LECTURE

RETURN TO OUR BASIC CONSERVATION EQN.

$$\boxed{\frac{d}{dt}\langle\psi|Q|\psi\rangle = \frac{i}{\hbar}\langle\psi|[H,Q]|\psi\rangle}$$

SO FAR STUDIED CONSEQUENCES FOR SIMPLEST CASE $Q = 1$

- NOW EXPLORE MORE GENERALLY

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

i) TOTAL ENERGY IS CONSERVED BECAUSE

$$[H,H] = HH - HH = 0$$

SO $\frac{d}{dt}\langle\psi|H|\psi\rangle = 0$ FOR ALL $|\psi\rangle$

ii) NOW CONSIDER MOM'M p

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

$$= [\frac{p^2}{2m}, p] + [V(x), p]$$

$$= \frac{1}{2m}\underbrace{(p^2p - pp^2)}_{0} + [V(x), p]$$

$$= [V(x), p]$$

BUT $[V(x), p] = [V(x), -i\hbar\, \partial/\partial x]$

TO WORK THIS OUT PUT ARBITRARY FN ON RHS

$$[V(x), p] f(x) = \left\{ V(x)\left(-i\hbar \frac{\partial}{\partial x}\right) + i\hbar \frac{\partial}{\partial x} V(x) \right\} f(x)$$

$$= -i\hbar V(x) \frac{\partial f}{\partial x} + i\hbar \frac{\partial V}{\partial x} f + i\hbar V \frac{\partial f}{\partial x}$$

$$= i\hbar \frac{\partial V}{\partial x} . f$$

$$\Rightarrow \quad [V(x), p] = i\hbar \frac{\partial V}{\partial x} \qquad \underline{\text{NOT ZERO}}$$

THEREFORE

$$[H, p] = i\hbar \frac{\partial V}{\partial x} \qquad \text{AND}$$

$$\boxed{\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} \right\rangle} \qquad (*)$$

NOTE SIMILARITY OF (*) TO CLASSICAL EQN OF MOTION

(*) SHOWS THAT $d\langle p\rangle/dt$ CANNOT BE ZERO UNLESS $\partial V/\partial x = 0$. BUT $\partial V/\partial x = 0$ SAYS $V = $ CONST, AND FIND LINEAR MOM'M

CONSERVATION ONLY WHEN H INDEP'T OF POSITION (SYSTEM INDEP'T OF POSITION)

iii) NOW TAKE $Q = x$

$$[H, x] = \left[\frac{p^2}{2m} + V, x\right]$$

$$= \left[\frac{p^2}{2m}, x\right] + \underbrace{[V(x), x]}_{\substack{V(x)x - xV(x) \\ = 0}}$$

USEFUL TO HAVE EXPRESSION FOR $[A^2, B]$

$$[A^2, B] = A^2 B - BA^2$$

$$= AAB - \underbrace{(ABA - ABA)}_{0} - BAA$$

$$= A(AB - BA) + (AB - BA)A$$

$$= A[A, B] + [A, B]A$$

APPLYING THIS

$$[H, x] = \frac{1}{2m}\left\{p[p, x] + [p, x]p\right\}$$

NOW CALCULATE $[p, x]$ BY ACTING ON ARBITRARY $f(x)$

$$[p,x]f(x) = \left(-i\hbar\frac{\partial}{\partial x}\,x + x\,i\hbar\frac{\partial}{\partial x}\right)f$$

$$= -i\hbar\left\{\frac{\partial x}{\partial x}f + \cancel{x\frac{\partial f}{\partial x}} - \cancel{x\frac{\partial f}{\partial x}}\right\}$$

$$= -i\hbar f(x)$$

$$\boxed{[p,x] = -i\hbar}$$

FUNDAMENTAL PROPERTY OF X AND p OPS.

HENCE

$$[H,x] = \frac{1}{2m}\left\{p(-i\hbar) + (-i\hbar)p\right\}$$

$$= -i\hbar\frac{p}{m}$$

THUS

$$\boxed{\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}} \quad (\dagger)$$

AND POSITION IS NOT CONSERVED UNLESS IN SPECIAL STATE WITH $\langle p\rangle = 0$

NOTE: $(\dagger)$ IS QM ANALOGUE TO CLASSICAL

$$\dot{x} = p/m$$

FROM $(*)$ AND $(\dagger)$ SEE THAT CLASSICAL EQNS OF MOTION ARE OBEYED <u>ON THE AVERAGE</u> IN QM (EHRENFEST THM.)

MORE ON COMMUTATORS

- HAVE SEEN HOW $[H, Q] = 0$ IMPLIES $\frac{d\langle Q\rangle}{dt} = 0$ IN Q.M.

- SO FAR HAVE ALWAYS BEEN WORKING WITH EXPECTATION VALUES (AVERAGES).

- DOES $[H, Q] = 0$ HAVE SPECIAL CONSEQUENCES FOR INDIVIDUAL MEASUREMENTS

YES...

- WE KNOW E'STATES OF H SATISFY

$$H \phi_n = E_n \phi_n$$

REMEMBER THIS MEANS THAT IF

$$\psi(x,t) = \underbrace{e^{-iE_n t/\hbar} \phi_n(x)}_{\text{NOT A SUPERPOSITION}}$$

THEN WHEN WE MEASURE ENERGY WE WILL GET E_n (WITH PROB. $= 1$)

- NOW SUPPOSE THE SAME FUNCTIONS ϕ_n ARE ALSO E'STATES OF ANOTHER OP. Q

$$Q \phi_n = q_n \phi_n$$

THIS MEANS THAT IF PARTICLE DESCRIBED BY ϕ_n THEN IT ALSO HAS A DEFINITE VALUE OF Q GIVEN BY q_n

$$\text{PROB}(Q = q_n) = 1$$

- WHAT IS CONDITION THAT THIS IS POSSIBLE?

ACT ON $H\phi_n = E_n \phi_n$ WITH Q

$$QH\phi_n = E_n Q \phi_n = E_n q_n \phi_n$$

ALTERNATIVELY ACT ON $Q\phi_n = q_n \phi_n$ WITH H

$$HQ\phi_n = q_n H \phi_n = q_n E_n \phi_n$$ SAME

SUBTRACTING ABOVE EQNS

$$(HQ - QH)\phi_n = 0$$

SINCE, BY ASSUMPTION, TRUE FOR ALL ϕ_n

$$\Rightarrow \boxed{[H, Q] = 0}$$

THUS:

> IF $[H,Q]=0$ IT IS POSSIBLE FOR PARTICLE TO BE IN STATE OF DEFINITE ENERGY (A 'STATIONARY STATE') IN WHICH THE VALUE OF Q IS ALSO DEFINITE.

- WHAT HAPPENS IF $\psi(x,t)$ IS <u>NOT</u> AN E-EIGEN STATE?

EG. SUPERPOSITION OF 2 E'STATES

$$\psi(x,t) = a_1 \phi_1(x) e^{-iE_1 t/\hbar} + a_2 \phi_2(x) e^{-iE_2 t/\hbar}$$

WITH $1 = |a_1|^2 + |a_2|^2$

SO $\text{PROB}(E=E_1) = |a_1|^2$

$\text{PROB}(E=E_2) = |a_2|^2$

- LET'S COMPUTE $\langle Q \rangle$

$$\langle Q \rangle = \int \psi^* Q \psi \, dx$$

$$= \int \left(a_1^* \phi_1 e^{iE_1 t/\hbar} + a_2^* \phi_2 e^{iE_2 t/\hbar}\right) \left(a_1 q_1 \phi_1 e^{-iE_1 t/\hbar} + a_2 q_2 \phi_2 e^{-iE_2 t/\hbar}\right)$$

$$\underline{= q_1 |a_1|^2 + q_2 |a_2|^2}$$

THIS IS JUST

$$\langle Q \rangle = q_1 \times (\text{PROB IN STATE 1}) + q_2 \times (\text{PROB STATE 2})$$

SO IF WE <u>MAKE A MEASUREMENT OF BOTH H AND Q</u> WE FIND

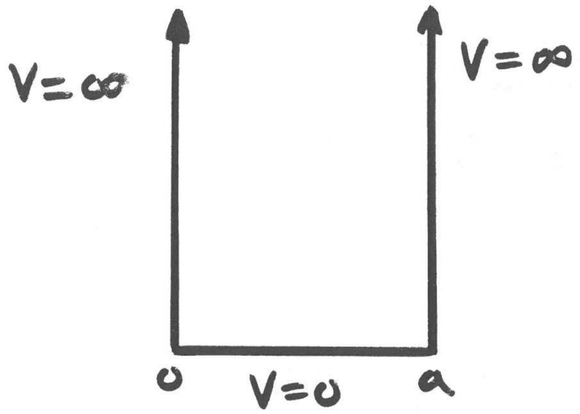
$$\boxed{\begin{array}{l} (E_1, q_1) \text{ WITH PROB} = |a_1|^2 \\ (E_2, q_2) \text{ WITH PROB} = |a_2|^2 \end{array}}$$

FUNDAMENTAL POINT IS

IF $[H, Q] = 0$ THEN CAN MEASURE BOTH QUANTITIES AND SIMULTANEOUSLY FIND PRECISE VALUES OF BOTH H AND Q

- WHAT HAPPENS IF $[H, Q] \neq 0$?

