup>n</sup>)

$$J(q) \Big|_{q=-\infty} = J(q) \Big|_{q=\infty}$$

①  $E < V_1, V_2$

$$\text{As } q \rightarrow \infty, \quad \psi(q) \rightarrow e^{-\kappa_2 q}$$

$$J \rightarrow 0$$

$$\text{As } q \rightarrow -\infty, \quad \psi(q) \rightarrow B(E) e^{\kappa_1 q} \quad (\because A=0)$$

$$J \rightarrow 0$$

②  $V_1 < E < V_2$

As  $q \rightarrow \infty$ ,  $\Psi(q) \rightarrow e^{-k_2 q}$

As  $q \rightarrow -\infty$   $J \rightarrow 0$

$\Psi(q) \rightarrow A e^{ik_1 q} + B e^{-ik_1 q}$

$$J = \Psi^* \frac{d\Psi}{dq} - \frac{d\Psi^*}{dq} \Psi$$

$$= (A^* e^{-ik_1 q} + B^* e^{ik_1 q}) (ik_1 A e^{ik_1 q} - ik_1 B e^{-ik_1 q})$$

$$- (A e^{ik_1 q} + B e^{-ik_1 q}) (-ik_1 A^* e^{-ik_1 q} + ik_1 B^* e^{ik_1 q})$$

$$= 2ik_1 (|A|^2 - |B|^2)$$

But  $J = 0$  for  $q \rightarrow \infty$

$|A|^2 = |B|^2$

③  $E > V_1, V_2$

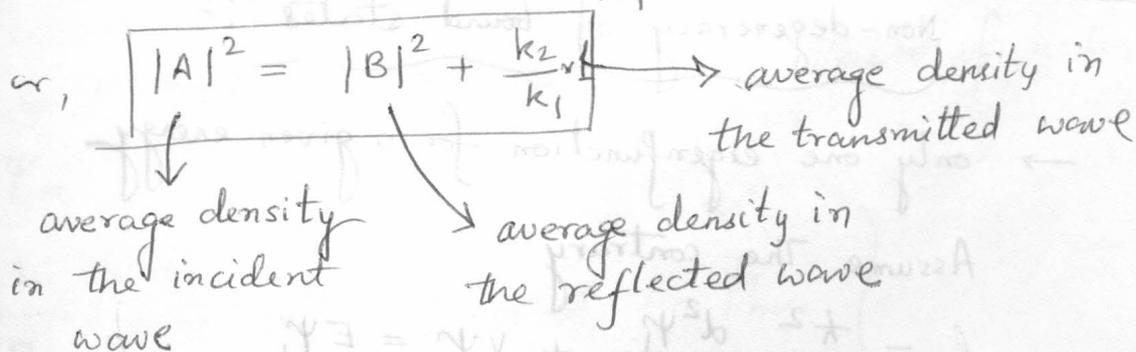
$\Psi(q) \rightarrow e^{ik_2 q}$  as  $q \rightarrow \infty$

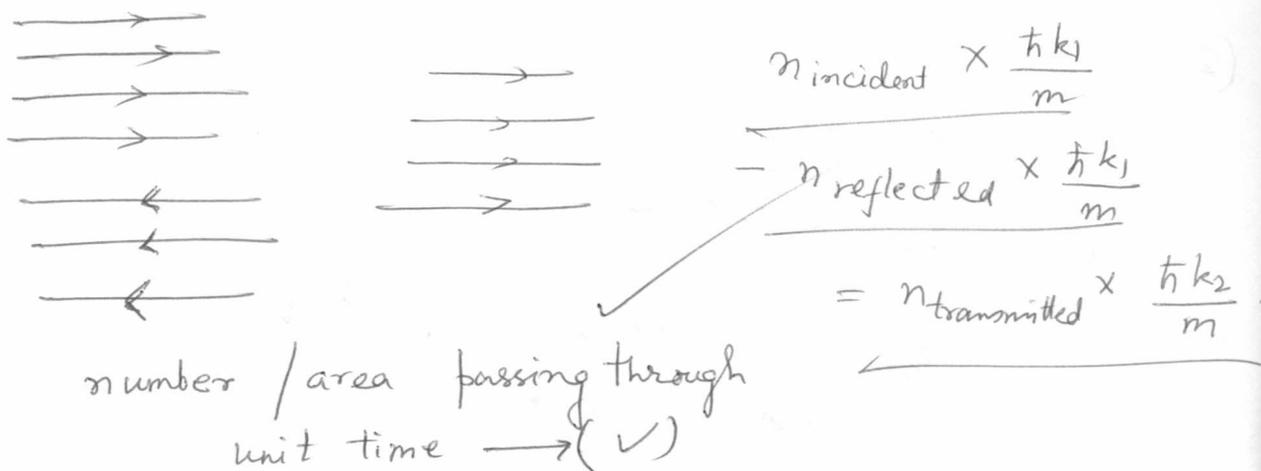
$\rightarrow A e^{ik_1 q} + B e^{-ik_1 q}$  as  $q \rightarrow -\infty$

$J \rightarrow 2ik_1 (A^* A - B^* B)$

$q \rightarrow \infty$   $\rightarrow J = 2ik_2$

$\Rightarrow A^* A - B^* B = \frac{k_2}{k_1}$





$$1 = \frac{|B|^2}{|A|^2} + \frac{k_2}{k_1} \left| \frac{1}{A} \right|^2$$

or,  $1 = |r(E)|^2 + \frac{k_2}{k_1} |t(E)|^2$

$\Downarrow$   $R(E)$  (fraction which gets reflected back)     
  $\Downarrow$   $T(E)$  (fraction which gets transmitted)

Oscillation theorem

Suppose, we arrange the energy eigenvalues as  $E_0 < E_1 < E_2 < \dots$   
 & the corresponding wavefunctions are  $\Psi_0(q), \Psi_1(q), \dots$   
 Then,  $\Psi_n(q)$  has precisely  $n$  nodes. ( $n$  zeros other than  $\pm \infty$ ).

19.08.2014

Non-degeneracy of bound states :-

$\rightarrow$  only one eigenfunction for a given energy

Assume the contrary

$$\left\{ \begin{array}{l} -\frac{\hbar^2}{2m} \frac{d^2 \Psi_1}{dq^2} + V \Psi_1 = E \Psi_1 \\ -\frac{\hbar^2}{2m} \frac{d^2 \Psi_2}{dq^2} + V \Psi_2 = E \Psi_2 \end{array} \right.$$

Ex. Show that  $\frac{d}{dq} \left( \psi_1 \frac{d\psi_2}{dq} - \psi_2 \frac{d\psi_1}{dq} \right) = 0$ .

$\therefore \psi_1 \frac{d\psi_2}{dq} - \psi_2 \frac{d\psi_1}{dq} = C$  (Independent of  $q$ )

What is  $C$ ?

$C=0$

At  $q = \infty$ ,  $\psi_1, \psi_2 \rightarrow 0$

$\therefore \psi_1 \frac{d\psi_2}{dq} = \psi_2 \frac{d\psi_1}{dq}$

or,  $\frac{1}{\psi_1} \frac{d\psi_1}{dq} = \frac{1}{\psi_2} \frac{d\psi_2}{dq}$

or,  $\ln \psi_1 = \ln \psi_2 + k$  ( $k = \text{integration constant}$ )

$\Rightarrow \psi_1 = e^k \psi_2$

$\Rightarrow$   ~~$\psi_1, \psi_2$  are basis~~  $\psi_1, \psi_2$  describe the same state.

