3) We now know that non-commuting operators (say A & B) cannot be observed precisely at the same time. To what extent the observation of $\langle A \rangle$ is imprecise in the presence of B, and $\langle B \rangle$ is imprecise in the presence of A, is answered by <u>Heisenberg's</u> <u>Uncertainty</u> <u>Relation</u>. In general, we claim...

$$\boxed{\text{If } A \,\&\, B \text{ are Hermitian operators that obey the commutation rule } [A,B] = iC, \text{ then the product of variances is: } \Delta A\, \Delta B \geq \tfrac{1}{2}|\langle C \rangle|.} \tag{12}$$

The "variances" ΔA & ΔB are just the rms deviations defined in Eq.(4) above. The expectation value $\langle C \rangle = \langle \psi | C \psi \rangle = \int \psi^* C \psi \, dx$ is evaluated w.r.t. the same wavefcn ψ used to define ΔA & ΔB. If (12) is true, then a precise statement of the position-momentum, and energy-time, uncertainty relations is//

$$\underline{\Delta x \Delta p \geq \tfrac{1}{2}\hbar}, \quad \underline{\Delta E \Delta t \geq \tfrac{1}{2}\hbar}. \tag{13}$$

Equality holds only if the QM system is specified by a certain special wavefcn ψ; for other wavefcns, the inequality ($>$) is in force. Later, we will find the special ψ... for now, we want to prove Eq.(12).

Proof of the Schwarz Inequality.

The proof of Heisenberg's Relation in Eq. (12) uses a mathematical result known as the Schwarz Inequality, which we now proceed to prove.

Let P be a positive definite Hermitian operator, i.e. $\langle\psi|P\psi\rangle$ is real and $\geqslant 0$ for all ψ. Let $\psi = f + \lambda g$, w/ f & g ~ arbitrary fcns, and λ = cnst (to be chosen). Then it follows that: $\underline{\underline{\langle f|Pf\rangle\langle g|Pg\rangle \geqslant |\langle f|Pg\rangle|^2}}$. (14)

PROOF With $\psi = f + \lambda g$, we calculate...

$$\rightarrow \langle\psi|P\psi\rangle = \langle f+\lambda g|P(f+\lambda g)\rangle = \langle f|Pf\rangle + \lambda\langle f|Pg\rangle +$$

$$+ \lambda^*\langle g|Pf\rangle + |\lambda|^2\langle g|Pg\rangle \geqslant 0. \quad (15A)$$

Now choose λ = cnst to be...

$$\rightarrow \lambda = -\langle g|Pf\rangle/\langle g|Pg\rangle = -\langle f|Pg\rangle^*/\langle g|Pg\rangle \quad (15B)$$

have used P = Hermitian in 2nd eqtn here.

Put this λ into (15A) to get...

$$\rightarrow \langle f|Pf\rangle - \left(\frac{\langle f|Pg\rangle^*}{\langle g|Pg\rangle}\right)\langle f|Pg\rangle - \left(\frac{\langle g|Pf\rangle^*}{\langle g|Pg\rangle}\right)\langle g|Pf\rangle + \frac{|\langle g|Pf\rangle|^2}{\langle g|Pg\rangle^2}\langle g|Pg\rangle \geqslant 0,$$

or//

$$\langle f|Pf\rangle\langle g|Pg\rangle - |\langle f|Pg\rangle|^2 - \underbrace{|\cancel{\langle g|Pf\rangle}|^2 + |\cancel{\langle g|Pf\rangle}|^2}_{\text{cancel}} \geqslant 0,$$

i.e.//

$$\underline{\underline{\langle f|Pf\rangle\langle g|Pg\rangle \geqslant |\langle f|Pg\rangle|^2}} \quad (15C)$$

for P a (+)ve definite Hermitian operator, and f & g arbitrary fcns. **QED**

REMARKS On Schwarz' Inequality, Eq. (15C).

1. Choose $P=1$ (manifestly a (+)ve definite Hermitian "operator"). Then (15C) $\Rightarrow$

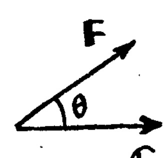
$$\boxed{\langle f|f\rangle\langle g|g\rangle \geqslant |\langle f|g\rangle|^2}, \text{ i.e.// } \left(\int f^* f\,dx\right)\left(\int g^* g\,dx\right) \geqslant \left|\int f^* g\,dx\right|^2. \quad (15D)$$

This relation is usually called Schwarz' Inequality, even with (15C) available.

