DIRAC FORMULATION OF QM

MORE POWERFUL AND MORE GENERAL THAN WAVEFUNCTIONS. ALL SERIOUS PHYSICISTS USE IT.

LET'S ABSTRACT GENERAL FEATURES OF QM

- WAVEFUNCTIONS CAN BE LINEARLY SUPERPOSED WITH COMPLEX COEFFS

MATHEMATICAL STRUCTURE IS COMPLEX LINEAR VECTOR SPACE

$$\boxed{\text{BASIC OBJECT IS 'STATE KET' } |\psi\rangle}$$

REPRESENTING STATE OF SYSTEM

A PARTICULAR SET OF STATES ARE ENERGY EIGENSTATES

$$H|n\rangle = E_n|n\rangle$$

WE ALSO HAVE COMPLEX CONJUGATES OF WAVEFUNCTIONS AND EIGENSTATES

REPRESENT THESE BY 'STATE BRAS'

$$\langle \psi | \quad \text{OR} \quad \langle n |$$

- THE <u>OVERLAP</u> OF WAVEFUNCTIONS

$$\int dx \, \phi(x)^* \, \psi(x)$$

<u>GENERALIZES TO</u>

UNITARY INNER PRODUCT FOR BRAS AND KETS

$\langle \phi | \psi \rangle$ = COMPLEX NUMBER GIVING OVERLAP OF $|\psi\rangle$ AND $|\phi\rangle$

$\langle \phi | \psi \rangle$ SATISFIES RULES EXPLAINED IN MATHS METHODS COURSE...

EG. $\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^*$

A KET IS NORMALIZED IF

$$\langle \psi | \psi \rangle = 1$$

AND $|\psi\rangle$ AND $|\phi\rangle$ ARE ORTHOGONAL IF

$$\langle \psi | \phi \rangle = \langle \phi | \psi \rangle = 0$$

MEANS WITH INNER PRODUCT

THIS UNITARY COMPLEX VECTOR SPACE $\langle \ldots | \ldots \rangle$

DESCRIBING THE POSSIBLE STATES OF THE SYSTEM IS CALLED THE

'<u>HILBERT SPACE</u>' OF THE SYSTEM

SOMETIMES DENOTED BY 'CURLY' $\mathcal{H}$

- LIKE ANY LINEAR VECTOR SPACE $\mathcal{H}$ HAS A DIMENSION DETERMINED BY MAXIMAL NUMBER OF LINEARLY INDEPENDENT VECTORS

$$c_1 |u_1\rangle + c_2 |u_2\rangle + \ldots + c_N |u_N\rangle = 0$$

SATISFIED ONLY IF $c_1 = c_2 = \ldots = c_N = 0$

A DIFFERENCE WITH VECTOR SPACES YOU ARE FAMILIAR WITH IS THAT

DIMENSION OF $\mathcal{H}$ IS TYPICALLY ∞ !

EG. WE KNOW PARTICLE IN 1D SQUARE WELL HAS ∞ NUMBER OF ENERGY EIGENSTATES $\varphi_n(x) \longleftrightarrow |n\rangle$ WHICH ARE LINEARLY INDEP'T

HOWEVER LATER IN COURSE WE WILL MEET VERY IMPORTANT PHYSICAL SYSTEMS WHERE $\mathcal{H}$ IS FINITE DIMENSIONAL (SPIN, ...) AND <u>CANNOT</u> BE DESCRIBED BY WAVEFUNCTIONS

- EXISTENCE OF INNER PRODUCT $\langle \,|\, \rangle$ ALLOWS US TO CONSTRUCT COMPLETE SETS OF ORTHONORMAL KETS (A <u>BASIS</u> FOR $\mathcal{H}$) VIA SCHMIDT PROCEDURE

  $|u_m\rangle$ WITH $\langle u_n | u_m \rangle = \delta_{nm}$

IF HAVE SUCH A BASIS THEN ANY STATE $|\psi\rangle$ OF SYSTEM CAN BE EXPANDED

$$\boxed{|\psi\rangle = \sum_{n=1}^{\dim \mathcal{H}} c_n |u_n\rangle}$$

c_n'S DETERMINED BY TAKING INNER PRODUCT OF THIS EQN WITH $\langle u_m|$

$$\langle u_m|\psi\rangle = \sum_{n=1}^{\dim \mathcal{H}} c_n \underbrace{\langle u_m|u_n\rangle}_{\delta_{mn}}$$

$$= c_m \qquad \therefore \; c_n = \langle u_n|\psi\rangle$$

THUS EXPANSION FOR $|\psi\rangle$ IS

$$\boxed{|\psi\rangle = \sum_{n=1}^{\dim \mathcal{H}} |u_n\rangle c_n = \underbrace{\sum_{n=1}^{\dim \mathcal{H}} |u_n\rangle\langle u_n|\psi\rangle}_{\text{EASILY REMEMBERED FORM}}}$$

THE BRAS AND KETS ARE RELATED BY TAKING THE ADJOINT (COMPLEX CONJUGATE TRANSPOSE FOR USUAL VECTORS) SO EQN

$$|\psi\rangle = \sum_{n=1}^{\dim \mathcal{H}} |u_n\rangle c_n$$

IMPLIES

$$(|\psi\rangle)^\dagger = \left(\sum_{n=1}^{\dim \mathcal{H}} |u_n\rangle c_n\right)^\dagger$$

$$\boxed{\langle\psi| = \sum_{n=1}^{\dim \mathcal{H}} c_n^* \langle u_n|}$$

NOTE C^* COEFF.