IN FACT ALREADY STUDIED THIS WHEN LOOKED AT $Q = p$ IN CASE OF INFINITE SQUARE WELL...



$$[H,p] = i\hbar \frac{\partial V}{\partial x} \neq 0$$

SINCE AT $x=0$ $\frac{\partial V}{\partial x} \to -\infty$

AND AT $x=a$ $\frac{\partial V}{\partial x} \to \infty$

IN THIS CASE WE SAW THAT

<u>IF</u> PARTICLE HAS <u>DEFINITE ENERGY</u>

$\psi(x,t) = e^{-iE_n t/\hbar} \phi_n(x)$ <u>THEN</u>

> ψ IS A SUPERPOSITION OF STATES WITH <u>DIFFERENT</u> <u>MOMENTA</u>

EQUIV:

> WE CANNOT KNOW BOTH E AND p FOR SURE SINCE $[H,p] \neq 0$

GENERAL RESULT IN QM

*

> IF A AND B ARE PHYSICAL (HERMITIAN) OPS. WITH $[A,B] \neq 0$ THEN CANNOT IN GENERAL SIMULTANEOUSLY KNOW VALUES OF A AND B

COMPLETE SETS OF QUANTUM NUMBERS

SUPPOSE WE HAVE TWO OPS. Q_1, Q_2

SATISFYING

$$\underline{[H, Q_1] = 0} \quad \text{AND} \quad \underline{[H, Q_2] = 0}$$

THEN

$$\frac{d\langle Q_1\rangle}{dt} = 0 \quad \text{AND} \quad \frac{d\langle Q_2\rangle}{dt} = 0$$

AND BOTH OBSERVABLES ARE CONSERVED

- **HOWEVER** IF $[Q_1, Q_2] \neq 0$ THEN WILL NOT BE ABLE TO MAKE DEFINITE MEASUREMENTS OF BOTH

- ON OTHER HAND IF $\underline{[Q_1, Q_2] = 0}$ THEN ALWAYS POSSIBLE TO FIND SIMULTANEOUS E'STATES OF Q_1 AND Q_2 AND H

$$\psi(x,t) = e^{-iE_n t/\hbar}\phi_n(x)$$

WHICH HAS

$$\left.\begin{array}{lll} \text{DEFINITE} & \text{ENERGY} & E_n \\ \text{''} & Q_1 & q_1 \\ \text{''} & Q_2 & q_2 \end{array}\right\} \text{THE 'QUANTUM NUMBERS' OF STATE } \psi$$

- IN CASE $[Q_1, Q_2] = 0$ Q_1 AND Q_2 ARE '<u>COMPATIBLE</u>'
- IN CASE $[Q_1, Q_2] \neq 0$

  Q_1 AND Q_2 ARE '<u>INCOMPATIBLE</u>'

  AND IT IS <u>POSSIBLE</u> FOR US TO HAVE STATE

  $$\psi(x,t) = e^{-iEt/\hbar}\phi(x)$$

  WITH <u>EITHER</u>

  $$\begin{cases} \text{DEFINITE ENERGY } E \\ \quad '' \quad\quad Q_1 \quad q_1 \end{cases}$$

  <u>OR</u>

  $$\begin{cases} \text{DEFINITE ENERGY } E \\ \quad '' \quad\quad Q_2 \quad q_2 \end{cases}$$

  <u>BUT NOT BOTH</u>

- <u>EG.</u> SINCE $[p, x] = -i\hbar$ WE CAN <u>NEVER HAVE A STATE IN WHICH BOTH p AND x HAVE DEFINITE VALUES</u>

- WE SAY THAT $E, \ldots$ FORM A <u>COMPLETE SET OF QUANTUM NUMBERS</u> IF <u>MAXIMAL</u> NUMBER OF SIMULTANEOUS E'VALUES ARE SPECIFIED

THE UNCERTAINTY PRINCIPLE

- PREVIOUSLY LOOKED AT STATES WHICH ARE EIGENFUNCTIONS OF MORE THAN ONE OBSERVABLE.

  THESE ARE RATHER SPECIAL STATES...

  ALSO WANT TO KNOW WHAT HAPPENS WHEN WE MAKE MEASUREMENTS ON SOME GENERAL SUPERPOSITION

- CONSIDER, EG, ENERGY SUPERPOSITION

$$\psi(x,t) = a_1 \phi_1 e^{-iE_1 t/\hbar} + a_2 \phi_2 e^{-iE_2 t/\hbar}$$

SUPPOSE MEASUREMENT OF ENERGY AT $t = t_0$ GIVES RESULT E_1

$\rightarrow$ MEANS WE NOW KNOW FOR SURE THAT ENERGY IS E_1

BUT THIS IMPLIES THAT NOW (IE. FOR $t \geqslant t_0$) SYSTEM MUST BE IN ENERGY E'STATE

$$\psi(x, t > t_0) = \phi_1 e^{-iE_1 t/\hbar}$$

THUS

> ① THE PART OF THE ORIGINAL ψ WHICH HAS A DIFFERENT ENERGY TO THE ONE MEASURED <u>DISAPPEARS</u>
>
> ② THE REMAINING PART HAS IT'S <u>COEFF CHANGED</u> SO THAT THE NEW WAVEF'N IS CORRECTLY NORMALIZED

- THIS PROCEDURE IS THE SO-CALLED '<u>COLLAPSE OF THE WAVEFUNCTION</u>'
- IT APPLIES WHEN <u>ANY</u> QUANTITY (NOT JUST ENERGY) <u>IS MEASURED</u>
- 'COLLAPSE OF THE WAVEFUNCTION' (ALSO KNOWN AS THE 'PROJECTION POSTULATE' OF QM) <u>APPEARS TO BE A DISTINCT TYPE OF TIME EVOLUTION FROM THE TDSE</u>
    - THE COPENHAGEN INTERPRETATION OF BOHR ETAL ACCEPTS THIS
    - OTHERS HAVE TRIED TO DERIVE 'COLLAPSE' FROM TDSE FOR LARGE OBJECTS (EG. YOU)

ACTING AS MEASURING DEVICE INTERACTING WITH SYSTEM

- FINALLY THERE ARE RADICAL PROPOSALS SUCH AS 'MANY WORLDS' WHICH TRY TO EXPLAIN WHY WE EXPERIENCE COLLAPSE

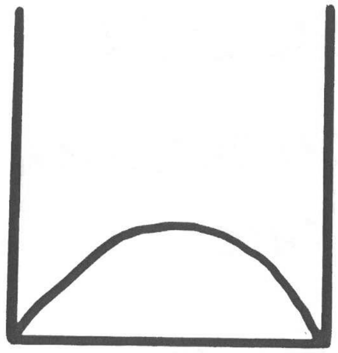
THIS PART OF QM IS STILL CONTROVERSIAL (AND EG. LEADS TO SUCH FUN AS SCH'S CAT...)

BUT <u>IMPORTANT TO STRESS</u>

EVERY EXPERIMENT EVER PERFORMED LEADS TO RESULTS CONSISTENT WITH THE SIMPLE 'COLLAPSE' POSTULATE AND DON'T REQUIRE ANYTHING FANCIER

LET'S SEE WHAT IT PREDICTS FOR A SERIES OF MEASUREMENTS

1) START WITH



$$\psi(x,t) = \phi_1(x)\, e^{-iE_1 t/\hbar}$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$

$$\phi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

2) MEASURE ENERGY

RESULT : E_1 $\qquad \psi_a(x,t) = \phi_1(x)\, e^{-iE_1 t/\hbar}$

3) MEASURE MOMENTUM

TO WORK OUT POSSIBLE RESULTS MUST REWRITE ψ_a AS A SUM OF MOM'M E'STATES

$$\psi_a = e^{-iE_1 t/\hbar} \sqrt{\frac{2}{a}}\, \frac{1}{2i} \left\{ e^{i\pi x/a} - e^{-i\pi x/a} \right\}$$

MOM'M $+\frac{\pi\hbar}{a}$ $\qquad$ MOM'M $-\frac{\pi\hbar}{a}$

SUPPOSE WE FIND $+\pi\hbar/a$

$\Longrightarrow$ WAVEFUNCTION COLLAPSES TO

$$\psi_b = e^{-iE_1 t/\hbar}\, \frac{e^{i\pi x/a}}{\sqrt{a}}$$

4) NOW MEASURE ENERGY AGAIN

TO WORK OUT POSSIBLE RESULTS MUST REWRITE ψ_b AS A SUM OF ENERGY E'STATES

$$\frac{e^{i\pi x/a}}{\sqrt{a}} = \frac{1}{\sqrt{a}}\left(\cos\frac{\pi x}{a} + i\sin\frac{\pi x}{a}\right)$$

HAPPENS TO BE AN ENERGY E'STATE

MUST USE FOURIER SERIES TO WRITE THIS AS

$$\frac{1}{\sqrt{a}}\cos\frac{\pi x}{a} = \sum_{n=1}^{\infty} a_n \underbrace{\left(\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\right)}$$

REMEMBER THIS IS AN ENERGY E'FN.

$$a_n = \frac{1}{\sqrt{a}}\int_0^a \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\cos\frac{\pi x}{a}\,dx$$

$$= \begin{cases} 0 & \text{IF } n = \text{ODD} \\ \dfrac{2\sqrt{2}\,n}{\pi(n^2-1)} & \text{IF } n = \text{EVEN} \end{cases}$$

THUS

$$\frac{e^{i\pi x/a}}{\sqrt{a}} = \frac{i}{\sqrt{2}}\left(\phi_1(x)\right) + \sum_{n\ \text{EVEN}} \frac{2\sqrt{2}\,n}{\pi(n^2-1)}\left(\phi_n(x)\right)$$

SO WHEN MEASURE ENERGY WE GET (!)