2. (15D) is similar to the vector inequality...

$$(\mathbb{F}\cdot\mathbb{F})(\mathbb{G}\cdot\mathbb{G}) \geqslant (\mathbb{F}\cdot\mathbb{G})^2;$$

i.e.// $F^2G^2 \geqslant (FG\cos\theta)^2$, or: $1 \geqslant \cos^2\theta$



NOTE: equality holds only when $\mathbb{F}$ & $\mathbb{G}$ collinear. (15E)

Proof of Heisenberg's Proposition in Eq. (12).

4) With the Schwarz Inequality in hand, proof of Heisenberg's Relation in Eq. (12) is straightforward. We want the rms deviations...

$$(\Delta A)^2 = \langle\psi|(A-\langle A\rangle)^2|\psi\rangle = \langle(A-\langle A\rangle)\psi|(A-\langle A\rangle)\psi\rangle, \text{ A is Hermitian;}$$

and//

$$(\Delta B)^2 = \langle(B-\langle B\rangle)\psi|(B-\langle B\rangle)\psi\rangle, \text{ similarly.} \tag{16}$$

Now define: $\underline{f = (A-\langle A\rangle)\psi}$, $\underline{g = (B-\langle B\rangle)\psi}$. The Schwarz Inequality of Eq. (15D) allows us to write... (w/ A & B Hermitian)...

$$\rightarrow (\Delta A)^2(\Delta B)^2 \geqslant |\underbrace{\langle(A-\langle A\rangle)\psi|(B-\langle B\rangle)\psi\rangle}|^2$$

$$= \langle\psi|(A-\langle A\rangle)(B-\langle B\rangle)\psi\rangle. \tag{17}$$

Rewrite the operator appearing here, i.e. $(A-\langle A\rangle)(B-\langle B\rangle)$, as...

$$\rightarrow (A-\langle A\rangle)(B-\langle B\rangle) = R + S; \tag{18}$$

w// $\underline{\underline{R}} = \frac{1}{2}[(A-\langle A\rangle)(B-\langle B\rangle) + (B-\langle B\rangle)(A-\langle A\rangle)]$, $\surd$ symmetrized product

&// $\underline{\underline{S}} = \frac{1}{2}[(A-\langle A\rangle)(B-\langle B\rangle) - (B-\langle B\rangle)(A-\langle A\rangle)]$. $\surd$ antisymmetrized product

Upon simplification, S reduces to...*

$$\rightarrow S = \frac{1}{2}(AB - BA) = \frac{1}{2}[A,B] = \frac{1}{2}iC \quad \surd \text{ by hypothesis... } [A,B] = iC, \text{ in Eq. (12).} \tag{19}$$

So// Eq. (17) $\Longrightarrow$ $\underline{\underline{(\Delta A)^2(\Delta B)^2 \geqslant |\langle\psi|(R+\frac{1}{2}iC)\psi\rangle|^2}}$. (20)

Note that both R & C are <u>Hermitian</u> operators, since A & B are Hermitian (show this as an exercise), so both $\langle R\rangle$ and $\langle C\rangle$ are <u>real</u>. Then, in (20)...

$$\rightarrow (\Delta A)^2(\Delta B)^2 \geqslant |\langle R\rangle + \tfrac{1}{2}i\langle C\rangle|^2 = \langle R\rangle^2 + \tfrac{1}{4}\langle C\rangle^2 \geqslant |\tfrac{1}{2}\langle C\rangle|^2,$$

i.e.// $\boxed{\Delta A\,\Delta B \geqslant \frac{1}{2}|\langle C\rangle| = \frac{1}{2}|\langle[A,B]\rangle|}$. **QED** (21)

This proves Heisenberg's proposition as quoted in Eq. (12) on p. Prop. 20.

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* Similarly, a reduction for R shows that: $\langle R\rangle = \langle\frac{1}{2}[A,B]\rangle + \langle BA\rangle - \langle B\rangle\langle A\rangle$.

The "special" wavefcn ψ for which $\Delta A\,\Delta B \to \frac{1}{2}|\langle[A,B]\rangle|$, minimum.