Oscillation theorem

Suppose, the eigenvalues of the Hamiltonian are  $E_0 < E_1 < E_2 < \dots$  & the eigenfunctions are

$\psi_0, \psi_1, \psi_2, \dots$

Then,  $\psi_n$  has  $n$  nodes. ( $n$  points where it vanishes)

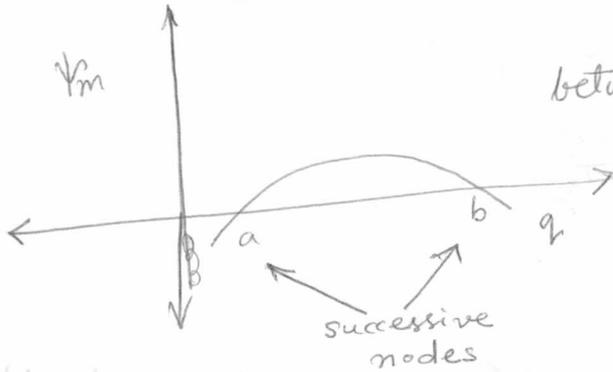
Suppose,  $\psi_m$  and  $\psi_n$  are two eigenfunctions of energy  $E_m$  and  $E_n$  with  $E_m < E_n$ .

Then, we'll show that  $\psi_n$  has larger number of nodes than  $\psi_m$ .

$$\left\{ \begin{array}{l} -\frac{\hbar^2}{2m} \frac{d^2 \psi_m}{dq^2} + V(q) \psi_m = E_m \psi_m \\ -\frac{\hbar^2}{2m} \frac{d^2 \psi_n}{dq^2} + V(q) \psi_n = E_n \psi_n \end{array} \right.$$

Ex. Show that 
$$\frac{d}{dq} \left( \psi_n \frac{d\psi_m}{dq} - \psi_m \frac{d\psi_n}{dq} \right) = (E_m - E_n) \psi_m \psi_n \quad \left( -\frac{2m}{\hbar^2} \right)$$

We'll show that between any two nodes of  $\psi_m$  there is a node of  $\psi_n$ .



Assume that  $\psi_m$  is positive between  $a$  and  $b$ . Then

$$\left[ \begin{array}{l} \frac{d\psi_m}{dq} > 0 \text{ at } q=a \\ \text{and } \frac{d\psi_m}{dq} < 0 \text{ at } q=b \end{array} \right]$$

We now integrate  $\frac{d}{dq} \left( \psi_n \frac{d\psi_m}{dq} - \psi_m \frac{d\psi_n}{dq} \right)$  from

$a$  to  $b$ .

$$\int_a^b \frac{d}{dq} \left( \psi_n \frac{d\psi_m}{dq} - \psi_m \frac{d\psi_n}{dq} \right) dq = -\frac{2m}{\hbar^2} (E_m - E_n) \int_a^b \psi_m \psi_n dq$$

$$\text{LHS} = \left. \psi_n \frac{d\psi_m}{dq} \right|_a^b$$

Suppose,  $\psi_n$  has no zero between  $a$  and  $b$ .

Let's assume that  $\psi_n > 0$  in  $[a, b]$ .

$$\left[ \begin{array}{l} \text{L.H.S.} = \text{negative } (< 0) \\ \text{R.H.S.} > 0 \end{array} \right] \left. \begin{array}{l} > 0 \\ < 0 \end{array} \right\} \begin{array}{l} \text{if } \psi_n \\ \text{is -ve} \end{array}$$

So, there's a contradiction.

$\therefore \psi_n$  must change sign between  $a$  &  $b$ .



x : nodes of  $\psi_m$

o : nodes of  $\psi_n$

# o > # x

### General proof :-

Define  $F_2 = \frac{1}{f_2} \frac{\partial f_2}{\partial q}$ ,  $G_2 = \frac{1}{g_2} \frac{\partial g_2}{\partial q}$

Why partial derivatives?  $\rightsquigarrow [f_2, g_2 \text{ depends on energy } E]$

Ex 0:  $F_2$  and  $G_2$  satisfy the same 1st order differential equation

$$F = \frac{1}{\psi} \frac{d\psi}{dq}$$

$$\begin{aligned} \frac{\partial F}{\partial q} &= \frac{1}{\psi} \frac{\partial^2 \psi}{\partial q^2} - \frac{1}{\psi^2} \left( \frac{\partial \psi}{\partial q} \right)^2 \\ &= -\frac{2m}{\hbar^2} (E - V(q)) - F^2 \end{aligned}$$

Ex. (1) For generic  $E$ ,  $F_2 \rightarrow -\kappa_2$  as  $q \rightarrow \infty$   
 $\rightarrow -\kappa_1$  as  $q \rightarrow -\infty$

$$\begin{aligned} G_2 &\rightarrow \kappa_2 \text{ for } q \rightarrow \infty \\ &\rightarrow \kappa_1 \text{ for } q \rightarrow -\infty \end{aligned}$$

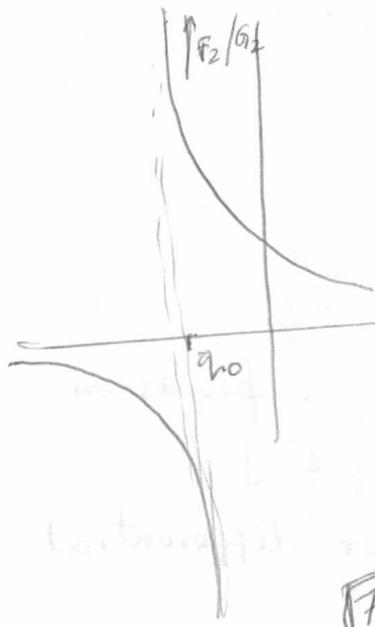
(2) If  $E = \text{energy of a bound state}$ , then

$$\begin{aligned} F_2 = G_2 &\rightarrow -\kappa_2 \text{ as } q \rightarrow \infty \\ &\rightarrow \kappa_1 \text{ as } q \rightarrow -\infty. \end{aligned}$$

(3) If  $F_2$  (or  $G_2$ ) has singularity of the

form  $\left[ \frac{A}{(q - q_0)^n} \right]$  then  $A = 1, n = 1$ .

(use diff. eq.)