THUS NORMALIZATION IMPLIES

$$1 = \langle\psi|\psi\rangle = \sum_{n=1}^{\dim \mathcal{H}} c_n^* \langle u_n| \sum_{m=1}^{\dim \mathcal{H}} |u_m\rangle c_m$$

$$= \sum_{n,m} c_n^* c_m \underbrace{\langle u_n|u_m\rangle}_{\delta_{nm}}$$

$$= \sum_n |c_n|^2$$

- IN QM ALSO HAVE (HERMITIAN) OPERATORS WHICH REPRESENT OBSERVABLES

A KEY PRINCIPLE OF QM IS THAT <u>ALL OPERATORS ARE LINEAR</u>, I.E., IF

$$|\psi\rangle = c_1|u_1\rangle + c_2|u_2\rangle$$

THEN

$$\hat{O}|\psi\rangle = c_1(\hat{O}|u_1\rangle) + c_2(\hat{O}|u_2\rangle)$$

TO BE TRUTHFUL THERE IS ONE, AND ONLY ONE EXCEPTION TO THIS, THE 'TIME-REVERSAL' OPERATOR $\hat{T}$ WHICH IS 'ANTILINEAR' — THIS IS AN ADVANCED (AND INTERESTING!) TOPIC...

OPERATORS ALSO ACT ON THE VECTOR SPACE OF BRAS LINEARLY ($\hat{O}$ CAN ACT 'LEFT' OR 'RIGHT')

$$\langle\psi|\hat{O} = (c_1^*\langle u_1| + c_2^*\langle u_2|)\hat{O}$$
$$= c_1^*(\langle u_1|\hat{O}) + c_2^*(\langle u_2|\hat{O})$$

SINCE BRAS AND KET EXCHANGED BY TAKING ADJOINT, USEFUL TO DEFINE ACTION OF ADJOINT ON OPERATORS TOO

ADJOINT $\hat{A}^{+}$ OF OP. $\hat{A}$ <u>DEFINED</u> BY

$$\boxed{\langle\psi|\hat{A}^{+}|\varphi\rangle \equiv \langle\varphi|A|\psi\rangle^{*}}$$

<u>HERMITIAN (OR 'SELF-ADJOINT'</u>) OPERATORS SATISFY

$$\boxed{\hat{A}^{+} = \hat{A}}$$

SO FOR HERMITIAN OPS (<u>ONLY</u>)

$$\langle\varphi|\hat{A}|\psi\rangle^{*} = \langle\psi|\hat{A}|\varphi\rangle$$

THE QUANTITY $\langle\varphi|\hat{A}|\psi\rangle$ IS CALLED THE 'MATRIX ELEMENT' OF $\hat{A}$ BETWEEN STATES $|\varphi\rangle$ AND $|\psi\rangle$.

IF $|u_n\rangle$ IS AN ORTHONORMAL BASIS THEN $\langle u_m|\hat{A}|u_n\rangle \equiv A_{mn}$ IS MATRIX ELEMENT IN CONVENTIONAL SENSE.

- A SURPRISINGLY USEFUL OPERATOR SECRETLY APPEARS IN THE EXPANSION OF GENERAL $|\psi\rangle$

$$|\psi\rangle = \sum_{n=1}^{\dim\mathcal{H}} |u_n\rangle\langle u_n|\psi\rangle$$

SINCE THIS HOLDS FOR ANY KET $|\psi\rangle$ WE CAN CANCEL $|\psi\rangle$ FROM BOTH LHS AND RHS, SO

$$\boxed{\hat{I} = \sum_{n=1}^{\dim\mathcal{H}} |u_n\rangle\langle u_n|}$$

WHERE $\hat{I}$ IS THE 'IDENTITY OPERATOR'

WHICH LEAVES ALL STATES UNCHANGED

$$\hat{I}|\varphi\rangle = \sum_{n=1}^{\dim\mathcal{H}} |u_n\rangle\langle u_n|\varphi\rangle$$

$$= |\varphi\rangle$$ BY EXPANSION THM FOR $|\varphi\rangle$

THE MATRIX ELEMENT OF $\hat{I}$ IS (IN A BASIS)

$$\langle u_p|\hat{I}|u_q\rangle = \sum_{n=1}^{\dim\mathcal{H}} \underbrace{\langle u_p|u_n\rangle}_{\delta_{pn}}\underbrace{\langle u_n|u_q\rangle}_{\delta_{nq}}$$

$$= \delta_{pq}$$

THUS WRITTEN EXPLICITLY AS A MATRIX $\hat{I}$ IS REPRESENTED AS

$$\hat{I} \longleftrightarrow \underbrace{\begin{pmatrix} \ddots & & & & & \\ & 1 & & & 0 & \\ & & 1 & & & \\ & & & 1 & & \\ & 0 & & & 1 & \\ & & & & & 1 \\ & & & & & & \ddots \end{pmatrix}}_{\dim \mathcal{H}} \Bigg\} \dim \mathcal{H}$$

THE <u>UNIT</u> MATRIX!