5) At bottom of p. Prop. 20, we said we would find the "special" wavefcn ψ for which the uncertainty product is a minimum, i.e. that ψ for which: $\Delta A\,\Delta B = \frac{1}{2}|\langle C\rangle|$, in Eq. (21). We can now write an operator equation for the ψ that guarantees this condition. Thus, we address the question:

$$\rightarrow \text{For what } \psi \text{ does: } \Delta A\,\Delta B \to \tfrac{1}{2}|\langle C\rangle|, \text{ minimum?} \tag{22}$$

Start from the full inequality in Eq. (21), viz.

$$\rightarrow (\Delta A)^2(\Delta B)^2 \geqslant \langle R\rangle^2 + \tfrac{1}{4}\langle C\rangle^2 \geqslant |\tfrac{1}{2}\langle C\rangle|^2 \tag{23}$$

get equality only when $\langle R\rangle \equiv 0$.

In the language of the Schwarz Inequality, Eq. (15D), the requirement is:

$$\rightarrow \langle f|f\rangle\langle g|g\rangle \geqslant |\langle f|g\rangle|^2, \tag{24}$$

get equality only when $g = \mu f$, w/ μ = cnst — i.e. the "vectors" g & f are collinear

w/ $f = (A - \langle A\rangle)\psi$ & $g = (B - \langle B\rangle)\psi$, per definitions below Eq. (16), p. Prop. 22. The "collinearity" condition on g & f here imposes a condition on ψ, viz.

$$(B - \langle B\rangle)\psi = \mu\,(A - \langle A\rangle)\psi, \text{ w/ } \mu = \text{cnst}. \tag{25}$$

So the following expectation values can be written in the form...

$$\begin{cases} \langle\psi|(A-\langle A\rangle)(B-\langle B\rangle)\psi\rangle = \mu\langle\psi|(A-\langle A\rangle)^2\psi\rangle = \mu(\Delta A)^2; & (26A) \\ \langle\psi|(B-\langle B\rangle)(A-\langle A\rangle)\psi\rangle = \frac{1}{\mu}(\Delta B)^2. & (26B) \end{cases}$$

These follow from Eq. (25), and the def$^{\underline{n}}$ of the QM variance in Eq. (5)

Now, add and subtract these eqtns...

$$\begin{cases} (26A) + (26B) = \mu(\Delta A)^2 + \frac{1}{\mu}(\Delta B)^2 = 2\langle R\rangle = 0; \\ (26A) - (26B) = \mu(\Delta A)^2 - \frac{1}{\mu}(\Delta B)^2 = 2\langle S\rangle = i\langle C\rangle. \end{cases} \tag{27}$$

The operators R & S in (27) are as defined in Eq. (18) above. The condition that $\langle R\rangle = 0$ follows from Eq. (23), while: $2S = iC$, was established in Eq. (19). Solving Eqs. (27) for the cnst μ, we find...

$$\rightarrow 2\mu(\Delta A)^2 = i\langle C\rangle, \quad \text{i.e.}/\!/ \quad \underline{\underline{\mu = i\langle C\rangle/2(\Delta A)^2}}. \tag{28}$$

Insert this result in Eq. (25) to find, finally...

$$\boxed{(B-\langle B\rangle)\psi = [i\langle C\rangle/2(\Delta A)^2](A-\langle A\rangle)\psi}. \tag{29}$$

For that ψ which satisfies this general operator eqtn, the uncertainty product: $(\Delta A)(\Delta B) = \frac{1}{2}|\langle[A,B]\rangle|$, is a minumum.

EXAMPLE $\underline{\psi(\text{minimum uncertainty}) \text{ for position-momentum operators}}$.

Let: $A = x$, $B = p = -i\hbar\frac{\partial}{\partial x}$, so that $\langle C\rangle = |\langle[x,p]\rangle| = \hbar$.

$$\text{Eq. (29)} \Rightarrow -\left(i\hbar\frac{\partial}{\partial x} + \bar{p}\right)\psi = \left[\frac{i\hbar}{2(\Delta x)^2}\right](x-\bar{x})\psi \quad \int^{\text{W}} \bar{p} = \langle p\rangle,\ \bar{x} = \langle x\rangle,\ (\Delta x)^2 = \langle(x-\bar{x})^2\rangle;$$

or// $$\underline{\frac{\partial\psi}{\partial x} = \left[-\frac{(x-\bar{x})}{2(\Delta x)^2} + i\bar{k}\right]\psi}, \text{ where } \bar{k} = \bar{p}/\hbar \text{ (mean wave \#)}. \tag{30}$$

The solution to this first-order ODE is a $\underline{\text{Gaussian}}$...