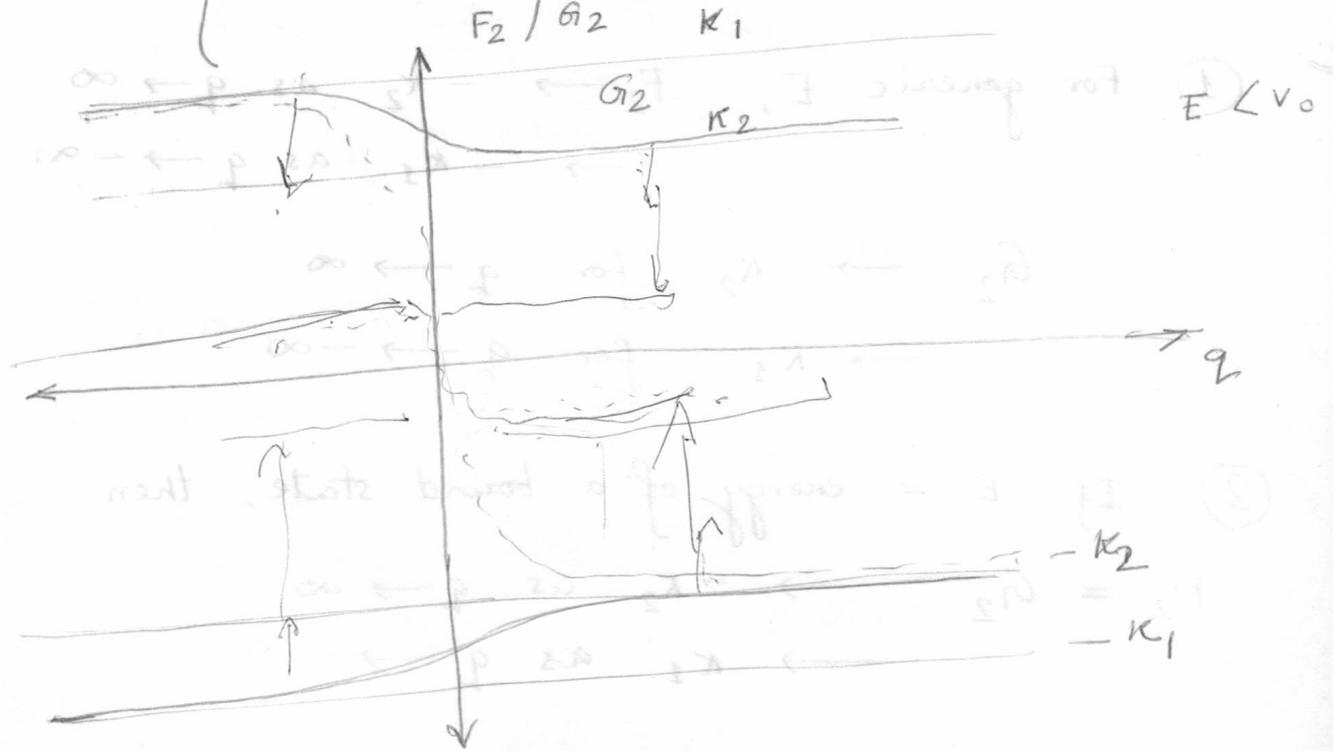
4. If ~~2~~  $F_2 = G_2$  at any one point, then  $F_2(q) = G_2(q)$ .

5.  $F_2$  (or  $G_2$ ) goes as  $\frac{1}{q - q_0}$  implies

7.  $f_2$  (or  $g_2$ )  $\approx C(q - q_0)$  [near  $q = q_0$ ]

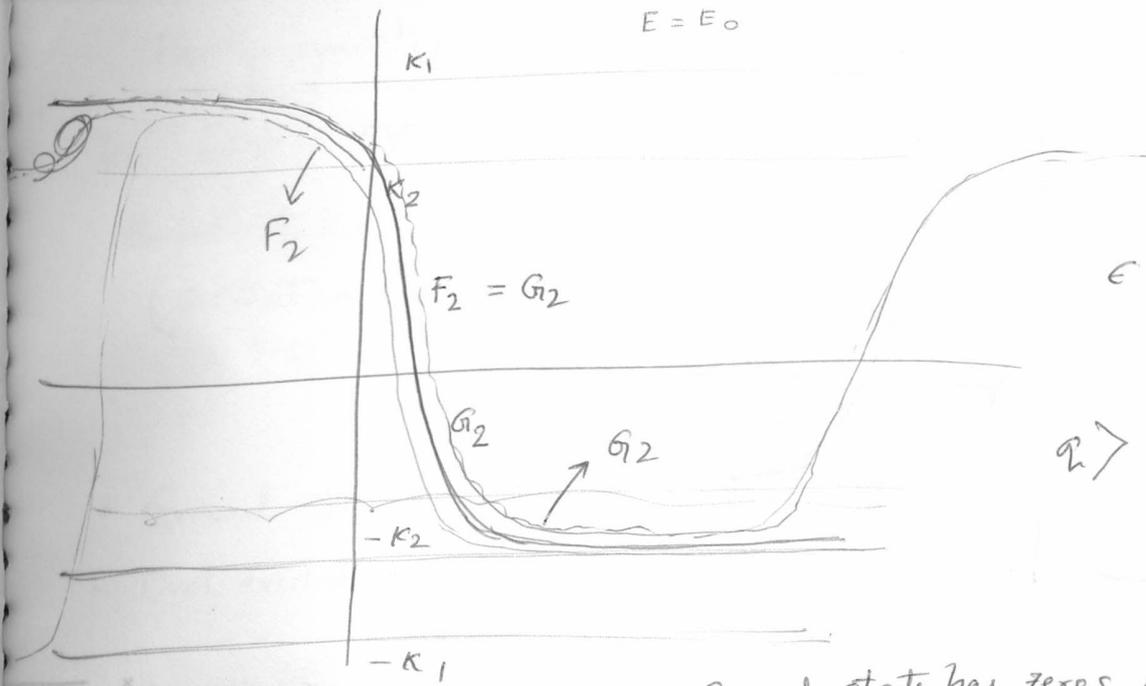
5. If  $E < V_0$ , then  $F_2(q) < 0$ ,  $G_2(q) > 0$

6.  $\left\{ \begin{array}{l} \frac{\partial}{\partial E} F_2(q, E) > 0 \\ \frac{\partial}{\partial E} G_2(q, E) < 0 \end{array} \right\}$



What happens if  $E = E_0$  ?

$E = E_0$

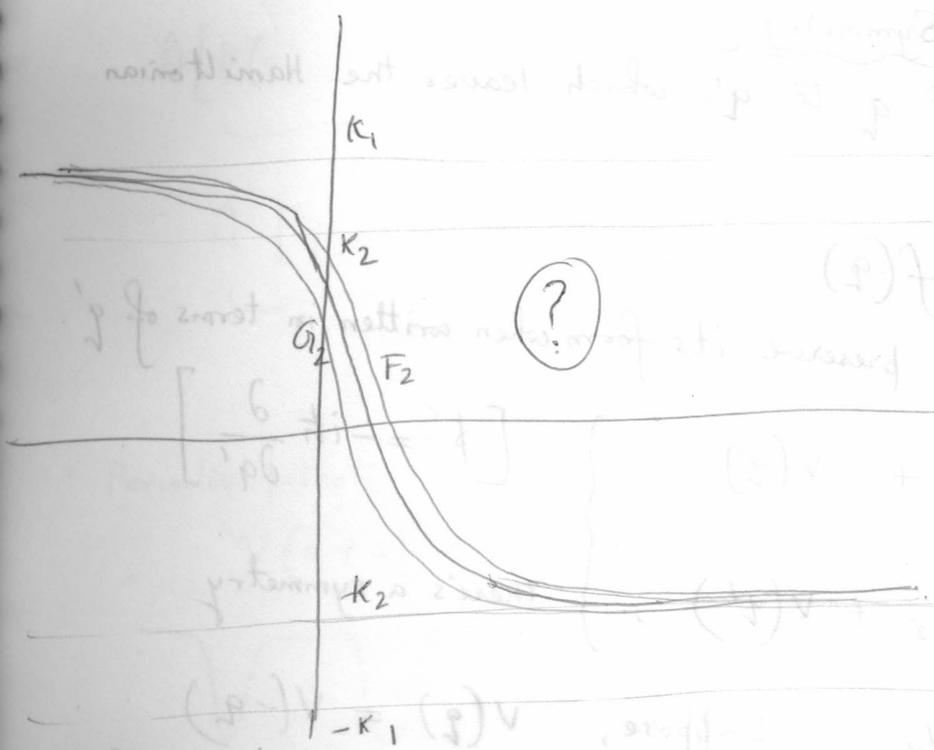


$$\epsilon e^{k_2 q} + e^{-k_2 q}$$

$$q > \frac{1}{2k_2} \ln\left(\frac{1}{\epsilon}\right)$$

→ Ground state has zeros only at  $\pm\infty$ .