- ANOTHER USEFUL EXAMPLE IS THE MATRIX ELEMENT OF A PRODUCT OF OPERATORS

$$\underbrace{\langle u_p | \hat{A} \hat{B} | u_q \rangle}_{(AB)_{pq}} = \langle u_p | \hat{A} \, \hat{I} \, \hat{B} | u_q \rangle$$

CAN ALWAYS INSERT $\hat{I}$ OPERATOR!

$$= \sum_n \langle u_p | A | u_n \rangle \langle u_n | B | u_q \rangle$$

$$= \underbrace{\sum_n A_{pn} B_{nq}}$$

JUST USUAL MATRIX MULTIPLICATION OF MATRICES REPRESENTING $\hat{A}$ AND $\hat{B}$

OUR EARLIER DEF'N OF $\hat{A}^\dagger$ AGREES WITH ADJOINT OF A MATRIX

$$
\begin{aligned}
(\hat{A}^\dagger)_{mn} &\equiv \langle u_m | \hat{A}^\dagger | u_n \rangle \\
&= \langle u_n | \hat{A} | u_m \rangle^* \\
&= (\hat{A})^*_{\underline{nm}} \quad \text{INDICES TRANSPOSED} \\
&= (\hat{A}_{mn})^{*T} \quad \checkmark
\end{aligned}
$$

BY FORMULA ON p. 8

BACK TO PHYSICS...

* FUNDAMENTAL POSTULATES OF QM *

I) STATES OF A SYSTEM ARE REPRESENTED BY **NORMALIZED** KETS $|\psi\rangle$ OR BRAS $\langle\varphi|$ IN A HILBERT SPACE (WHICH VARIES FROM SYSTEM TO SYSTEM)

II) OBSERVABLES ARE REPRESENTED BY **LINEAR** **HERMITIAN** **OPERATORS** ACTING ON KETS OR BRAS

III) ALL SUCH HERMITIAN OPS. $\hat{A}$ ARE ASSUMED TO POSSESS A <u>COMPLETE SET</u> OF ORTHONORMAL EIGENSTATES

$\|1\rangle$	WITH	EIGENVALUE	a_1
$\|2\rangle$	"	"	a_2
$\|3\rangle$	"	"	a_3
$\vdots$	$\vdots$	$\vdots$	$\vdots$

'COMPLETE SET' MEANS THAT $|1\rangle, |2\rangle, \ldots$ FORMS A BASIS FOR THE SPACE, SO <u>ANY</u> $|\psi\rangle$ CAN BE <u>EXPANDED IN EIGENSTATES OF $\hat{A}$</u> (FOR <u>ANY</u> $\hat{A}$)

$$|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

IV) THE <u>FUNDAMENTAL PROBABILITY POSTULATE FOR MEASUREMENTS</u> IS

i) POSSIBLE RESULTS OF MEASUREMENT OF A ARE <u>EIGENVALUES</u> OF $\hat{A}$ <u>ONLY</u>

ii) $\text{PROB}(A = a_n) = |\langle n|\psi\rangle|^2$

iii) <u>AFTER MEASUREMENT</u> OF $\hat{A}$ WITH RESULT a_n THE STATE $|\psi\rangle$ IS <u>REDUCED</u> TO ('COLLAPSES TO')

$$|\psi_{after}\rangle = |n\rangle$$

COEFF CHANGED TO 1

EIGENKET OF $\hat{A}$ WITH $\hat{A}|n\rangle = a_n|n\rangle$

[NOTE: IF a_n IS A DEGENERATE EIGENVALUE (IE IF MORE THAN ONE LINEARLY INDEP'T KET HAS SAME a_n EIGENVALUE) THE PROCEDURE OF REDUCTION IS SLIGHTLY MORE INVOLVED – THIS IS AN ADVANCED TOPIC.]