$$\left[\!\left[\ \psi(x) = \underbrace{\left(1/[2\pi(\Delta x)^2]^{1/4}\right)}_{\text{norm}^{\underline{\text{z}}}\text{n cnst chosen so that } \int_{-\infty}^{\infty}|\psi(x)|^2 dx = 1.} \exp\left\{-\frac{(x-\bar{x})^2}{4(\Delta x)^2} + i\bar{k}x\right\}, \right.\right. \tag{31}$$

for which $|\psi(x)|^2$ signifies a perfectly random process. For this wavefcn, the uncertainty product $\Delta x\Delta p = \frac{1}{2}\hbar$ is as small as possible. Not surprisingly, the momentum wavefcn is also $\underline{\text{Gaussian}}$ (random):

$$\left[\!\left[\ \varphi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)e^{-ikx}dx = \left(1/[2\pi(\Delta k)^2]^{\frac{1}{4}}\right)\exp\left\{-\frac{(k-\bar{k})^2}{4(\Delta k)^2} - i(k-\bar{k})x\right\}. \right.\right. \tag{32}$$

SUMMARY : Schrödinger's Eqtn and Properties of Wave Mechanics.

Derivation of Schrödinger's Eqtn for m in an External Field

- Retain notion of a QM system described by a (localized) wavefunction ψ.
- Impose classical forms for (expectation value) motion of m : $\langle p\rangle = m\frac{d}{dt}\langle x\rangle$, $\langle F\rangle = \frac{d}{dt}\langle p\rangle$.

① find : $\boxed{i\hbar(\partial\psi/\partial t) = \mathcal{H}\psi}$ w/ $\mathcal{H} = (\mathbb{p}^2/2m) + V(\mathbf{r},t)$) $\mathbb{p} = -i\hbar\nabla$, momentum op$^{\text{r}}$, V = P.E. of the external field.

② the P.E. fcn V must be real to ensure probability conservation (i.e. $\int_\infty |\psi|^2 d^3r = 1$).

③ continuity eqtn still applies : $\boxed{\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbb{J} = 0}$) w/ $\rho = \psi^*\psi = |\psi|^2$, and $\mathbb{J} = \mathrm{Re}\{\psi^*(\hbar/im)\nabla\psi\}$, even w/ $V \neq 0$.

④ $\mathcal{H} = i\hbar\,\partial/\partial t$ is the system's Hamiltonian, i.e. the total energy operator.

⑤ when V is time-independent, system wavefcn is : $\psi(\mathbf{r},t) = u(\mathbf{r})e^{-(i/\hbar)Et}$, i.e. a "stationary state" w/ energy E = cnst, and : $\mathcal{H}u = [-(\hbar^2/2m)\nabla^2 + V]u = Eu$.

Properties of the QM Hamiltonian operator $\mathcal{H}$

- From the form of Schrödinger's Eqtn : $i\hbar(\partial\psi/\partial t) = \mathcal{H}\psi$, and its interpretation, conclude :

① $\mathcal{H}$ is a linear operator, for which a superposition of solutions ψ is possible.

② since probability is conserved ($\frac{\partial}{\partial t}\int_\infty |\psi|^2 d^3r = 0$), then $\mathcal{H}$ is a Hermitian operator, w/ $\int_\infty (\mathcal{H}\psi)^*\psi\, d^3r = \int_\infty \psi^*(\mathcal{H}\psi)\, d^3r$. The expectation value $\langle\mathcal{H}\rangle$ is therefore real.

③ now adopt Dirac's bra-ket notation : $\langle f|g\rangle = \int_\infty f^* g\, d^3r$.

④ $\mathcal{H}$ Hermitian $\Rightarrow$ $\mathcal{H}$ is "self-adjoint" : $\langle f|\mathcal{H}^\dagger g\rangle = \langle \mathcal{H}f|g\rangle = \langle f|\mathcal{H}g\rangle$, so/ $\mathcal{H}^\dagger = \mathcal{H}$.

⑤ the stationary-state eigenvalue eqtn : $\mathcal{H}u = Eu$, (usu.) generates a discrete set of "eigenfunctions" $\{u_n\}$ as solutions. The state u_n has a discrete "eigenenergy" E_n. For different energies, states m & n are "orthonormal" : $\langle u_m|u_n\rangle = \delta_{mn}$ (result of $\mathcal{H}$ Herm$^{\text{n}}$).