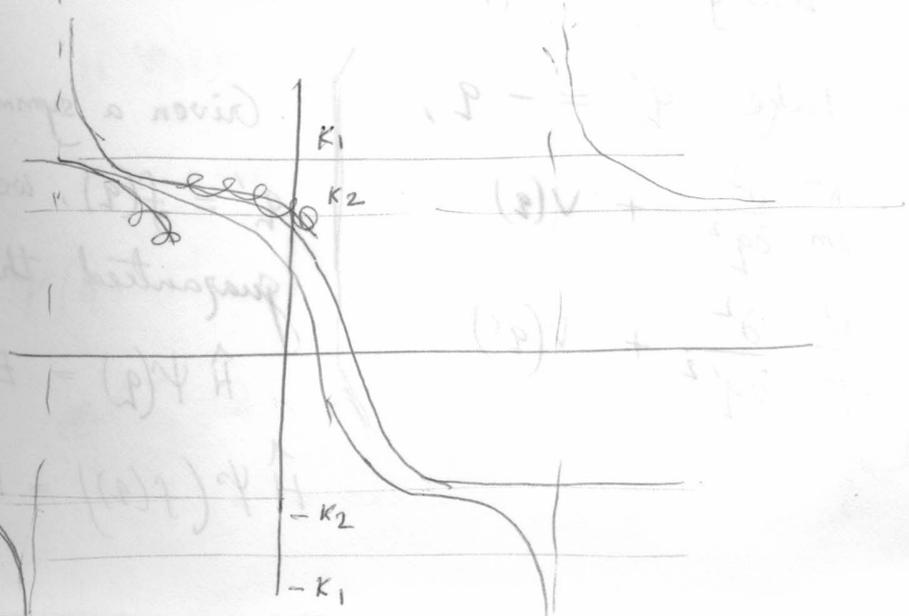
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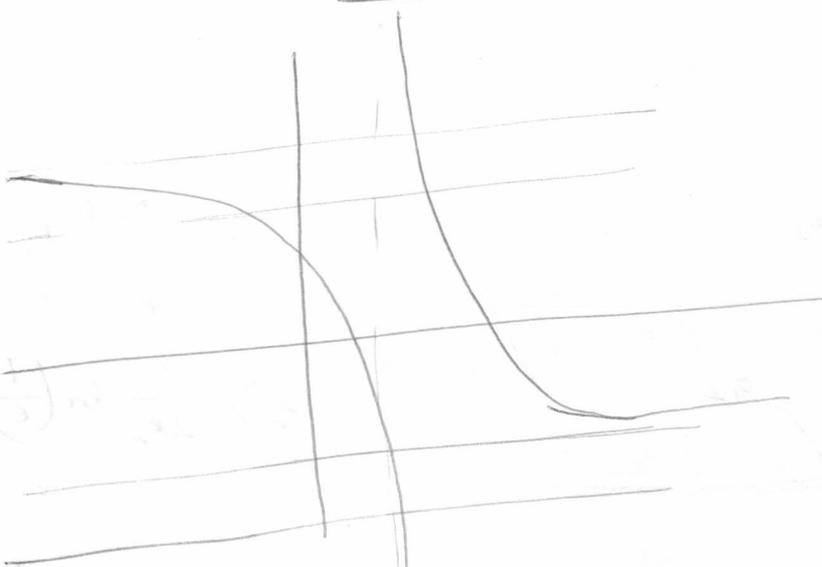
Transformation of  $\psi$  to  $\phi$  with  $\phi = \psi$  unchanged.

$\psi = \phi$

$$H = \frac{p^2}{2m} + V(x)$$



$$E = E_1$$



24.08.2011

Symmetry :-

→ Transformation of  $q$  to  $q'$  which leaves the Hamiltonian unchanged.

$$q' = f(q)$$

$\hat{H}$  should preserve its form when written in terms of  $q'$ .

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q)$$

$$\left[ p' = -i\hbar \frac{\partial}{\partial q'} \right]$$

If  $H' = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q'^2} + V(q')$ ,

there's a symmetry

Example: Parity. Suppose,  $V(q) = V(-q)$

If we take  $q' = -q$ ,

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q)$$

$$= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q'^2} + V(q')$$

Given a symmetry  $q' = f(q)$ , we are guaranteed that if  $\hat{H}\psi(q) = E\psi(q)$  then  $\hat{H}\psi(f(q)) = E\psi(f(q))$

## Parity symmetry

If  $\hat{H}\psi(q) = E\psi(q)$ , then  $\hat{H}\psi(-q) = E\psi(-q)$ .

Bound states :  $\psi(-q) = \lambda\psi(q)$  for some  $\lambda$   
(oscillation theorem)  $= \lambda^2\psi(-q)$

$\lambda = \pm 1$   $\rightarrow$  { eigenvalues of parity operator }

• Ground state  $\rightarrow$  even parity

• First excited "  $\rightarrow$  odd "

(no. of nodes)

$$\psi(q) \neq \lambda\psi(-q)$$

What if "scattering states" are there?

$$\hat{H}[\psi(q) + \psi(-q)] = E[\psi(q) + \psi(-q)]$$

even

• Not useful in scattering

$$\hat{H}[\psi(q) - \psi(-q)] = E[\psi(q) - \psi(-q)]$$

odd

## Another example

• Periodic potential

$$V(q+a) = V(q)$$



$$q' = q + a$$

$$\hat{H} = \left\{ \begin{array}{l} -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \\ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q'^2} + V(q') \end{array} \right\}$$

If  $\hat{H}\psi(q) = E\psi(q)$ , then

$$\hat{H}\psi(q+a) = E\psi(q+a)$$

$$\psi(q+a) = \lambda\psi(q) \quad (\text{one can choose})$$

$$\lambda = e^{i\alpha}$$

( $\alpha \rightarrow$  real)

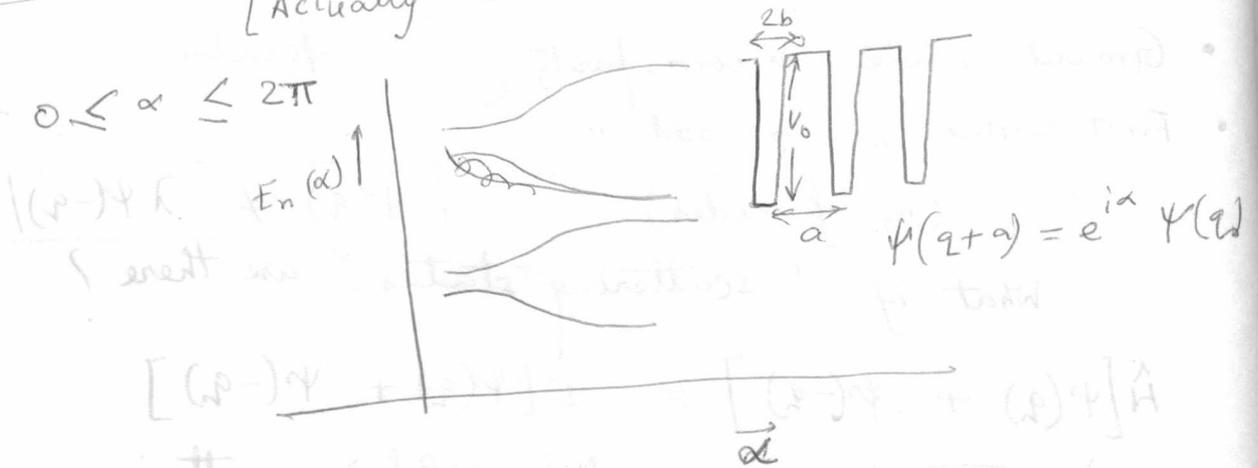
$|\lambda|$  must be 1.