NOTE: SUBSEQUENT MEASUREMENTS OF SAME $\hat{A}$ ON $|\psi_{after}\rangle = |n\rangle$ RETURN a_n WITH PROBABILITY = 1 AS LONG AS NO MEASUREMENTS OF OTHER OPS $\hat{B}$ ARE MADE AT INTERMEDIATE TIMES (MORE ON THIS LATER)

V) IN THE <u>ABSENCE</u> OF A <u>MEASUREMENT</u> THE TIME EVOLUTION OF THE KET $|\psi(t)\rangle$ DESCRIBING THE STATE OF THE SYSTEM AT TIME t CHANGES <u>SMOOTHLY</u> IN TIME ACCORDING TO THE TDSE

$$\boxed{i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle}$$

NOTES: i) THE <u>TDSE IS A LINEAR EQN, WHICH IS ALSO DETERMINISTIC</u>, IE GIVEN THE STATE AT $t=0$ $|\psi(0)\rangle$ THE STATE AT A LATER TIME t IS UNIQUELY DETERMINED AS LONG AS NO MEASUREMENTS ARE PERFORMED!

ii) THUS THE PROBALISTIC, NON-DETERMINISTIC ASPECTS OF QM ARE <u>PURELY DUE TO THE COLLAPSE OF THE STATE UPON MEASUREMENT</u>!

iii) $\hat{H}$ IS THE HAMILTONIAN — THE OPERATOR CORRESPONDING TO THE ENERGY OF THE SYSTEM

iv) WE CAN FORMALLY INTEGRATE THE TDSE FROM TIME $= t_0$ TO t_f

$$|\psi(t_f)\rangle = e^{-i\hat{H}(t_f - t_0)/\hbar} |\psi(t_0)\rangle$$

WHERE THE EXPONENTIAL IS DEFINED BY ITS POWER SERIES

EG. $$e^{\hat{O}} = 1 + \hat{O} + \frac{\hat{O}^2}{2!} + \dots$$

SINCE $\hat{H} = \hat{H}^\dagger$ (HERMITIAN) THE OPERATOR

$$U \equiv e^{-i\hat{H}(t_f - t_0)/\hbar}$$

IS <u>UNITARY</u>

$$U^\dagger U = e^{i\hat{H}^\dagger(t_f - t_0)/\hbar} e^{-i\hat{H}(t_f - t_0)/\hbar}$$

$$= e^{i\hat{H}(t_f - t_0)/\hbar - i\hat{H}(t_f - t_0)/\hbar}$$

$$= 1$$

SO TIME EVOLUTION IS "UNITARY EVOLUTION"

HOW DO WE RECOVER WAVEFUNCTIONS?

CONSIDER POSITION OPERATOR $\hat{X}$. THIS HAS A CONTINUOUS SPECTRUM OF EIGENVALUES

$$\hat{X}\,|x\rangle = x\,|x\rangle$$

THE EIGENKETS $|x\rangle$ ARE NORMALIZED AS

$$\langle x | x' \rangle = \delta(x - x')$$

THIS IS ANALOGUE OF $\langle n|m\rangle = \delta_{nm}$ IN DISCRETE CASE

THE EXPANSION OF A NORMALIZED STATE $|\psi\rangle$ OF THE PARTICLE IN TERMS OF POSITION EIGENKETS READS

$$|\psi\rangle = \int dx \underbrace{\,|x\rangle\langle x|\psi\rangle}$$

ANALOGUE OF $\sum_n$

ANALOGUE OF $|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$

THE GENERAL RULES OF THE DIRAC FORMALISM TELL US THE INTERPRETATION OF $\langle x|\psi\rangle$

$\langle x|\psi\rangle$ = PROBABILITY AMPLITUDE THAT PARTICLE IN STATE $|\psi\rangle$ IS LOCATED AT x

IE, $\langle x|\psi\rangle$ IS <u>PRECISELY</u> WHAT WE PREVIOUSLY CALLED <u>THE WAVEFUNCTION</u>!

THE DESCRIPTION OF STATES BY WAVEFUNCTIONS IS CALLED THE "X-REPRESENTATION" (OR "COORDINATE REP'N"), AND SCHROEDINGER'S WAVE MECHANICS IS THE FORM QM TAKES IF THE COORDINATES OF A PARTICLE ARE ALL ONE CARES ABOUT (EG. IF NO SPIN, NO ANTIPARTICLE CREATION, ...)

WORTHWHILE TO EMPHASIZE THAT <u>ALL</u> ASPECTS OF WAVE MECHANICS CAN BE DERIVED FROM DIRAC

EG. OVERLAP

$$\langle \psi | \varphi \rangle = \langle \psi | \underbrace{\left(\int dx\, |x\rangle\langle x| \right)}_{\substack{\text{INSERTING THE} \\ \text{IDENTITY OPERATOR} \\ \text{IN X-REP'N,} \\ \text{c.f. } \hat{I} = \sum_n |n\rangle\langle n|}} | \varphi \rangle$$

$$= \int dx\, \langle \psi | x \rangle \langle x | \varphi \rangle$$

$$= \int dx\, \langle x | \psi \rangle^* \langle x | \varphi \rangle$$

$$= \int dx\, \psi^*(x)\, \varphi(x) \quad \checkmark$$

IN SUMMARY, WE HAVE SEEN THAT THE <u>PROBABILITY AMPLITUDE</u> IS THE CRUCIAL OBJECT IN QM THAT WE MUST COMPUTE TO SOLVE A PROBLEM FULLY

RULES FOR AMPLITUDES

- IN THE X-REPRESENTATION (IE USUAL WAVEFUNCTIONS) THE AMPLITUDES ARE JUST FOUND BY SOLVING THE TISE WITH APPROPRIATE BOUNDARY CONDITIONS (AND $\hat{H}$!)

