3. BRAs, KETs & OPERATORS – THE MATHEMATICS OF QUANTUM MECHANICS

This section will be a little more formal, but hopefully you'll recognise what we've already seen as a specific case of the generalities.

KETS

The state vectors we've been using $|\alpha\rangle$, form what is known as a complex vector space and which may be finite (as in the previous example), or infinite in which case it is known as a 'Hilbert' space.

Dirac called the object $|\alpha\rangle$ a "ket", the label α should tell us all that can be asked physically about the state.

There are mathematical rules for kets:

* Kets can be added : $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$, the result is also a ket

* multiplying a ket by a complex number gives another ket
  $c|\alpha\rangle = |\alpha\rangle c$ (numbers "commute" with kets)

* the physical state corresponding to $c|\alpha\rangle$ is the same as that for $|\alpha\rangle$

* observables (things like momentum, position ...) can be represented by <u>operators</u> which act on kets from the left giving another ket

$$A|\alpha\rangle = |\beta\rangle$$

there are a certain set of kets that when acted on by A become a constant times themself, ie.

$$A|a_i\rangle = a_i|a_i\rangle$$

these are known as the <u>eigenkets</u> or the <u>eigenstates</u> of A. The numbers a_i are known as the <u>eigenvalues</u>.

→ we've already seen these – the eigenkets of the operator S were $|S+\rangle$ with eigenvalue $+\frac{1}{2}$ $\quad S|S+\rangle = +\frac{1}{2}|S+\rangle$
& $|S-\rangle$ with eigenvalue $-\frac{1}{2}$. $\quad S|S-\rangle = -\frac{1}{2}|S-\rangle$

(BRAS)

We've also been using objects denoted $\langle\alpha|$ – this is called a "bra". The space of bra's is considered to be "dual" to the space of kets. This is fancy mathematical language – basically for each ket there is a corresponding bra:

$$|\alpha\rangle \leftrightarrow \langle\alpha|$$

the 'dual' to the sum is straightforward $\quad |\alpha\rangle + |\beta\rangle \leftrightarrow \langle\alpha| + \langle\beta|$

there is a slight subtlety with $c|\alpha\rangle$: $\quad c|\alpha\rangle \leftrightarrow c^*\langle\alpha|$

The name for the amplitude contraction we've been using, $\langle\beta|\alpha\rangle$ is the <u>inner product</u>. In order to have conservation of probability we required that

$$\underline{\langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle}$$

(origin of the names - bra-ket = bracket)

It follows that $\langle\alpha|\alpha\rangle$ is real since $\langle\alpha|\alpha\rangle^* = \langle\alpha|\alpha\rangle$. We also insist that $\langle\alpha|\alpha\rangle \geq 0$.

We say that two kets, $|\alpha\rangle, |\beta\rangle$ are <u>orthogonal</u> if $\langle\alpha|\beta\rangle = 0$, or equivalently $\langle\beta|\alpha\rangle = 0$.

We already saw that the basis states $|S+\rangle, |S-\rangle$ have this property.
Another example would be

$$\left.\begin{aligned} |\alpha\rangle &= |S+\rangle + |S-\rangle \\ |\beta\rangle &= |S+\rangle - |S-\rangle \end{aligned}\right\} \langle\alpha|\beta\rangle = \langle S+|S+\rangle - \langle S-|S-\rangle = \underline{0}$$

We will usually normalise states such that $\langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1$, this is easily done by multiplying by a real number $\quad |\tilde{\alpha}\rangle = \frac{1}{\sqrt{\langle\alpha|\alpha\rangle}}|\alpha\rangle$

OPERATORS

Operators act on kets to give other kets $X|\alpha\rangle = |\beta\rangle$.
Two operators X, Y are equal if $X|\alpha\rangle = Y|\alpha\rangle$ for any ket in the vector space.
Operators can be added, this is commutative & associative, just like addition of regular numbers

$$X + Y = Y + X$$
$$X + (Y + Z) = (X + Y) + Z$$

We'll mostly deal with <u>linear</u> operators, i.e.

$$X\left(c|\alpha\rangle + d|\beta\rangle\right) = cX|\alpha\rangle + dX|\beta\rangle$$

Operators act on bras from the right $\langle\alpha|X = \langle\beta|$.

In general <u>$\langle\alpha|X$ is not dual to $X|\alpha\rangle$</u>, rather the duality is

between $X|\alpha\rangle \longleftrightarrow \langle\alpha|X^{\dagger}$ where the operator

$X^{\dagger}$ is called the Hermitian adjoint of X. An operator is hermitian if $X^{\dagger} = X$.