(normalization)

$$\Psi(q) = e^{i\alpha q/a} \phi(q) \quad [\text{Defn of } \phi(q)]$$

$$\therefore \phi(q+a) = \phi(q)$$

• Solve SE in a period. Use  $\Psi(q+a) = \Psi(q)$ .  
 Fix one  $\alpha$  → Vary  $\alpha$  over a continuous range.  
 [Actually continuous spectrum]



Delta function pot.

$$V(q) = a \delta(q - q_0)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dq^2} + a \delta(q - q_0) \Psi = E \Psi$$

Away from  $q_0$ , we have free particle.

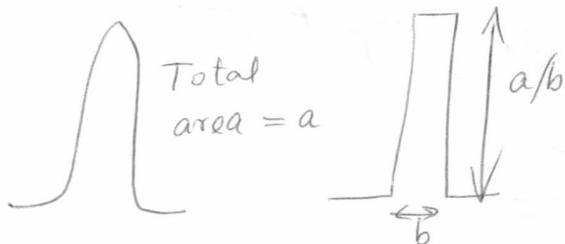
Near  $q_0$ , integrate the eq. from  $(q_0 - \epsilon)$  to  $(q_0 + \epsilon)$ .

$$-\frac{\hbar^2}{2m} \int_{q_0 - \epsilon}^{q_0 + \epsilon} \frac{d^2 \Psi}{dq^2} dq = a \int_{q_0 - \epsilon}^{q_0 + \epsilon} dq \delta(q - q_0) \Psi = E \int_{q_0 - \epsilon}^{q_0 + \epsilon} \Psi(q) dq$$

$$\Rightarrow \left( -\frac{\hbar^2}{2m} \left( \frac{d\Psi}{dq} \Big|_{q_0 + \epsilon} - \frac{d\Psi}{dq} \Big|_{q_0 - \epsilon} \right) + a \Psi(q_0) \right) = 0(\epsilon)$$

$$\frac{d\Psi}{dq} \Big|_{q_0 + \epsilon} - \frac{d\Psi}{dq} \Big|_{q_0 - \epsilon} = \frac{2ma}{\hbar^2} \Psi(q_0) \quad (\epsilon \rightarrow 0)$$

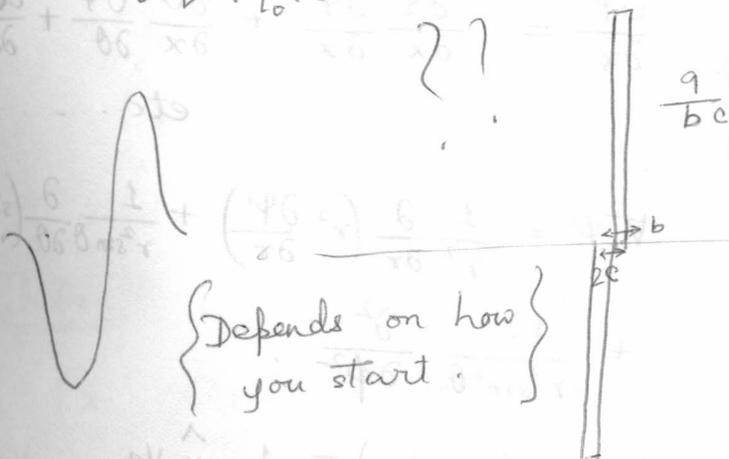
$$\Psi|_{q_0+\epsilon} = \Psi|_{q_0-\epsilon} \text{ for } \epsilon \rightarrow 0$$



$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dq^2} + a \delta'(q-q_0) \Psi = E\Psi$$

$$\Rightarrow -\frac{\hbar^2}{2m} \left\{ \frac{d\Psi}{dq} \Big|_{q_0+\epsilon} - \frac{d\Psi}{dq} \Big|_{q_0-\epsilon} \right\} - a \Psi'(q_0) = 0$$

$$\Rightarrow \frac{d\Psi}{dq} \Big|_{q_0+\epsilon} - \frac{d\Psi}{dq} \Big|_{q_0-\epsilon} = \frac{2m}{\hbar^2} a \left( -\frac{d\Psi}{dq} \right) \Big|_{q_0}$$



25.08.2011

$$\Psi \circ f_2(E) \text{ \& } f_2(E+\delta E)$$

$$\frac{d}{dq} \left( f_2(E) \frac{df_2(E+\delta E)}{dq} - f_2(E+\delta E) \frac{df_2(E)}{dq} \right) = \int_0^q$$

divide by  $f_2(E) f_2(E+\delta E) = F_2(E+\delta E) - F_2(E)$

### 3-dimensional systems

Three coordinates :  $x, y, z$

$\Rightarrow$  operators :  $\hat{x}, \hat{y}, \hat{z}$

$$\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{p}_y = \frac{\hbar}{i} \frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i} \frac{\partial}{\partial z}$$

$$H = \frac{\hat{p}^2}{2m} + V(x, y, z) \Rightarrow \text{Quantize}$$

$$\hat{H} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(\hat{x}, \hat{y}, \hat{z})$$

Energy eigenvalue equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(x, y, z) \psi = E \psi$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (\text{Laplacian operator})$$

→ Central potential  $V = V(r)$

Spherical polar coordinates

$$\begin{cases} x = r \sin \theta \cos \phi \\ y = r \sin \theta \sin \phi \\ z = r \cos \theta \end{cases}$$

$$\frac{\partial \psi}{\partial x} = \frac{\partial x}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\partial \theta}{\partial x} \frac{\partial \psi}{\partial \theta} + \frac{\partial \phi}{\partial x} \frac{\partial \psi}{\partial \phi}$$

etc. . . .

Using these, show that,

$$\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2}$$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) - \frac{1}{r^2} \hat{K} \psi$$

$$\hat{K} \psi = \left[ -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) - \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right]$$

operator

$$\hat{H} \psi = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{\hbar^2}{2m} \hat{K} \psi + V \psi$$

Now, we consider central potentials.  $[V = V(r)]$

$$\text{Then: } \hat{H} \hat{K} \psi = \hat{K} \hat{H} \psi$$

$$[\hat{H}, \hat{K}] = 0$$

Choose  $\psi$  to be an eigenstate of  $\hat{K}$ .

$(\hat{L}_x, \hat{L}_y, \hat{L}_z)$

$$\hat{K} \psi = \lambda \psi$$

$$\Rightarrow \hat{H} \psi = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \left[ \frac{\hbar^2 \lambda}{2m r^2} + V \right] \psi$$

$\Rightarrow$  One dimensional problem (effectively)

$[r \rightarrow 0 \text{ to } \infty]$

We want to find eigenfunctions and eigenvalues of  $\hat{K}$ .