- USEFUL TO STATE SOME VERY GENERAL RULES FOR PROB. AMPLITUDES THAT CAN BE DERIVED FROM DIRAC FORMULATION

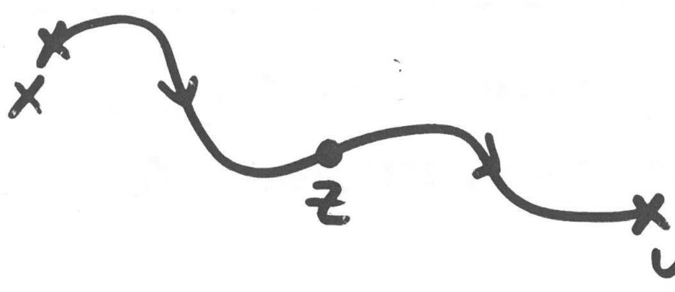
> LET'S DEFINE 'AN EVENT' IN AN EXPERIMENT TO BE A SITUATION IN WHICH ALL OF THE INITIAL AND FINAL CONDITIONS OF THE EXP'T ARE COMPLETELY SPECIFIED

IE, ALL POSITIONS, ANGULAR MOM'M, ..., OF ALL PARTICIPATING PARTICLES SPECIFIED

RULE 1: WHEN AN EVENT CAN OCCUR IN SEVERAL ALTERNATIVE WAYS, THE AMPLITUDE IS THE SUM OF THE AMPLITUDES FOR EACH WAY CONSIDERED SEPARATELY (SO GET INTERFERENCE)

RULE 2: THE AMPLITUDE FOR EACH SEPARATE WAY AN EVENT CAN OCCUR CAN BE WRITTEN AS THE PRODUCT OF THE AMPLITUDE FOR PART OF THE EVENT OCCURING THAT WAY WITH THE AMPLITUDE OF THE REMAINING PART

E.G. AMP (PARTICLE X $\rightarrow$ y)



$$\mathrm{Amp}(x \rightarrow y) = \mathrm{Amp}(x \rightarrow z) \cdot \mathrm{Amp}(z \rightarrow y)$$

$$\Longleftrightarrow \langle y|x\rangle = \langle y|z\rangle\langle z|x\rangle$$

CONVENTION

RULE 3: IF AN EXPERIMENT IS PERFORMED WHICH IS CAPABLE IN PRINCIPLE OF DETERMINING WHICH OF THE ALTERNATIVE WAYS ACTUALLY IS TAKEN (SO IN FACT NOT ALL FINAL CONDITIONS ARE THE SAME)

NOTE! NOT AMPLITUDES

THEN TOTAL PROBABILITY IS SUM OF PROBABILITIES FOR EACH ALTERNATIVE

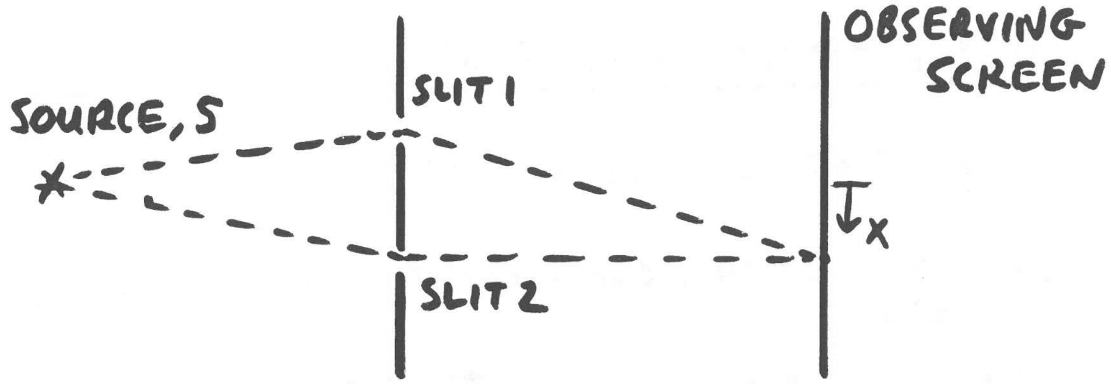
$$P_{TOT} = P_1 + P_2 + \ldots$$

(INTERFERENCE IS LOST)

NOTE: 'CAPABLE IN PRINCIPLE' DOESN'T MEAN THAT IT'S NECESSARY FOR A HUMAN (OR OTHER SENTIENT BEING) TO CHECK THAT ALL FINAL CONDITIONS ARE THE SAME (IT'S ENOUGH FOR THE STATE OF ONE ATOM TO BE DIFFERENT WHETHER WE'RE AWARE OR NOT!)