Operators can be multiplied, they are in general <u>not</u> commutative,

$$\underline{XY \neq YX}$$

but they are associative

$$X(YZ) = (XY)Z = XYZ$$

<u>$(XY)^{\dagger} = Y^{\dagger}X^{\dagger}$</u> since $XY|\alpha\rangle = X|\beta\rangle$; $Y|\alpha\rangle = |\beta\rangle$
$X|\beta\rangle \leftrightarrow \langle\beta|X^{\dagger}$; $Y|\alpha\rangle \leftrightarrow \langle\alpha|Y^{\dagger}$
$XY|\alpha\rangle \leftrightarrow \langle\alpha|Y^{\dagger}X^{\dagger}$.

Operators can be formed by the <u>outer product</u> of bras & kets : $|\alpha\rangle\langle\beta|$

Objects of great interest to us will be things like

$$\langle\beta|X|\alpha\rangle$$

which will be suggestively referred to as "matrix elements".

note that $\langle\beta|X|\alpha\rangle = \langle\beta|\gamma\rangle = \left(\langle\gamma|\beta\rangle\right)^{*} = \left(\langle\alpha|X^{\dagger}|\beta\rangle\right)^{*}$

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X^{\dagger}|\beta\rangle^{*}$$

HERMITIAN OPERATORS

We'll have cause to deal mostly with Hermitian operators, ie those satisfying $A^\dagger = A$, since we'll find that these often represent an observable.

Hermitian operators have two important properties
1. their eigenvalues are real
2. their eigenkets form an orthogonal set

let's prove these statements:

$$A|a_i\rangle = a_i|a_i\rangle \qquad \text{"eigen-equation"}$$

$$\Rightarrow \langle a_j|A^\dagger = \langle a_j|A = \langle a_j|a_j^*$$

$$\left.\begin{aligned} \text{hence } \langle a_j|A|a_i\rangle &= a_i\langle a_j|a_i\rangle \\ \& \langle a_j|A|a_i\rangle &= a_j^*\langle a_j|a_i\rangle \end{aligned}\right\} \; 0 = (a_i - a_j^*)\langle a_j|a_i\rangle$$

now say $i=j$ then $a_i - a_i^* = 0 \Rightarrow \underline{a_i \text{ is real}}$

say $i \neq j$ then $(a_i - a_j)\langle a_i|a_j\rangle = 0$ & provided there are not two eigenkets with the same eigenvalue, $\langle a_i|a_j\rangle = 0$

$\Rightarrow |a_i\rangle, |a_{j\neq i}\rangle$ are orthogonal.

If we normalise to 1 we have an "orthonormal" set $\langle a_i|a_j\rangle = \delta_{ij}$

The set is proposed to be complete - the whole ket space is spanned by the eigenkets $|a_i\rangle$.

We can use these eigenkets as "basis" kets (just like we used $|S+\rangle, |S-\rangle$, or in conventional vector analysis we use $\hat{x}, \hat{y}, \hat{z}$). We can expand an arbitrary ket in terms of these basis kets:

$$\underline{|\alpha\rangle = \sum_i c_i |a_i\rangle} \qquad \text{where the } c_i \text{ are complex numbers}$$

$$\langle a_j|\alpha\rangle = \sum_i c_i \langle a_j|a_i\rangle = \sum_i c_i \delta_{ij} = c_j \qquad \underline{c_j = \langle a_j|\alpha\rangle}$$

recall the transformation from S-basis to T-basis previously

$$\underline{|\alpha\rangle = \sum_i |a_i\rangle\langle a_i|\alpha\rangle}$$

we can consider $\sum_i |a_i\rangle\langle a_i|$ to be an operator that leaves a state unchanged upon multiplication. This is the identity operator

$$\mathbb{1} = \sum_i |a_i\rangle\langle a_i| \qquad \text{"completeness" or "closure"}$$

MATRIX REPRESENTATIONS

This abstract notion of bra's, ket's and operators is all well and good, but we've all put effort into learning a bunch of mathematical techniques for more concrete objects like matrices & functions. Is there any way that we can 'represent' our system in terms of these things?

Fortunately there is. Consider using the eigenkets of some Hermitian operator A as a basis. Since $1 = \sum_i |a_i\rangle\langle a_i|$ we can write the following for an operator X:

$$X = \sum_i \sum_j |a_j\rangle\langle a_j|X|a_i\rangle\langle a_i| \; .$$

If there are N eigenkets $|a_i\rangle$, there are N^2 complex numbers $\langle a_j|X|a_i\rangle$.