Definitions: Angular momentum operators

$$\vec{L} = \vec{r} \times \vec{p} \quad (\text{classically})$$

$$L_x = y p_z - z p_y, \dots$$

$$\hat{L}_z = x \hat{p}_y - y \hat{p}_x$$

$$\hat{L}_x \psi = -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \psi$$

$$\hat{L}_z \psi = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \psi$$

$$\hat{L}_x = y \hat{p}_z - z \hat{p}_y$$

$$\hat{L}_y = -(x \hat{p}_z - z \hat{p}_x)$$

Define  $\hat{L}^2 \psi = (\hat{L}_x \hat{L}_x \psi + \hat{L}_y \hat{L}_y \psi + \hat{L}_z \hat{L}_z \psi)$

Ex: Check the following

$$\left\{ \begin{array}{ll} [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z & [\hat{L}_x, \hat{L}^2] = 0 \\ [\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x & [\hat{L}_y, \hat{L}^2] = 0 \\ [\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y & [\hat{L}_z, \hat{L}^2] = 0 \end{array} \right.$$

Define  $\left\{ \begin{array}{l} L_+ = L_x + iL_y \\ L_- = L_x - iL_y \end{array} \right\} \left\{ \begin{array}{l} [L_+, L_-] = 2\hbar L_z \\ [L_z, L_+] = \hbar L_+ \\ [L_z, L_-] = -\hbar L_- \end{array} \right.$  Check

Ex Check that

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}, \quad L_- = e^{-i\phi} \left( -\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$$

$$\hat{L}_+ = e^{i\phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$$

$$\hat{L}^2 \psi = \left\{ \frac{1}{2} (\hat{L}_+ \hat{L}_- + \hat{L}_- \hat{L}_+) + \hat{L}_z \hat{L}_z \right\} \psi$$

$$= -\hbar^2 \left[ \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) \right]$$

[Use the above formulae]

$$\hat{L}^2 \psi = \lambda \hbar^2 \psi \quad \hat{K} \psi = \lambda \psi$$

$$\hat{L}^2 \psi = \lambda \hbar^2 \psi$$

Use  $[\hat{L}^2, \hat{L}_x] = 0$ ,  $[\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z]$

$$\Rightarrow [\hat{L}^2, L_+] = 0, [\hat{L}^2, L_-] = 0$$

Choose them to be eigenstates of  $\hat{L}_z$  with eigenvalue  $m\hbar$ . ( $m = \text{real number}$ )

Call this eigenstate  $\psi_{\lambda, m}$ . This satisfies

$$\hat{L}_z \psi_{\lambda, m} = m\hbar \psi_{\lambda, m}$$

$$\hat{L}^2 \psi_{\lambda, m} = \lambda \hbar^2 \psi_{\lambda, m}$$

$$\hat{L}_z \hat{L}_+ \psi_{\lambda, m} = \left\{ [\hat{L}_z, \hat{L}_+] + L_+ L_z \right\} \psi_{\lambda, m}$$

$$= \hbar \hat{L}_+ \psi_{\lambda, m} + m\hbar \hat{L}_+ \psi_{\lambda, m}$$

$$= (m+1)\hbar \hat{L}_+ \psi_{\lambda, m}$$

$\left\{ \begin{array}{l} L_+ \rightarrow \text{raising operator} \\ L_- \rightarrow \text{lowering operator} \end{array} \right\}$

$$\hat{L}^2 \hat{L}_+ \psi_{\lambda, m} = \left\{ [\hat{L}^2, \hat{L}_+] + \hat{L}_+ \hat{L}^2 \right\} \psi_{\lambda, m}$$

$$= \lambda \hbar^2 \hat{L}_+ \psi_{\lambda, m}$$

$$\langle L_+ \Psi_{\lambda, m} | L_+ \Psi_{\lambda, m} \rangle = \langle \Psi_{\lambda, m} | (L_+)^{\dagger} L_+ \Psi_{\lambda, m} \rangle$$

$$\left\{ \begin{aligned} L_- L_+ - L_+ L_- &= -2\hbar L_z \\ L_- L_+ + L_+ L_- &= 2(\hat{L}^2 - \hat{L}_z^2) \end{aligned} \right.$$

$$\therefore L_- L_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar L_z$$

$$= \langle \Psi_{\lambda, m} | L_- L_+ \Psi_{\lambda, m} \rangle$$

$$= \hbar^2 (\lambda - m^2 - m) \langle \Psi_{\lambda, m} | \Psi_{\lambda, m} \rangle \quad (2)$$

If  $\lambda = m(m+1)$ , then  $L_+ \Psi_{\lambda, m} = 0$  possible

If  $\lambda > m(m+1)$ , then  $L_+ \Psi_{\lambda, m} \neq 0$  (1)

$$\Psi_{\lambda, m+1} = \frac{1}{\hbar \sqrt{\lambda - m^2 - m}} L_+ \Psi_{\lambda, m} \quad (2)$$

If  $\lambda < m(m+1)$ : not possible (non-normalizable solutions) normalized

If  $\lambda > m(m+1)$ , we can construct a new eigenstate of  $(\hat{L}^2, \hat{L}_z)$  of ev.  $(\lambda \hbar^2, (m+1)\hbar)$ .

$$L_+ \Psi_{\lambda, m+1} = 0 \text{ if } \lambda = (m+1)(m+2)$$

$$\neq 0 \text{ if } \lambda > (m+1)(m+2)$$

$\Rightarrow$  define  $\Psi_{\lambda, m+2}$   
(not possible if  $\lambda < (m+1)(m+2)$ .)

Step 1.  $\lambda \geq m(m+1)$

Step 2.  $\lambda \geq (m+1)(m+2)$

$\lambda \geq (m+2)(m+3)$

$$(m+p) \Rightarrow \lambda \begin{matrix} \text{must be} \\ \text{for integer } p > 0 \end{matrix} (m+p)(m+p+1)$$

$\lambda = (m+p)(m+p+1)$  for some non-negative integer

$$l = m+p \rightarrow \text{definition of } l.$$

Repeat this with  $L_-$

$L_- \Psi_{\lambda, m} \Rightarrow$  (1) Exercise show that this has  $(L^2, L_z)$  e.v.  $(\lambda \hbar^2, (m-1)\hbar)$

$$(2) (L_- \Psi_{\lambda, m}, L_- \Psi_{\lambda, m}) = \hbar^2 (\lambda - m(m-1))$$

Possibilities

$$(1) \lambda = m(m-1) \Rightarrow L_- \Psi_{\lambda, m} = 0$$

$$(2) \lambda < m(m-1) \Rightarrow \text{not possible}$$

$$(3) \lambda > m(m-1) \Rightarrow \Psi_{\lambda, m-1} = \frac{1}{\hbar \sqrt{\lambda - m(m-1)}} L_- \Psi_{\lambda, m}$$