USEFUL TO MANIPULATE AMPLITUDES EVEN WHEN DON'T KNOW (YET) EXACTLY THEIR VALUE

EG. <u>TWO-SLIT INTERFERENCE</u>



$\langle 1|S\rangle$ = AMPLITUDE FOR PARTICLE TO GO FROM S TO SLIT 1

$\langle x|1\rangle$ = AMP. FOR SLIT 1 TO X ON SCREEN

SIMILAR FOR $\langle 2|S\rangle$ AND $\langle x|2\rangle$

SO <u>TOTAL AMP. FROM SOURCE S TO</u> X

$$AMP_{1+2} = \langle x|1\rangle\langle 1|S\rangle + \langle x|2\rangle\langle 2|S\rangle$$

<u>MULTIPLY AMPS. ALONG ROUTE</u>

<u>ADD DIFFERENT ROUTES</u>

$$\Rightarrow PROB(S \to X) = |TOTAL\ AMP.|^2$$

BECAUSE OF INTERFERENCE TERMS $\longrightarrow$ $\underline{\neq}$ $PROB(S\to 1\to X) + PROB(S\to 2\to X)$

$$= |\langle x|1\rangle\langle 1|S\rangle|^2 \qquad = |\langle x|2\rangle\langle 2|S\rangle|^2$$

LECTURE : CONSERVED QUANTITIES

IN CLASSICAL PHYSICS MANY CONSERVED QUANTITIES (ENERGY, MOM'M, ANG. MOM'M, ...)

WHAT ABOUT Q.M?

- CONSIDER EXPECTATION VALUE OF SOME OP. Q WHICH DOES NOT HAVE ANY EXPLICIT TIME-DEP. (EG. x OR $-i\hbar\,\partial/\partial x$)

$$\langle Q\rangle_\psi = \int_{-\infty}^{\infty} \psi^*(x,t)\, Q\, \psi(x,t)\, dx$$

BECAUSE ψ IS FUNCTION OF t WE WILL FIND, IN GENERAL, THAT $\langle Q\rangle_\psi$ IS A FUNCTION OF t ...

$$\frac{d\langle Q\rangle_\psi}{dt} = \int_{-\infty}^{\infty} \left\{ \left(\frac{\partial\psi^*}{\partial t}\right) Q\,\psi + \psi^* Q \frac{\partial\psi}{\partial t} \right\} dx$$

USE TDSE $H\psi = i\hbar \dfrac{\partial\psi}{\partial t}$ TO REPLACE t-DERIVATIVES

$$\frac{d\langle Q\rangle}{dt} = \int_{-\infty}^{\infty} \left\{ \left(\frac{H\psi}{i\hbar}\right)^* Q\,\psi + \psi^* Q\left(\frac{H\psi}{i\hbar}\right) \right\} dx$$

$$\text{RHS} = \frac{1}{i\hbar}\int_{-\infty}^{\infty}\left\{-\psi^* HQ\psi + \psi^* \underbrace{QH}\psi\right\}dx$$

BECAUSE H IS HERMITIAN

NOTE: BEING CAREFUL WITH ORDER!

$$= \frac{i}{\hbar}\int_{-\infty}^{\infty}\psi^*(HQ-QH)\psi\, dx$$

$$= \frac{i}{\hbar}\langle (HQ-QH)\rangle_\psi$$

- **Q IS A CONSERVED QUANTITY IF $\frac{d\langle Q\rangle}{dt}=0$ NO MATTER WHAT STATE ψ THE PARTICLE IS IN**

THIS CAN ONLY HAPPEN IF

$$\boxed{(HQ-QH)\psi = 0} \quad (*)$$

FOR ANY NORMALIZABLE FUNCTION ψ.

- THE OBJECT $HQ-QH$ IS CALLED THE COMMUTATOR OF H AND Q, DENOTED

$$[H,Q] \stackrel{\text{def}}{=} HQ-QH$$

THE STATEMENT THAT $[H, Q] = 0$ MEANS (*). WHEN WORKING OUT COMMUTATORS OF DIFFERENTIAL OPS. REMEMBER TO HAVE THEM ACT ON SOME ARBITRARY FN TO AVOID MISTAKES

EXAMPLE

SIMPLEST CASE IS $Q = 1$

$$\frac{d}{dt}\langle\psi|\psi\rangle = \frac{i}{\hbar}\langle\psi|\underbrace{[H,1]}|\psi\rangle = 0$$

AS $[A, 1] = 0$ FOR ANY OP. A

NAMELY, THE PROBABILITY IS CONSERVED INDEP'T OF TIME

$$\langle\psi|\psi\rangle = 1$$

IN FACT PROBABILITY (AND ALL OTHER CONSERVED QUANTITIES) ARE CONSERVED LOCALLY

$\Rightarrow$ IT FLOWS AROUND SATISFYING A LOCAL CONSERVATION EQN.