E_1	WITH	PROB	$P(E_1) = 1/2$
E_2	"	"	$P(E_2) = \frac{32}{9\pi^2}$
E_4	"	"	
E_6	"	"	$P(E_n) = \frac{8n^2}{(n^2-1)^2\pi^2}$
$\vdots$	$\vdots$	$\vdots$	

THUS EVEN THOUGH WE STARTED WITH AN ENERGY E' STATE, BY MAKING A MEAS. OF MOM'M (AN OP. INCOMPATIBLE WITH H) WE HAVE LEFT PARTICLE IN A STATE OF VERY INDEFINITE ENERGY!

- CONSIDERATIONS SUCH AS THESE LEAD HEISENBERG TO HIS FAMOUS UNCERTAINTY PRINCIPLE

- THE U.P. IS NOT A SEPERATE AXIOM OF QM. IT IS SIMPLY A CONSEQUENCE OF RULES ALREADY STATED...

WHEN THERE IS UNCERTAINTY IN OUTCOME OF MEAS. USEFUL TO QUANTIFY: <u>DEFINE UNCERTAINTY AS</u>

$$\boxed{(\Delta q)^2 \stackrel{\text{def}}{=} \langle q^2 \rangle - \langle q \rangle^2}$$

$\Delta q = 0$ IF q TAKES A SINGLE VALUE

<u>HEISENBERG'S U.P.</u> CONSIDERS x AND p (REMEMBER $[x, p] = i\hbar$) AND STATES

$$\boxed{\Delta x \, \Delta p \geq \hbar/2}$$

BEFORE PROVING THIS LET'S INVESTIGATE SOME ASPECTS OF ITS MEANING

IT SAYS THAT IF WE PREPARE A PARTICLE IN A STATE WHEREBY ITS LOCATION x IS KNOWN TO WITHIN Δx, THEN THE UNCERTAINTY IN ITS MOMENTUM IS AT <u>LEAST</u> $\hbar / 2\Delta x$

EXAMPLE:

SUPPOSE GAUSSIAN WAVEF'N

$$\phi(x) = \frac{1}{a^{1/2}\pi^{1/4}} e^{-x^2/2a^2}$$

CLEARLY $\langle x \rangle = \int_{-\infty}^{\infty} x\,|\phi(x)|^2 dx = 0$

ALSO

$$\langle x^2 \rangle = \frac{1}{a\pi^{1/2}} \int_{-\infty}^{\infty} x^2 e^{-x^2/a^2} dx$$

$$= a^2/2$$

$$\Longrightarrow \quad \underline{\Delta x} = \left[\langle x^2 \rangle - \langle x \rangle^2\right]^{1/2} = \underline{\frac{a}{\sqrt{2}}}$$

NOW FOR p:

$$\langle p \rangle = \frac{-i\hbar}{a\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/2a^2} \frac{\partial}{\partial x} e^{-x^2/2a} dx = 0$$

$$\langle p^2 \rangle = \frac{-\hbar^2}{a\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/2a^2} \frac{\partial^2}{\partial x^2} e^{-x^2/2a^2} dx$$

$$= \frac{-\hbar^2}{a\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/2a^2} \left(\frac{x^2}{a^4} - \frac{1}{a^2}\right) dx$$

$$= \hbar^2/2a^2$$

$$\Longrightarrow \quad \underline{\Delta p = \frac{\hbar}{a\sqrt{2}}}$$

THUS

$$\Delta p \, \Delta x = \frac{\hbar}{a\sqrt{2}} \frac{a}{\sqrt{2}} = \hbar/2$$

EXACTLY SATURATING H.U.P. BOUND

IN FACT A GAUSSIAN WAVEFUNCTION GIVES THE LEAST POSSIBLE VALUE FOR $\Delta p \Delta x$

- SINCE $\Delta p \neq 0$ INTERESTING TO ASK WHAT THE MOM'N DISTRIBUTION IS

WE KNOW X-SPACE WAVEFUNCTION

$$\phi(x) = \frac{1}{a^{1/2}\pi^{1/4}} e^{-x^2/2a^2}$$

IN DIRAC NOT'N THIS IS $\langle x | \phi \rangle$

'AMPLITUDE FOR PARTICLE IN STATE ϕ TO BE FOUND AT X'

WE WANT $\langle p | \phi \rangle$

'AMPLITUDE FOR PARTICLE IN STATE ϕ TO BE MEASURED WITH MOM'M p'

THIS IS JUST FOURIER TRANSFORM OF $\phi(x)$

$$\boxed{\hat{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar}\, \phi(x)}$$

SO $\int_{-\infty}^{\infty} dp\, |\hat{\phi}|^2 = 1$

OR IN DIRAC

$$\langle p|\phi\rangle = \sum_{\substack{\text{ALL } x \\ \text{VALUES}}} \langle p|x\rangle\langle x|\phi\rangle$$

LIKE 2-SLIT INTERFERENCE

[NOTE:

$$\langle p|x\rangle = \langle x|p\rangle^* = \left(\frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}}\right)^* = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$]

INTEGRAL FOR $\hat{\phi}(p)$ CAN BE DONE BY COMPLETING THE SQUARE

$$\bar{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\; e^{-\frac{1}{2a^2}\left\{(x - ipa^2/\hbar)^2 + p^2a^4/\hbar^2\right\}}$$

$$= \sqrt{\frac{a}{\hbar\pi^{1/2}}}\; e^{-p^2a^2/2\hbar^2}$$

<u>ANOTHER GAUSSIAN</u> (SHOULD RECALL THIS FROM THEORY OF FOURIER TRANSFORMS)

PROOF OF GENERAL U.P. (NON-EXAMINABLE)

SUPPOSE WE HAVE 2 HERMITIAN OPS A AND B WITH $[A,B] \neq 0$

DEFINE
$$\bar{A} = A - \langle A \rangle$$
$$\bar{B} = B - \langle B \rangle$$

AND CONSIDER FOLLOWING WAVEF'N

$$\phi_\lambda = \bar{A}\psi + i\lambda\bar{B}\psi$$

REAL A PARAMETER WE'RE GOING TO VARY

AND NORMALIZATION INTEGRAL

$$I(\lambda) = \int_{-\infty}^{\infty} dx\, \phi_\lambda^* \phi_\lambda \geq 0$$

SINCE A AND B HERMITIAN, SO ARE $\bar{A}, \bar{B}$, SO

$$I(\lambda) = \int dx (\bar{A}\psi + i\lambda\bar{B}\psi)^*(\bar{A}\psi + i\lambda\bar{B}\psi)$$

EXPANDING
$$= \int dx \left\{ |\bar{A}\psi|^2 + \lambda^2 |\bar{B}\psi|^2 + i\lambda\left[(\bar{A}\psi)^*(\bar{B}\psi) - (\bar{B}\psi)^*(\bar{A}\psi)\right]\right\}$$

USING HERMITIAN $\bar{A}, \bar{B}$
$$= \int dx\, \psi^* (\bar{A}^2 + \lambda^2 \bar{B}^2 + i\lambda[\bar{A},\bar{B}])\psi$$

USING DEF OF $(\Delta A)^2$ ETC
$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \int dx\, \psi^* [\bar{A},\bar{B}]\psi$$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \langle [A,B] \rangle$$

SINCE CONST. PIECES $\langle A \rangle, \langle B \rangle$ CANCEL IN $[\ ,\ ]$

THUS WE LEARN

$$(\Delta A)^2 + (\Delta B)^2 + i\lambda \langle [A,B] \rangle \geq 0$$

AND MINIMUM MUST EXIST WHEN $dLHS/d\lambda = 0$

$$2\lambda (\Delta B)^2 + i \langle [A,B] \rangle = 0$$

SUBST. SOL'N OF THIS INTO $I(\lambda)$ WE GET

$$(\Delta A)^2 - \frac{\langle [A,B] \rangle^2}{4(\Delta B)^2} + \frac{\langle [A,B] \rangle^2}{2(\Delta B)^2} \geq 0$$

$$\Longrightarrow \boxed{(\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \langle i[A,B] \rangle^2}$$

USEFUL TO KNOW!