Keep repeating with  $\Psi_{\lambda, m-1}, \Psi_{\lambda, m-2}, \dots$

After  $q^{\text{th}}$  step, we'll get  $\lambda \geq (m-q)(m-q+1)$

At some value of  $q$ ,

$$\lambda = (q-m)(q-m-1) = l(l+1)$$

Quadratic in  $q$

Solutions

$$q-m = l+1, -l = m+p+1, -m-p$$

$$q > 0, p > 0$$

$$\therefore q-m = m+p+1$$

$$\text{or, } q = 2m+p+1$$

$$\text{or, } 2m = q-p-1$$

$$2l - 2p = q - p - 1$$

$$p \geq 0, q \geq 1$$

integer p

$$\text{or, } 2l = p + q - 1 = \text{integer} \geq 0$$

$l = \text{non-negative}$  (either integer or  $(\text{integer} + \frac{1}{2})$ )

$l - m \rightarrow \text{integer (non-negative)}$

$\therefore m$  is integral.

$$m : l, l-1, l-2, \dots, -l$$

### LIMIT OF ALGEBRA

$$L_z \psi_{\lambda, m} = m\hbar \psi_{\lambda, m}$$

$$-i\hbar \frac{\partial}{\partial \phi} \psi_{\lambda, m} = m\hbar \psi_{\lambda, m}$$

$$\psi = \boxed{e^{-im\phi} f(r, \theta)}$$

$m \rightarrow \text{integer}$

$l \rightarrow \text{also an integer}$

$$F_2 = \frac{1}{f_2} \frac{\partial f_2}{\partial q}^2$$

$$\frac{\partial F_2}{\partial q} = \frac{1}{f_2} \frac{\partial^2 f_2}{\partial q^2} - \frac{1}{f_2^2} \frac{\partial f_2}{\partial q}^2$$

$L_z \psi_{\lambda, m}$

26.08.2011 Tutorial :- (Prof. A. Sen)

$$\frac{\partial}{\partial q} \left[ f_2(E) \frac{\partial f_2}{\partial q}(E+\delta E) - f_2(E+\delta E) \frac{\partial f_2}{\partial q}(E) \right]$$

$$= f_2(E) \frac{\partial^2 f_2}{\partial q^2}(E+\delta E) - f_2(E+\delta E) \frac{\partial^2 f_2}{\partial q^2}(E)$$

$$= -\frac{2m}{\hbar^2} (\delta E) f_2(E) f_2(E+\delta E) \quad (\text{By Schrödinger eq}^n)$$

$$\text{or, } \frac{1}{f_2(E+\delta E)} \frac{\partial^2 f_2(E+\delta E)}{\partial q^2} - \frac{1}{f_2(E)} \frac{\partial^2 f_2(E)}{\partial q^2} = -\frac{2m}{\hbar^2} (\delta E)$$

$$F_2 = \frac{1}{f_2} \frac{\partial f_2}{\partial q}^2 \quad \frac{\partial F_2}{\partial q} = \frac{1}{f_2} \frac{\partial^2 f_2}{\partial q^2} - \left( \frac{1}{f_2} \frac{\partial f_2}{\partial q} \right)^2$$

$$\therefore \frac{\partial}{\partial q} [F_2(E+\delta E) - F_2(E)] + F_2^2(E+\delta E) - F_2^2(E) = -\frac{2m}{\hbar^2} \delta E$$

$$\Rightarrow \frac{\partial}{\partial q} [F_2(E+\delta E) - F_2(E)] + \frac{\partial F_2^2(E)}{\partial q} \delta E = -\frac{2m}{\hbar^2} \delta E$$

$$\Rightarrow \frac{\partial}{\partial q} \frac{[F_2(E+\delta E) - F_2(E)]}{\delta E} = -\left[ \frac{2m}{\hbar^2} + 2F_2(E) \frac{\partial F_2(E)}{\partial E} \right] \delta E$$

Taking limit  $\delta E \rightarrow 0$ , we have

$$\frac{\partial F_2(E)}{\partial E} = -2 \int_{-\infty}^{\infty} \left[ \frac{m}{\hbar^2} + F_2(E) \frac{\partial F_2(E)}{\partial E} \right] dq' + P(E)$$

OR

$$f_2(E) \left[ -\frac{2m}{\hbar^2} (V(q) - E) f_2(E+\delta E) \right] - f_2(E+\delta E) \left[ \frac{2m}{\hbar^2} (V(q) - E) f_2(E) \right] = -\frac{2m}{\hbar^2} \delta E f_2(E) f_2(E+\delta E)$$

$$f_2(E) \frac{\partial f_2(E+\delta E)}{\partial q} - f_2(E+\delta E) \frac{\partial f_2(E)}{\partial q} = -\int_{-\infty}^{\infty} \frac{2m}{\hbar^2} \delta E f(E) f(E+\delta E) dq'$$

$$f_2 = e^{-\kappa_2 q}$$

$$\Rightarrow F_2(E+\delta E) - F_2(E) = -\frac{\delta E}{f_2(E) f_2(E+\delta E)} \int_{-\infty}^{\infty} \frac{2m}{\hbar^2} f_2^2(E) dq'$$

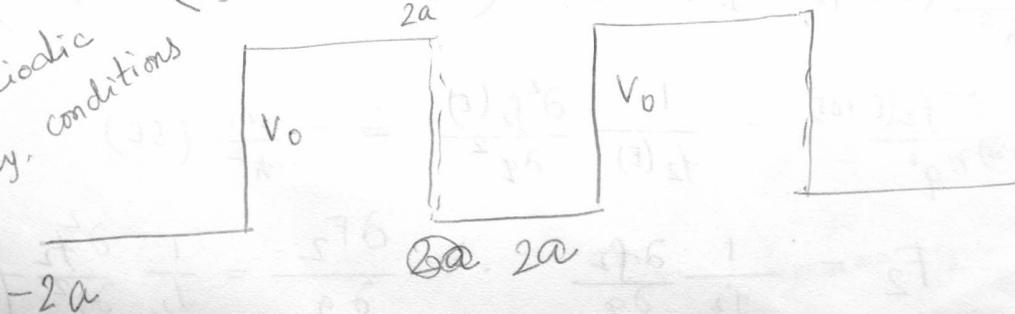
$$\Rightarrow \frac{\partial F_2}{\partial E} = -\frac{1}{f_2^2(E)} \frac{2m}{\hbar^2} \int_{-\infty}^{\infty} f_2^2(E) dq'$$

( $\delta E \rightarrow 0$ )

$$= \frac{1}{f_2^2(E)} \frac{2m}{\hbar^2} \int_{-a}^a f_2^2(E) dq'$$

( $f_2$  is real here)

Periodic  
bdy. conditions



$V = 0$  for  $-2a$  to  $0$ ,  $2a$  to  $4a$ ,  $6a$  to  $8a$ ,  
 $= V_0$  "  $0$  to  $2a$ ,  $4a$  to  $6a$ ,

$$\psi(x+a) = e^{i\alpha} \psi(x)$$

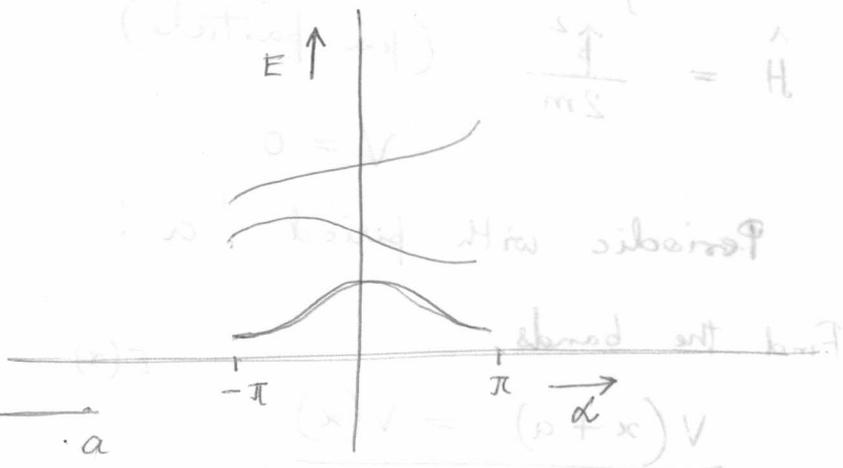
$\psi(x)$  &  $\psi(x+a)$  are <sup>both</sup> energy eigenfunctions