PROBABILITY CURRENT

$\rho = \psi^*\psi$ IS THE PROB. DENSITY

$$\Rightarrow \frac{\partial \rho}{\partial t} = \frac{\partial \psi^*}{\partial t}\psi + \psi^*\frac{\partial \psi}{\partial t} \qquad ①$$

BUT TDSE SAYS FOR 1D QM

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

$$\Rightarrow -i\hbar\frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* \qquad \text{(V IS REAL)}$$

THUS RHS OF ① ABOVE

$$= \frac{i}{\hbar}\left\{\left(-\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*\right)\psi - \psi^*\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right)\right\}$$

$$= -\frac{i\hbar}{2m}\left(\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right)$$

$$= -\frac{i\hbar}{2m}\underline{\nabla}\cdot\left(\psi\underline{\nabla}\psi^* - \psi^*\underline{\nabla}\psi\right)$$

DEFINING

$$\boxed{\underline{j} = \frac{i\hbar}{2m}\left(\psi\underline{\nabla}\psi^* - \psi^*\underline{\nabla}\psi\right)}$$

HAVE CONSERVATION EQN

$$\boxed{\frac{\partial \rho}{\partial t} + \underline{\nabla}\cdot\underline{j} = 0}$$

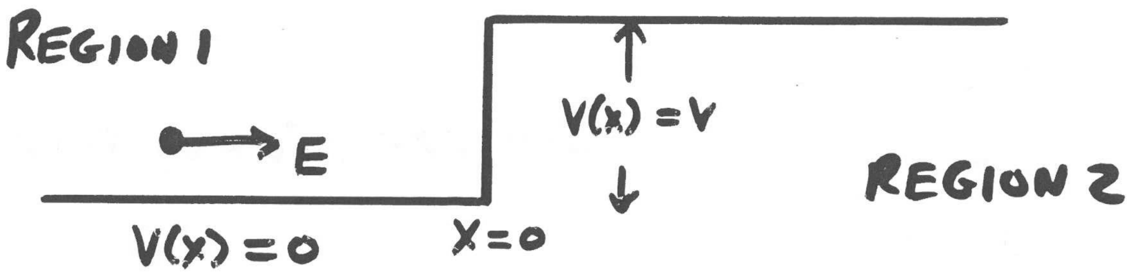
EXAMPLE: PLANE WAVE $e^{i(px-Et)/\hbar}$

$$j = \frac{-i\hbar}{2m}\left(e^{-ipx/\hbar}\frac{\partial}{\partial x}e^{ipx/\hbar} - c.c.\right)$$

$$= \frac{-i\hbar}{2m}\frac{2ip}{\hbar} = \frac{p}{m} = v$$

THE POTENTIAL STEP

APPLICATION OF CONS. OF PROB (AND SUPERPOSITION OF E'STATES)



CLASSICALLY A PARTICLE INCIDENT FROM LEFT WITH KE = E WITH E < V WILL BE REFLECTED BY BARRIER. WHAT HAPPENS IN QM?

PROCEDURE

- FIND GENERAL SOL'N TO TDSE IN EACH REGION

- MATCH SOL'NS AT $x=0$ USING **BOUNDARY CONDITIONS**

$$\boxed{\begin{array}{l} \text{i) } \psi(x,t) \text{ CONTINUOUS} \\ \text{ii) } \dfrac{\partial \psi(x,t)}{\partial x} \text{ CONTINUOUS} \end{array}}$$

NOTE: ii) APPLIES WHEN JUMP IN V IS **NOT** INFINITE

[• NORMALIZE SOL'N]

REGION 1

ALREADY KNOW THAT FREE ($V=0$) TDSE HAS SOL'N

$$\psi_1 = e^{-iEt/\hbar}\left(a e^{ikx} + b e^{-ikx}\right)$$

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

$p = \hbar k$
+ve TRAVELLING (INCOMMING)

$p = -\hbar k$
-ve TRVL'N WAVE (REFLECTED)

I WILL CHOOSE

$$a = 1, \quad b = r$$

SEE WHY SOON...

REGION 2:

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V\phi = E'\phi \qquad \psi_2 = \phi_2 e^{-iE't/\hbar}$$

SUPPOSE FOR MOMENT THAT $E > V$ THEN

$$\phi_2 = c e^{ik'x} + \underbrace{d e^{-ik'x}}_{} \qquad \frac{\hbar^2 k'^2}{2m} = E' - V$$

$-$ve TRAVELLING

BUT WE WANT PARTICLES ONLY INCIDENT FROM LEFT

SO $d = 0$

NOW IMPOSE BOUNDARY CONDITIONS:

i) $\psi_1(x,t) = \psi_2(x,t)$ AT $x = 0$ (FOR ALL t)

$\Rightarrow$ $E = E'$ (SO ENERGY CONS.)