SO IN GENERAL <u>ANY</u> 2 OPS. WITH $[\ ,\ ] \neq 0$ WILL HAVE UNCERTAINTY RELATION (THOUGH RHS WILL DEPEND ON DETAILS)

FOR PARTICULAR CASE OF $[p, x] = -i\hbar$ GET

$$\underline{\Delta x \, \Delta p \geq \hbar/2} \quad \checkmark$$

THE SIMPLE HARMONIC OSCILLATOR

BECAUSE MANY SYSTEMS TO LEADING APPROX'N ARE THE S.H.O. (OR MANY WEAKLY COUPLED S.H.O's) THIS IS AN <u>IMPORTANT</u> CASE...

THE POT'L ENERGY IS $V(x) = \frac{1}{2}kx^2$ SO TISE IS

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + \frac{1}{2}kx^2\phi = E\phi$$

VERY CONVENIENT TO RESCALE THE x VARIABLE BY $x = \alpha y$

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2\phi}{dy^2} + \frac{1}{2}k\alpha^2 y^2\phi = E\phi$$

AND INSIST THAT COEFFS OF K.E. AND P.E. ARE SAME

$$\frac{\hbar^2}{2m\alpha^2} = \frac{1}{2}k\alpha^2$$

$$\Rightarrow \alpha^2 = \frac{\hbar}{\sqrt{mk}}$$

THEN TISE

$$\hbar\sqrt{\frac{k}{m}}\,\frac{1}{2}\left(-\frac{d^2\phi}{dy^2} + y^2\phi\right) = E\phi$$

NOW $\sqrt{k/m} = \omega$ THE CLASSICAL ANGULAR FREQ., SO LET

$$\epsilon = E\Big/\left(\frac{\hbar\omega}{2}\right)$$

I.E., ϵ IS THE ENERGY IN UNITS OF $\hbar\omega/2$

THUS OUR TISE BECOMES

$$-\frac{d^2\phi}{dy^2} + y^2\phi = \epsilon\phi$$

IT'S EASY TO CHECK THAT

$$\boxed{\phi_0 = e^{-y^2/2}}$$

IS A SOLUTION (CLEARLY IT'S NORMALIZABLE)

LET'S DO IT...

$$\phi_0' = -y\,e^{-y^2/2}$$

$$\phi_0'' = y^2 e^{-y^2/2} - e^{-y^2/2}$$

SO TISE READS

$$-\left(y^2 e^{-y^2/2} - e^{-y^2/2}\right) + y^2 e^{-y^2/2} = \epsilon\, e^{-y^2/2}$$

$\Rightarrow$ SOL'N IF $\epsilon = 1$

THE ENERGY E'VALUE

IN FACT AS WE'LL SOON SEE THIS IS THE GROUND STATE

$$\boxed{E_0 = \frac{\hbar\omega}{2} > 0 \; !}$$

- THERE ARE 2 WAYS OF GETTING REST...

- I. TRY $\phi = H(y)\, e^{-y^2/2}$

THEN $\phi' = H' e^{-y^2/2} - y H e^{-y^2/2}$

$$\phi'' = H'' e^{-y^2/2} - 2y H' e^{-y^2/2} - H e^{-y^2/2} + y^2 H e^{-y^2/2}$$

SO TISE BECOMES

$$e^{-y^2/2}(-H'' + 2yH' + H) = \epsilon H e^{-y^2/2}$$

OR

$$H'' - 2yH' + H(\epsilon - 1) = 0$$

THIS IS CALLED HERMITE'S EQN, AND CAN BE SOLVED BY THE FROBEINIUS SERIES METHOD.

THERE ARE NORMALIZABLE SOL'NS FOR $\epsilon = 2n+1$; $H_n(y)$ IS A HERMITE POLYNOMIA

II) A MUCH MORE INSTRUCTIVE METHOD WHICH GENERALIZES TO MANY OTHER PROBLEMS...

IN y COORDS OUR HAMILTONIAN OP. IS

$$H = -\frac{d^2}{dy^2} + y^2$$

LET'S TRY TO 'FACTORIZE' THIS

DEFINE OPERATORS

$$a_+ = -\frac{d}{dy} + y$$

$$a_- = \frac{d}{dy} + y$$

ACTING ON ARBITRARY $f(y)$

$$a_+ a_- f = \left(-\frac{d}{dy} + y\right)\left(\frac{d}{dy} + y\right) f$$

$$= -\frac{d^2 f}{dy^2} + y\frac{df}{dy} - y\frac{df}{dy} - f + y^2 f$$

$$= \left(-\frac{d^2 f}{dy^2} + y^2 f\right) - f$$

SIMILARLY

$$a_- a_+ f = \left(-\frac{d^2 f}{dy^2} + y^2 f\right) + f$$

SO WE LEARN

- i) $\underline{[a_+, a_-]} = a_+ a_- - a_- a_+$

$$\underline{= -2}$$

- ii) WE CAN WRITE TISE AS

$$\boxed{(a_+ a_- + 1)\phi = \epsilon \phi} \qquad (1)$$

- iii) $\underline{a_- \phi_0} = \left(\frac{d}{dy} + y\right) e^{-y^2/2} \underline{= 0}$

THUS $(a_+ a_- + 1)\phi_0 = 1.\phi_0$

AND AGAIN HAVE FOUND $\epsilon_0 = 1$

- iv) NOW ACT ON TISE (THE ENERGY E'VALUE EQN) (1) WITH a_+ AND USE $[a_+, a_-]$

$$a_+(a_+ a_- + 1)\phi = \epsilon a_+ \phi$$

$$a_+(a_- a_+ - 2 + 1)\phi = \epsilon a_+ \phi$$

$$[a_+ a_- a_+ + (-2+1) a_+]\phi = \epsilon a_+ \phi$$

$$(a_+ a_- + 1) a_+ \phi = (\epsilon + 2) a_+ \phi$$

SO HAVE LEARNT

$$\boxed{\begin{array}{l}\text{IF } \phi \text{ HAS E'VALUE } \epsilon \\ a_+ \phi \text{ HAS E'VALUE } \epsilon + 2\end{array}}$$

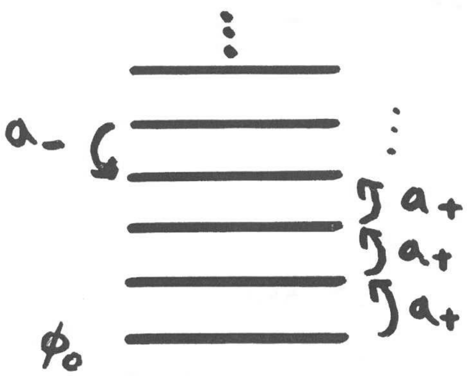
- v) SIMILARLY EASY TO SHOW THAT

$$\boxed{\begin{array}{l}\text{IF } \phi \text{ HAS E'VALUE } \epsilon \\ a_- \phi \text{ HAS E'VALUE } \epsilon - 2\end{array}}$$

SINCE $a_- \phi_0 = 0$ (WE SAY '<u>a_- ANNIHILATES ϕ_0</u>') THERE IS NO STATE WITH LOWER ENERGY THAN ϕ_0

$\Rightarrow$ ϕ_0 IS INDEED GROUND STATE, WITH $\epsilon = 1$

- vi) <u>BY REPEATED APPLICATION OF a_+ ON ϕ_0 WE GENERATE ENTIRE SPECTRUM!!</u>



a_+ AND a_- ARE KNOWN AS '<u>RAISING AND LOWERING</u>' OR '<u>LADDER</u>' OR '<u>CREATION AND ANNIHILATION</u>' OPS.

THUS SPECTRUM OF SHO IS

$$\epsilon_0 = 1 \qquad E_0 = \frac{\hbar\omega}{2} \qquad \phi_0 = e^{-y^2/2}$$

$$\epsilon_1 = 3 \qquad E_1 = (1+\tfrac{1}{2})\hbar\omega \qquad \phi_1 = \left(-\frac{d}{dy}+y\right)\phi_0 = 2y e^{-y^2/2}$$

$$\epsilon_2 = 5 \qquad E_2 = (2+\tfrac{1}{2})\hbar\omega \qquad \phi_2 = \left(\frac{-d}{dy}+y\right)\phi_1 = 2(2y^2-1)e^{-y^2/2}$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$\epsilon_n = 2n+1 \quad \boxed{\begin{aligned} &E_n = (n+1/2)\hbar\omega \\ &\phi_n = \left(-\frac{d}{dy}+y\right)^n \phi_0 = H_n(y)\,e^{-y^2/2} \end{aligned}}$$

A COMPLETE SOL'N OF PROBLEM !