$$\boxed{\psi(x+a) = \lambda \psi(x)}$$

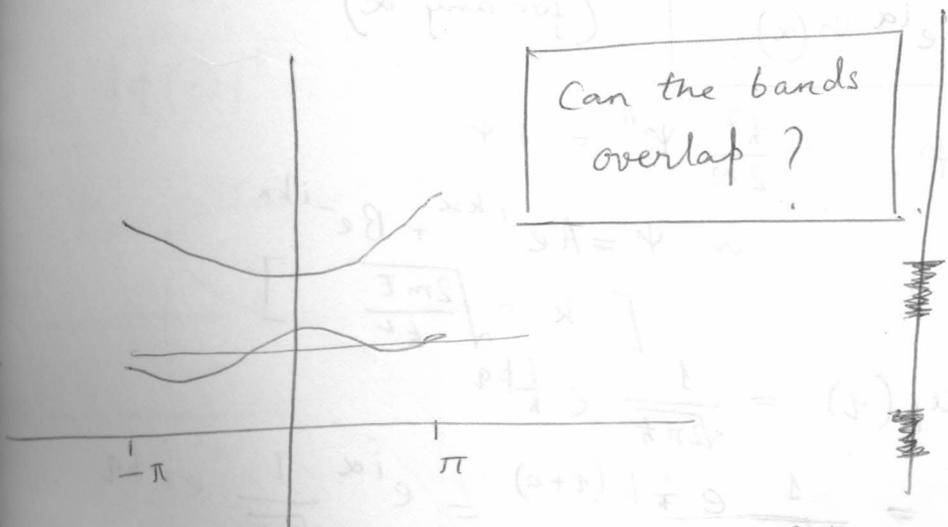
If not, try linear combinations

$$e^{-2i\beta} \psi(x-2a) + e^{-i\beta} \psi(x-a) + \dots + e^{i\beta} \psi(x+a) + \dots$$

For some  $\beta$ , these combinations may be zero.



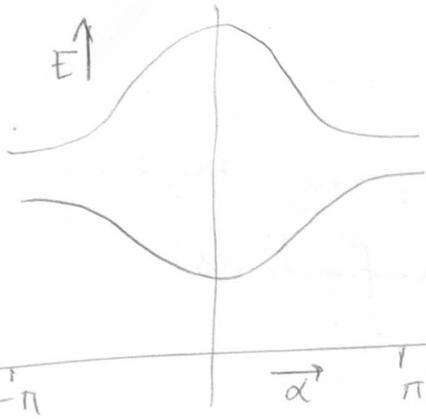
Can the bands overlap?



We can't have more than two solutions for any  $\alpha$ .

Can't cut more than twice.

$\psi \rightarrow \psi^*$  ✓  $E(\alpha)$  is always a symmetric fn of  $\alpha$



$$\psi(x+a) = e^{i\alpha} \psi(x)$$

$$\left\{ \begin{array}{l} H\psi = E\psi \\ H\psi^* = E\psi^* \end{array} \right.$$

For every  $E$ , we have two solutions.

- Therefore, the bands can't overlap.
- They can touch at  $\alpha = 0, \pm\pi$

Take  $\hat{H} = \frac{\hat{p}^2}{2m}$  (free particle)  
 $V = 0$ .

Periodic with period 'a'.

Find the bands.

$E(\alpha)$ .

$$V(x+a) = V(x)$$

$$\psi(x+a) = e^{i\alpha} \psi(x) \quad (\text{for any } \alpha)$$

$$\frac{\hat{p}^2}{2m} \psi = E\psi \quad - \quad \frac{\hbar^2}{2m} \psi'' = E\psi$$

or,  $\psi = A e^{ikx} + B e^{-ikx}$

$$\psi = \frac{2mE}{\hbar^2} \psi \quad \left[ k = \sqrt{\frac{2mE}{\hbar^2}} \right]$$

$$u_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p q}$$

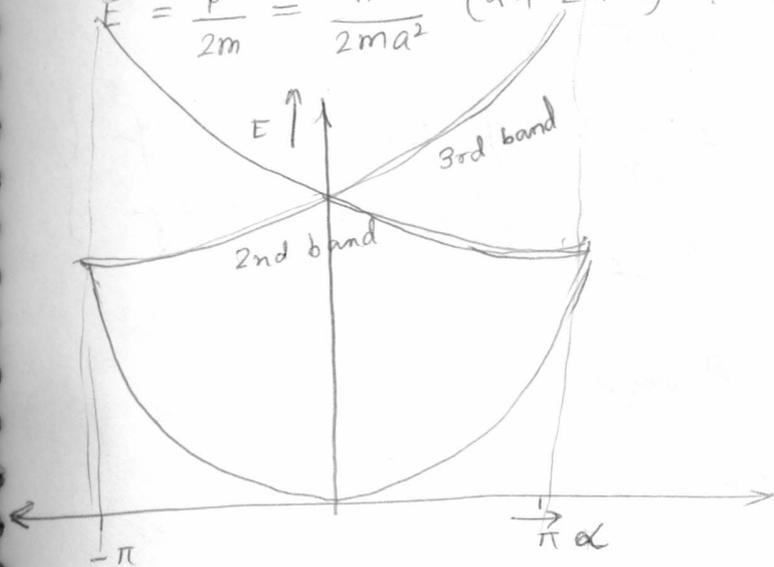
$$u_p(q+a) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p (q+a)} = e^{i\alpha} \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p q}$$

$$\alpha = \frac{p a}{\hbar}$$

$$p = \frac{\hbar \alpha}{a} + \frac{(2m\pi)\hbar}{a}$$

$$E = \left( \frac{\hbar^2 \alpha^2}{a^2} + \frac{4m^2 \pi^2 \hbar^2}{a^2} + \frac{4m\pi \hbar^2 \alpha}{a^2} \right)$$

$$E = \frac{p^2}{2m} = \frac{\hbar^2}{2ma^2} (\alpha + 2n\pi)^2 \quad (n = \text{integer})$$



1st problem

$$\psi_0 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

First measure position.

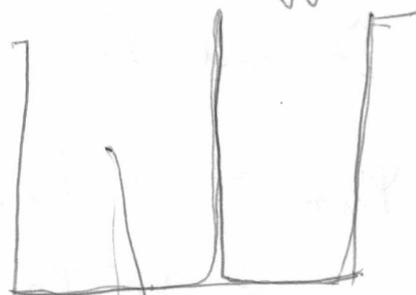
Next, " energy.

Calculate probability that the particle is within first measurement gives the result between  $L/4$  to  $L/2$  and second one gives the ground state energy.

$$P_1 = |\psi_0|^2 dq$$

$$|\phi(q)|^2 = \delta(q - q_0)$$

$\psi_0$  collapses to  $\phi_0$



$E \geq E_0$