ALSO $\phi_1(0) = \phi_2(0)$

$\Rightarrow$ $1 + r = c$

ii) $\phi_1'(0) = \phi_2'(0)$ ($e^{-iEt/\hbar}$ CANCEL)

$ik(1-r) = ik'c$

SO $$\boxed{r = \frac{1 - k'/k}{1 + k'/k}, \quad c = \frac{2}{1 + k'/k}}$$

<u>NOTE</u>: WE FIND $a \neq 0$ — A TRANSMITTED WAVE AS EXPECTED (FOR <u>E > V</u>)
<u>BUT ALSO $r \neq 0$</u> — THERE IS <u>A REFLECTED WAVE TOO</u> (<u>CLASSICALLY</u> FOR E > V, <u>NO REFLECTION</u>)!

• <u>LET'S NOW CALCULATE PROB. FLUXES</u>

• IN REGION 2

$$j_2 = \frac{-i\hbar}{2m}\left\{\left(c e^{i(k'x - Et/\hbar)}\right)^* \frac{\partial}{\partial x} c e^{i(k'x - Et/\hbar)} - c.c.\right\}$$

$$= \frac{\hbar k'}{m}|c|^2 \quad \text{(NOT JUST } |c|^2\text{!)}$$

• IN REGION 1 GET

$$j_1 = \underbrace{\frac{\hbar k}{m}}_{\text{INCIDENT}} + \underbrace{|r|^2 \frac{\hbar(-k)}{m}}_{\text{REFLECTED}}$$

WHAT WE CARE ABOUT IS PROBABILITY OF REFLECTION OR TRANSMISSION. THESE ARE GIVEN BY RATIOS

REFLECTED FLUX / INCIDENT FLUX $= R$

$$\text{TRANSMITTED FLUX} / \underbrace{\text{INCIDENT FLUX}} = T$$

SINCE WE DIVIDE BY THIS DO NOT NEED TO NORMALIZE REGION 1 WAVE (EASIEST TO TAKE COEFFS 1, r)

FIND

$$R = \frac{|r|^2 \hbar k/m}{\hbar k/m} = |r|^2 = \left(\frac{k-k'}{k+k'}\right)^2$$

$$T = \frac{\hbar k'/m \, |c|^2}{\hbar k/m} = \frac{k'}{k}|c|^2 = \frac{4kk'}{(k+k')^2}$$

NOTE THAT $R+T=1$ ✓ (TOT. PROB = 1)

WHAT HAPPENS IF $E<V$?

NOW SOL.'N IN REGION 2 IS

$$\phi_2 = c\,e^{-\kappa x} + \underbrace{d e^{\kappa x}} \qquad \frac{\hbar^2\kappa^2}{2m} = V-E$$

EXPLODES AS $x \to +\infty$
PHYSICALLY IMPOSSIBLE
$\Rightarrow d = 0$

AGAIN, MATCHING SOL'NS AT BOUNDARY

$$1 + r = c$$

$$ik(1-r) = -Kc$$

SO $$r = \frac{1 - iK/k}{1 + iK/k}, \quad c = \frac{2}{1 + iK/k}$$

NOW FIND

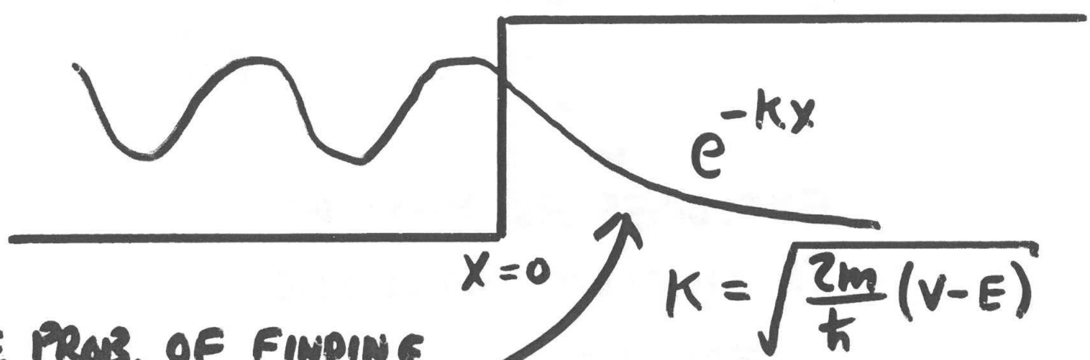
$$R = |r|^2 = 1$$ <u>ALL REFLECTED</u>

AND $$j_2 = \frac{-i\hbar}{2m} |c|^2 \left(e^{-kx} \frac{\partial}{\partial x} e^{-kx} - c.c. \right)$$

$$= 0$$ SO NONE TRANSMITTED ✓

NOTE HOWEVER THE

WAVEFUNCTION <u>DOES</u> PENETRATE INTO THE <u>CLASSICALLY FORBIDDEN REGION</u> !



FINITE PROB. OF FINDING PARTICLE HERE!