SO FAR HAVEN'T NORMALIZED WAVEF'NS ...

$$\text{E.G.} \quad \phi_0(x) = C e^{-x^2/2\alpha^2}$$

NOTE: MUST CONVERT BACK TO X

$$1 = \int_{-\infty}^{\infty} dx\, |\phi_0|^2 = C^2 \int_{-\infty}^{\infty} dx\, e^{-x^2/\alpha^2}$$

$$= C^2 \pi^{1/2} \alpha$$

$$\Rightarrow \quad C = \frac{1}{\alpha^{1/2}\pi^{1/4}}$$

RECALL

$$\alpha^2 = \frac{\hbar}{\sqrt{mk}}$$

- SIMILARLY CAN NORMALIZE HIGHER $\phi_n(x)$'s ...

- JUST AS IMPORTANT OUR WAVEF'NS ARE ALSO <u>ORTHOGONAL</u>

$$\boxed{\int_{-\infty}^{\infty} \phi_n(x)\, \phi_m(x)\, dx = 0 \qquad n \neq m}$$

[THIS <u>MUST BE TRUE</u> : THEY ARE E'FUNCTIONS OF HERMITIAN OPERATOR H WITH DIFFERENT E'VALUES ϵ_n AND ϵ_m.
C.F. 'STURM-LIOUVILLE' THEORY IN MATHS METHODS COURSE...]

- NOTE THAT THE $\phi_n(x)$ GO <u>EVEN-ODD-EVEN...</u> AND JUST LIKE THE ∞□U, <u>THE n^{th} EXCITED STATE HAS n NODES</u>.

- <u>FEATURES OF THE GROUND-STATE</u>

$$\phi_0(x) = \frac{1}{\alpha^{1/2}\pi^{1/4}} \exp\left(-\frac{x^2}{2\alpha^2}\right)$$

$$E_0 = \frac{\hbar\omega}{2} \qquad \alpha^2 = \frac{\hbar}{\sqrt{mk}}$$

A CLASSICAL PARTICLE OF TOTAL ENERGY $\hbar\omega/2$ WOULD BE CONFINED TO REGION WHERE

$$V(x) \leq E_0$$

$$\frac{1}{2}kx^2 \leq \frac{\hbar\omega}{2}$$

$$\Rightarrow x^2 \leq \frac{\hbar\omega}{k} = \frac{\hbar}{k}\sqrt{\frac{k}{m}} = \frac{\hbar}{\sqrt{mk}} = \alpha^2$$

I.E. $\quad -\alpha \leq x \leq \alpha$

IF GO BACK TO TISE

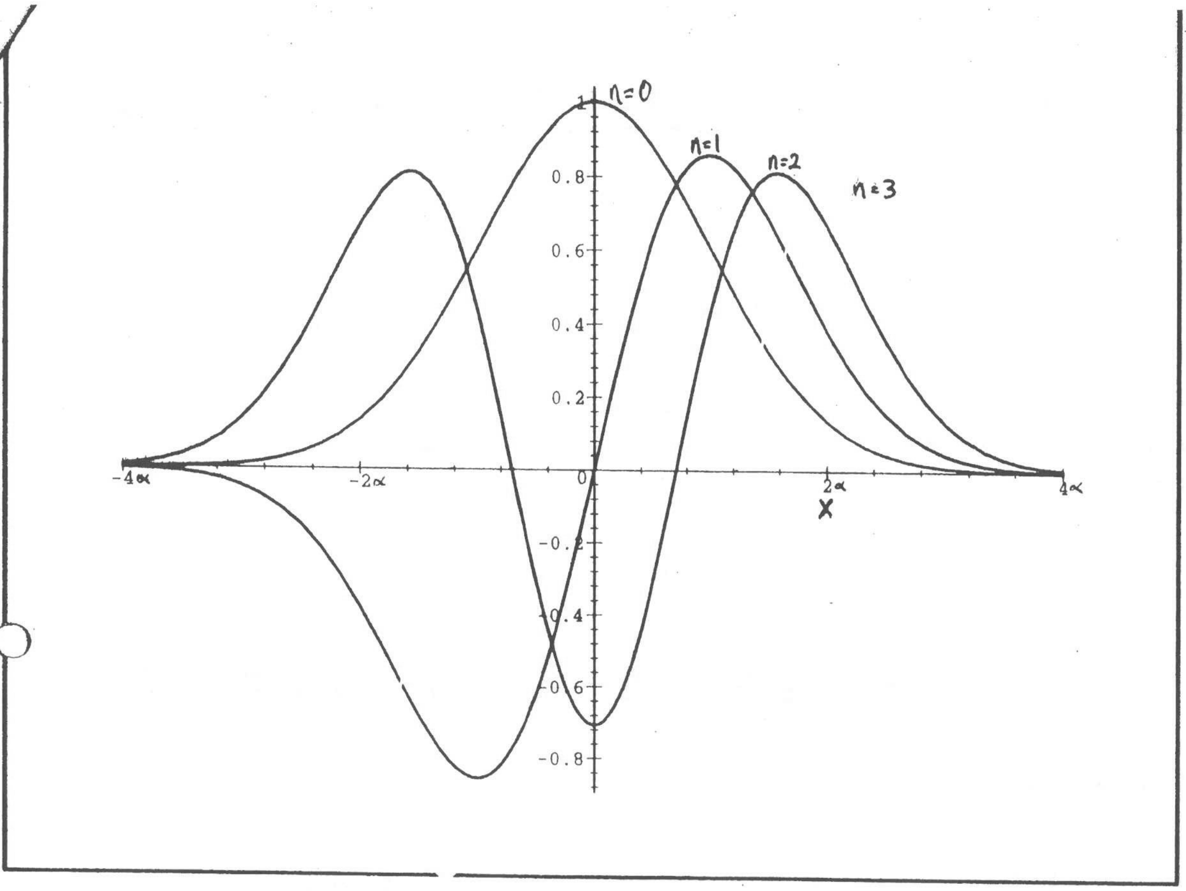
$$\frac{-\hbar^2}{2m}\frac{d^2\phi}{dx^2} + \frac{1}{2}kx^2\phi = E\phi$$