Functional Conditions on Acceptable System Wavefcns ψ

- When the P.E. fcn V is finite, ψ & $\nabla\psi$ should be finite & continuous everywhere. If $V\to\infty$ at some point, ψ remains finite & continuous there, while $\nabla\psi$ is finite but discontinuous

① these conditions $\leftrightarrow$ both position probabilities ($d\mathcal{P} = \psi^*[1]\psi\, d^3r$) and momentum changes ($d\mathbb{p} = \psi^*[-i\hbar\nabla]\psi\, d^3r$) are finite & continuous everywhere.

② these conditions alone are sufficient to ensure that in a bound-state problem : $\mathcal{H}u = Eu$, the wavefcns $u\to u_n$ and energies $E\to E_n$ will be discrete (i.e. eigenvalues).

(next page)

SUMMARY (cont'd)

Quantum-Mechanical Eqtn-of-Motion

- Assume: max$^{\underline{m}}$ information available re QM dynamical variable $Q = Q(\mathbf{r}, \mathbf{p}, t)$ is the expectation value: $\langle Q \rangle = \int_\infty \psi^*(\mathbf{r},t)\{Q\}\psi(\mathbf{r},t)\,d^3r$ = fcn of time t (possibly).
- With $i\hbar(\partial\psi/\partial t) = \mathcal{H}\psi$, and ψ governing $\langle Q \rangle$, $\mathcal{H}$ must govern t-dependence of $\langle Q \rangle$.

① combine these notions to find: $\boxed{\frac{d}{dt}\langle Q \rangle = \frac{i}{\hbar}\langle[\mathcal{H}, Q]\rangle + \langle \partial Q/\partial t \rangle}$, the QM eqtn-of-motion. The symbol $\underline{[A,B] = AB - BA}$ is the "commutator" of operators A & B.

② commutator examples: $[x_k, p_\ell] = i\hbar\delta_{k\ell}$, $[x, Q] = i\hbar(\partial Q/\partial p)$, $[Q, p] = i\hbar(\partial Q/\partial x)$.

③ ~ easily show: $\frac{d}{dt}\langle x \rangle = \langle \partial\mathcal{H}/\partial p \rangle$, $\frac{d}{dt}\langle p \rangle = \langle -\partial\mathcal{H}/\partial x \rangle$; Hamilton's eqtns hold.

QM Observability & Heisenberg's Uncertainty Relations

- For QM operators A & B, anticipate: $\underline{\Delta A \Delta B \sim |\langle[A,B]\rangle|}$ (suggested by $\Delta x \Delta p \sim \hbar$).
- Define QM uncertainty ΔA by variance: $\underline{(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle}$.
- QM observability $\begin{cases} \text{I. } \langle A \rangle = a, \text{ a definite (certain) value iff } \Delta A = 0; \\ \text{II. } \Delta A = 0 \text{ iff } A\psi = a\psi, \text{ state } \psi \text{ in question is an eigenfcn of A.} \end{cases}$

① A & B are both observable in the same state ψ iff $[A,B] = 0$.

② if $[A,B] = iC$, then $\boxed{\Delta A \Delta B \geq \frac{1}{2}|\langle C \rangle|}$, per Heisenberg.

If A & B do *not* commute, they cannot be observed simultaneously in state ψ.

③ for most states ψ (even eigenstates): $\Delta A \Delta B > \frac{1}{2}|\langle C \rangle|$. Equality results ($\Delta A \Delta B = \frac{1}{2}|\langle C \rangle|$) only when: $(B - \langle B \rangle)\psi = \mu(A - \langle A \rangle)\psi$, with: $\mu = i\langle C \rangle / 2(\Delta A)^2$.

NOTE We have arrived at the above listing of properties and characteristics of QM theory in an empirical and inductive fashion... this is the way the theory must work in order to accommodate wave-particle duality (as expressed by: $\Delta x \Delta p \geq \hbar/2$, and: $\Delta E \Delta t \geq \hbar/2$), and this is the way the theory should work so as to allow a dynamical interpretation (expressed by: $i\hbar\,\partial\psi/\partial t = \mathcal{H}\psi$, and: $\frac{d}{dt}\langle Q \rangle = \frac{i}{\hbar}\langle[\mathcal{H}, Q]\rangle + \langle \dot{Q} \rangle$)

Alternatively, it is possible to construct a QM theory in a purely theoretical and deductive fashion, by starting from a number of postulates. This is what Dirac did when (in ~1927) he was searching for a relativistic generalization of the above. We will cover Dirac's work later in this course. For now, it is worth surveying Dirac's postulates as abstractions of our theory so far.