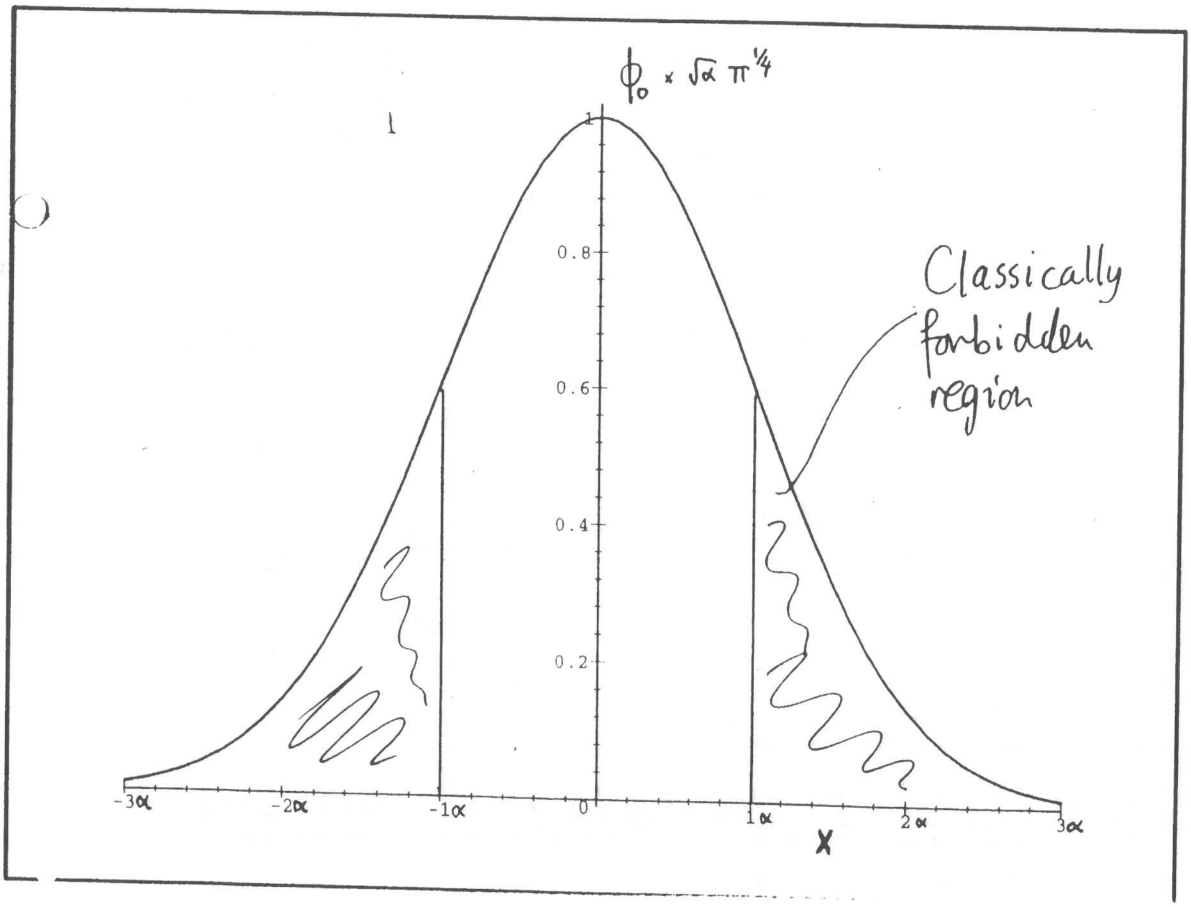
AT THE POINT WHERE $E = V(x)$ (THE LIMIT OF THE CLASSICAL MOTION) WE SEE THAT

$$\frac{d^2\phi}{dx^2} = 0$$ A POINT OF INFLEXION FOR ϕ

THIS IS TRUE FOR ANY STATE

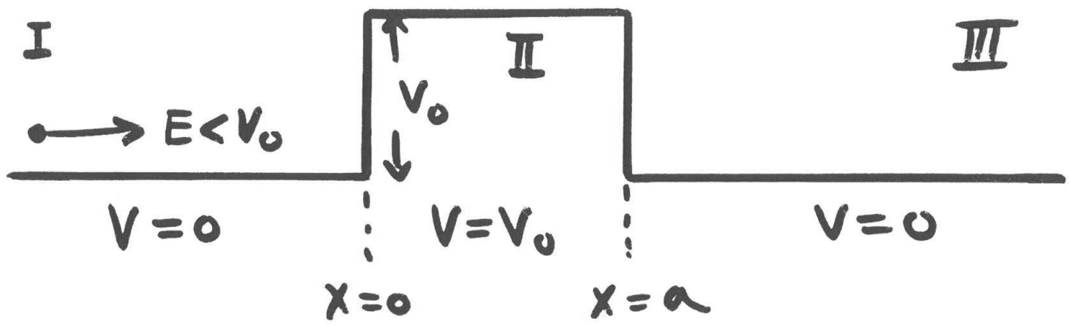
	PROB OUTSIDE CLASSICAL REGION	n
QUANTUM EFFECTS MOST SIGNIFICANT FOR LOW E STATES	0.157	0
	0.116	1
	0.095	2
	⋮	⋮


n=0
n=1
n=2
n=3
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-4α
-2α
2α
4α
x


$\phi_0 \times \sqrt{\alpha}\,\pi^{1/4}$
1
0.8
0.6
0.4
0.2
0
-3α
-2α
-1α
1α
2α
3α
x
Classically forbidden region

SCATTERING, TUNNELING, AND FINITE POTENTIAL WELLS

CONSIDER FOLLOWING $V(x)$



WITH PARTICLE OF ENERGY $E<V_0$ INCIDENT FROM LEFT

THREE REGIONS IN WHICH SOL'NS TO TISE ARE:

$$\psi_I = \underbrace{e^{ikx}}_{\text{INCIDENT}} + r\,\underbrace{e^{-ikx}}_{\text{REFLECTED}} \qquad \frac{\hbar^2 k^2}{2m} = E$$

$$\psi_{II} = A e^{\kappa x} + B e^{-\kappa x} \qquad \frac{\hbar^2 \kappa^2}{2m} = V_0 - E$$

$$\psi_{III} = \underbrace{t}_{\text{TRANSMITTED}}\, e^{+ikx} \qquad \frac{\hbar^2 k^2}{2m} = E$$

NOW MUST IMPOSE BOUNDARY CONDITIONS AT $x=0$ AND $x=a$ ...

AT $x=0$

ψ CONTINUOUS $\quad 1+r = A+B$

$\frac{\partial\psi}{\partial x}$ " $\quad ik(1-r) = K(A-B)$

AT $x=a$

ψ CONTINUOUS $\quad Ae^{Ka} + Be^{-Ka} = te^{ika}$

$\frac{\partial\psi}{\partial x}$ " $\quad K(Ae^{Ka} - Be^{-Ka}) = ikte^{ika}$

CLASSICALLY ZERO TRANSMISSION THROUGH BARRIER. WE WANT TO FIND t IN QM CASE...

FROM $x=0$ EQNS GET

$$1+r = A+B$$

$$1-r = \frac{-iK}{k}(A-B) \qquad \text{ADD AND FIND}$$

$$2 = A(1 - iK/k) + B(1 + iK/k) \qquad (1)$$

FROM $x=a$ EQNS GET

$$2Ae^{Ka} = (1+ik/K)te^{ika}$$

$$2Be^{-Ka} = (1-ik/K)te^{ika}$$

PUT THESE BACK INTO (1)

$$2 = t e^{ika}\left\{ \tfrac{1}{2} e^{-Ka}\left(1 - i\tfrac{K}{k}\right)\left(1 + ik/K\right) + \tfrac{1}{2} e^{Ka}\left(1 + i\tfrac{K}{k}\right)\left(1 - ik/K\right) \right\}$$

$$= t e^{ika}\left\{ \tfrac{1}{2} e^{-Ka}\left(2 + i\left[\tfrac{k}{K} - \tfrac{K}{k}\right]\right) + \tfrac{1}{2} e^{Ka}\left(2 - i\left[\tfrac{k}{K} - \tfrac{K}{k}\right]\right) \right\}$$

$$= t e^{ika}\left\{ 2\cosh Ka - i\left(\tfrac{k}{K} - \tfrac{K}{k}\right)\sinh Ka \right\}$$

$$\Rightarrow t = \frac{2e^{-ika}}{2\cosh Ka - i\left(\frac{k}{K} - \frac{K}{k}\right)\sinh Ka}$$

THUS PROB OF TRANSMISSION IS

$$\boxed{T = |t|^2 = \frac{4}{4\cosh^2 Ka + \frac{(k^2 - K^2)^2}{k^2K^2}\sinh^2 Ka}} \quad (2)$$

NB. THE FACTORS OF $\hbar k/m$ IN INCIDENT AND TRANSMITTED FLUX CANCEL. (AS k'S SAME)

THERE IS MUCH PHYSICS IN (2)

LET'S LOOK AT SOME CASES...

- WHEN Ka IS LARGE

$$T \simeq \frac{4\, e^{-2Ka}}{1 + (k^2 - K^2)^2 / 4k^2K^2} > 0 \quad !$$

THIS IS TYPICAL TUNNELLING BEHAVIOR, IN PARTICULAR THE <u>EXPONENTIAL DAMPING</u> OF THE TUNNELLING PROB. WITH THE <u>WIDTH</u> a OF BARRIER.

- WHEN $E = V_0$

$$K^2 = \frac{2m}{\hbar^2}(V_0 - E) = 0$$

AND THIS IMPLIES

$$T = \frac{4}{4 + k^2 a^2} < 1 \quad !$$

NOTE THAT EVEN THOUGH CLASSICALLY ONE WOULD GET PERFECT TRANSMISSION, HERE $T \neq 1$, AND <u>IN QM GET SOME REFLECTION</u>

$$R = 1 - T = \frac{k^2 a^2}{4 + k^2 a^2}$$

- **WHEN $E > V_0$**

$$K^2 = \frac{2m}{\hbar^2}(V_0 - E) < 0 \quad \text{SO WRITE}$$

$$K = i\hat{k} = i\left[\frac{2m}{\hbar}(E - V_0)\right]^{1/2}$$

THEN WITH THIS SUBST

$$t = \frac{2e^{-ika}}{2\cos\hat{k}a - \left(k/\hat{k} + \hat{k}/k\right) i \sin\hat{k}a}$$

GIVING

$$T = |t|^2 = \frac{4}{4\cos^2\hat{k}a + \left(\frac{k}{\hat{k}} + \frac{\hat{k}}{k}\right)^2 \sin^2\hat{k}a}$$

SO ZERO

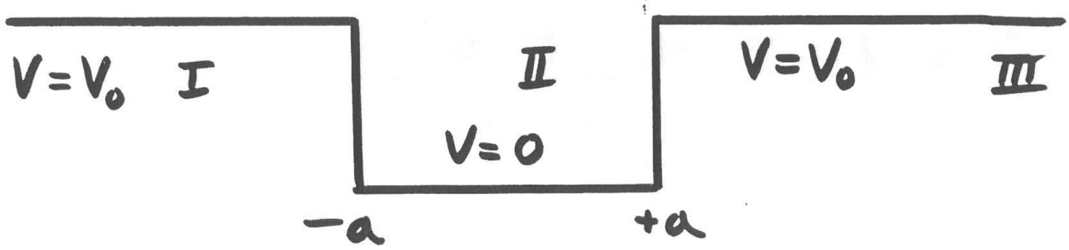
WHICH IS LESS THAN 1 UNLESS $\underbrace{\hat{k}a = n\pi}$

'RESONANT TRANSMISSION'

CF. CLASSICALLY

$T = 1$ FOR $E > V_0$!

SO FAR SQUARE BARRIER, NOW SQUARE WELL ...



NOTE

$$\psi_{I} = A e^{Kx} \qquad \frac{\hbar^2 K^2}{2m} = V_0 - E$$

$$\psi_{II} = B \cos kx + C \sin kx \qquad \frac{\hbar^2 k^2}{2m} = E$$

$$\psi_{III} = D e^{-Kx}$$

BOUNDARY CONDITIONS

$$A e^{-Ka} = B \cos ka - C \sin ka \qquad (1)$$

$$K A e^{-Ka} = kB \sin ka + kC \cos ka \qquad (2)$$

$$D e^{-Ka} = B \cos ka + C \sin ka \qquad (3)$$

$$-K D e^{-Ka} = -kB \sin ka + kC \cos ka \qquad (4)$$

THESE EQNS ARE A PAIN TO SOLVE BY HAND – NOWADAYS WE'D USE A SYMBOLIC MATH PROGRAM (E.G. MAPLE, MATHEMATICA, ...) BUT WORTHWHILE TO STUDY SOME FEATURES... WE CAN WRITE (1)...(4) AS

$$\begin{pmatrix} e^{-Ka} & -\cos ka & \sin ka & 0 \\ K e^{-Ka} & -k \sin ka & -k \cos ka & 0 \\ 0 & -\cos ka & -\sin ka & e^{-Ka} \\ 0 & k \sin ka & -k \cos ka & -K e^{-Ka} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0$$

FOR NON-TRIVIAL SOL'NS NEED

$$\det(\ ) = 0$$

$$\Rightarrow e^{-2\kappa a}(\kappa \cos ka - k \sin ka)(\kappa \sin ka + k \cos ka) = 0$$

THIS IMPLIES:

(I) $\boxed{\dfrac{\kappa}{k} = \tan ka}$ IN WHICH CASE

EVEN WAVEF'NS $\Leftarrow$ $\begin{cases} C = 0 \\ D = A \end{cases}$

$$B = \frac{e^{-\kappa a}}{\cos ka} A$$

OR

(II) $\boxed{\dfrac{\kappa}{k} = -\cot ka}$ IN WHICH CASE

ODD WAVEF'NS $\Leftarrow$ $\begin{cases} B = 0 \\ D = -A \end{cases}$

$$C = -A \frac{e^{-\kappa a}}{\sin ka}$$

WE NEED TO SOLVE (I) AND (II) TO GET ENERGIES. BUT THESE TRANSCENDENTAL EQNS CAN'T BE SOLVED ALGEBRAICALLY – SO USE GRAPHICAL METHOD ...

LET'S WRITE

$$E = \epsilon \frac{\hbar^2}{2ma^2} \qquad V_0 = \lambda \frac{\hbar^2}{2ma^2}$$

THEN EQNS (I), (II) BECOME

$$\sqrt{\frac{\lambda}{\epsilon} - 1} = \tan\sqrt{\epsilon} \quad \text{AND} \quad \sqrt{\frac{\lambda}{\epsilon} - 1} = -\cot\sqrt{\epsilon}$$

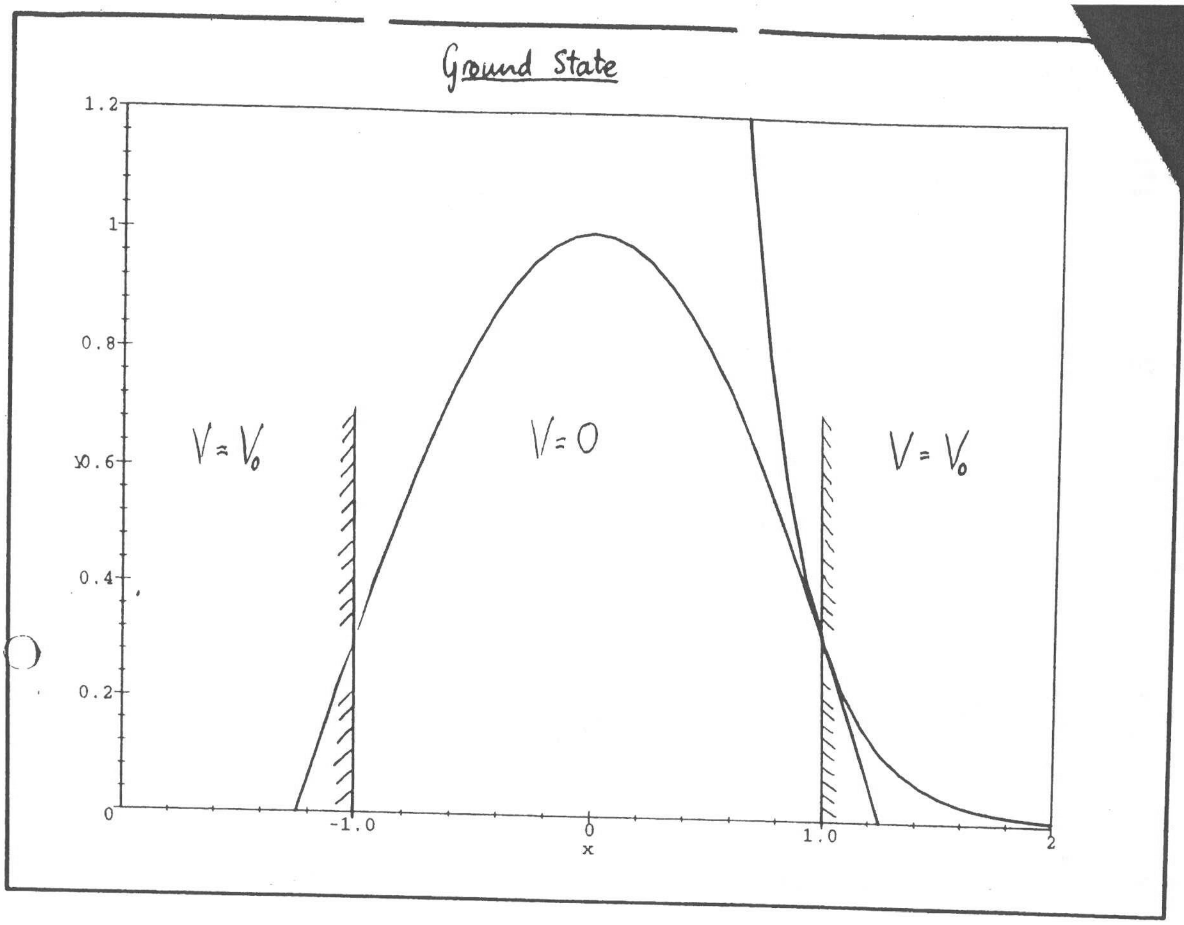
$\longrightarrow$ PICTURES OF METHOD OF SOL'N

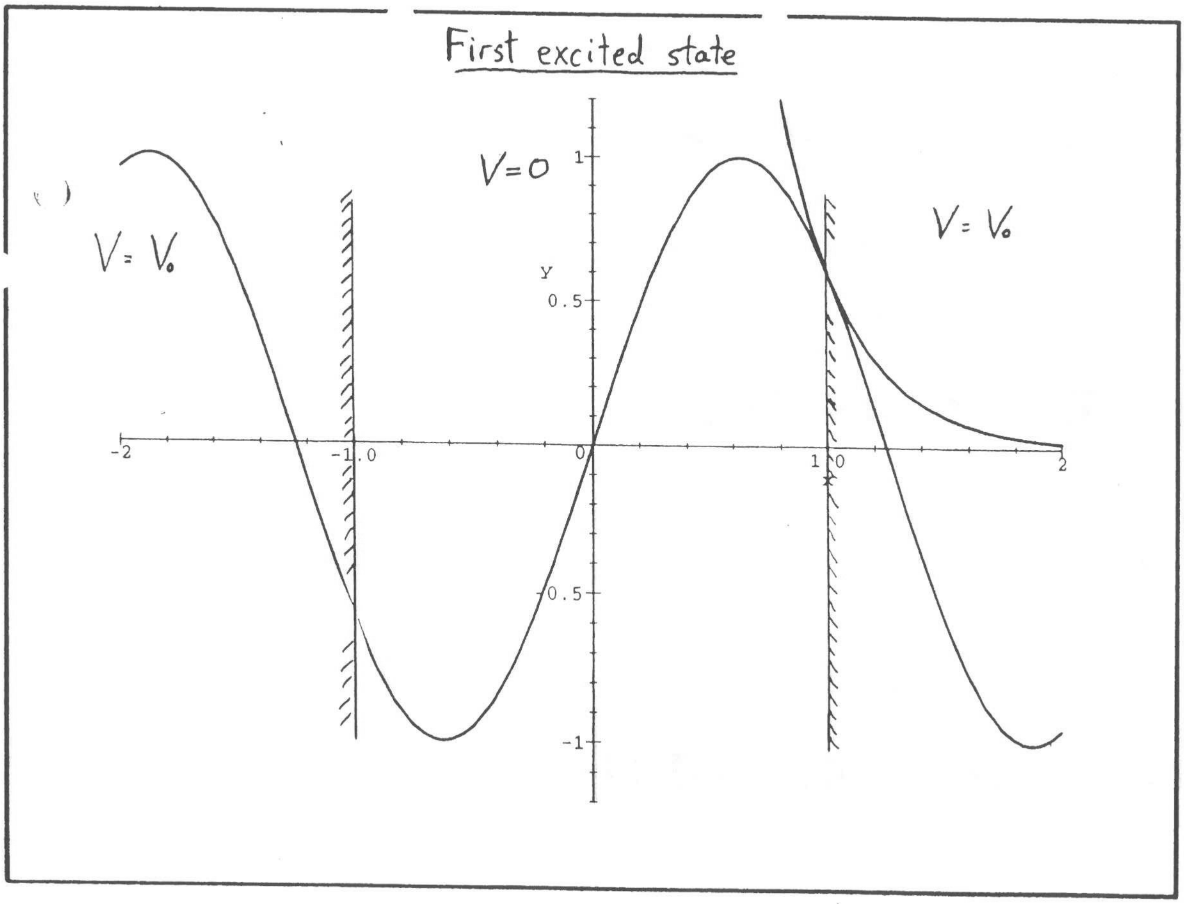
$\longrightarrow$ PICTURES OF WAVEFUNCTIONS

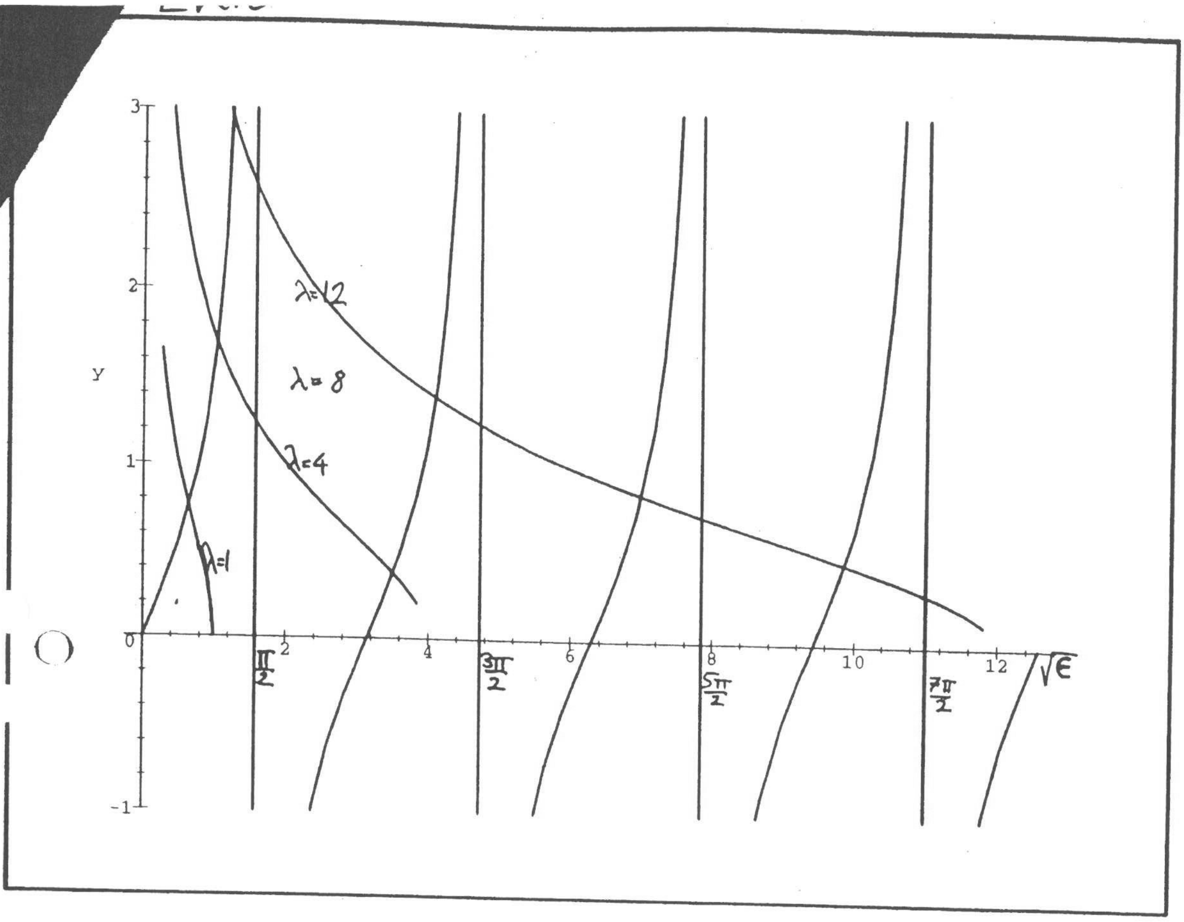
NOTE THERE IS <u>ALWAYS</u> ONE EVEN BOUND STATE NO MATTER HOW SMALL V_0

(THIS TRUE OF 1D TISE.)

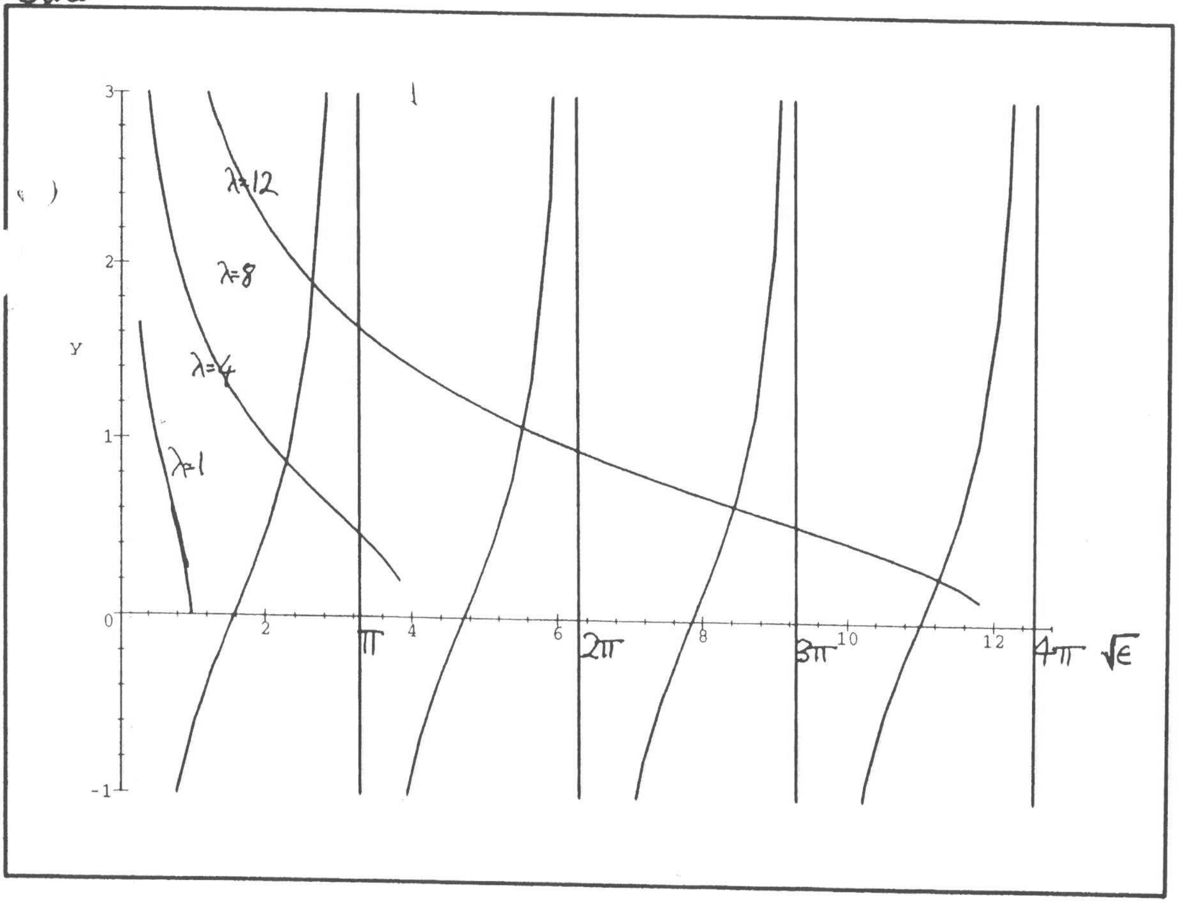
ONLY A FINITE NUMBER OF BOUND STATES FOR $V_0 < \infty$, AND FORMULA FOR ENERGIES NOT NEARLY SO SIMPLE AS ∞ □ ⊔ CASE.


Ground State
1.2
1
0.8
0.6
0.4
0.2
0
-1.0
0
x
1.0
2
V = V0
V = 0
V = V0


First excited state
V = V0
V=0
V = V0
1
y
0.5
-2
-1.0
0
1.0
2
-0.5
-1


y
3
2
1
0
-1
2
4
6
8
10
12
λ=12
λ=8
λ=4
λ=1
$\frac{\pi}{2}$
$\frac{3\pi}{2}$
$\frac{5\pi}{2}$
$\frac{7\pi}{2}$
$\sqrt{\epsilon}$

Odd


y
3
2
1
0
-1
2
4
6
8
10
12
λ=12
λ=8
λ=4
λ=1
π
2π
3π
4π
$\sqrt{\epsilon}$