We'll write these numbers as a matrix

$$X \rightsquigarrow \begin{bmatrix} \langle a_1|X|a_1\rangle & \langle a_1|X|a_2\rangle & \langle a_1|X|a_3\rangle & \cdots \\ \langle a_2|X|a_1\rangle & \langle a_2|X|a_2\rangle & \langle a_2|X|a_3\rangle & \cdots \\ \vdots & & \ddots & \end{bmatrix} = X_{ji}$$

Since $\langle a_j|X|a_i\rangle = \langle a_i|X^\dagger|a_j\rangle^*$ we see that the hermitian conjugate $X^\dagger$ is represented by the complex transpose of the matrix representing X.

If operators can be represented by matrices, products of operators should be represented by matrix products:

say $Z = XY$

then $\langle a_j|Z|a_i\rangle = \langle a_j|XY|a_i\rangle = \langle a_j|X \cdot 1 \cdot Y|a_i\rangle$

$$= \sum_k \langle a_j|X|a_k\rangle\langle a_k|Y|a_i\rangle$$

or $Z_{ji} = \sum_k X_{jk} Y_{ki}$ – the usual rule of matrix multiplication.

Notice that this representation extends to kets too:

say $|\beta\rangle = X|\alpha\rangle$

then $|\beta\rangle = \sum_j X|a_j\rangle\langle a_j|\alpha\rangle$ & $\langle a_i|\beta\rangle = \sum_j \langle a_i|X|a_j\rangle\langle a_j|\alpha\rangle$

$[\;] = [\,X\,][\alpha]$ or $\beta_i = \sum_j X_{ij}\alpha_j$ where we represent $|\alpha\rangle$ by a column vector: $|\alpha\rangle \rightsquigarrow \begin{bmatrix} \langle a_1|\alpha\rangle \\ \langle a_2|\alpha\rangle \\ \vdots \end{bmatrix} = \alpha_i$

Similarly bras can be represented by row vectors:

$$\langle\gamma| = \langle\alpha|X \quad \Rightarrow \quad \langle\gamma|a_i\rangle = \sum_j \langle\alpha|a_j\rangle\langle a_j|X|a_i\rangle$$

$$\langle\alpha| \rightsquigarrow [\langle\alpha|a_1\rangle, \langle\alpha|a_2\rangle \dots] = [\langle a_1|\alpha\rangle^*, \langle a_2|\alpha\rangle^* \dots] = \alpha_i^\dagger$$

$$\gamma_i^\dagger = \sum_j \alpha_j^\dagger X_{ji}$$

$$[\gamma^\dagger] = [\alpha^\dagger]\begin{bmatrix} X \end{bmatrix}$$

Inner products are clearly contractions of a row & a column vector:

$$\langle\beta|\alpha\rangle = \sum_k \langle\beta|a_k\rangle\langle a_k|\alpha\rangle \rightsquigarrow \sum_k \beta_k^\dagger \alpha_k$$

$$\rightsquigarrow [\langle a_1|\beta\rangle^*, \langle a_2|\beta\rangle^*, \dots]\begin{bmatrix} \langle a_1|\alpha\rangle \\ \langle a_2|\alpha\rangle \\ \vdots \end{bmatrix}$$

Outer products are the opposite combination:

$$|\beta\rangle\langle\alpha| \rightsquigarrow \begin{bmatrix} \langle a_1|\beta\rangle \\ \langle a_2|\beta\rangle \\ \vdots \end{bmatrix}[\langle a_1|\alpha\rangle^*, \langle a_2|\alpha\rangle^*, \dots] = \begin{bmatrix} \langle a_1|\beta\rangle\langle a_1|\alpha\rangle^* & \langle a_1|\beta\rangle\langle a_2|\alpha\rangle^* & \dots \\ \langle a_2|\beta\rangle\langle a_1|\alpha\rangle^* & \langle a_2|\beta\rangle\langle a_2|\alpha\rangle^* & \\ \vdots & & \ddots \end{bmatrix}$$

If an operator is represented in the basis of it's own eigenkets it has a simple, diagonal, form

$$A \rightsquigarrow \langle a_j|A|a_i\rangle = \langle a_j|a_i|a_i\rangle = a_i\langle a_j|a_i\rangle = a_i\delta_{ij}$$

$$A \rightsquigarrow \begin{bmatrix} a_1 & 0 & 0 & \dots \\ 0 & a_2 & 0 & \\ 0 & 0 & a_3 & \\ \vdots & & & \ddots \end{bmatrix}$$

We can get a concrete example by considering the S-apparatus from earlier. Since it splits beams in the z-direction we'll start calling it S_z.

Treated as an operator it has eigenkets $S_z|S_z+\rangle = +\frac{1}{2}|S_z+\rangle$

$$S_z|S_z-\rangle = -\frac{1}{2}|S_z-\rangle$$

We can express the operator S_z as an outer product of these basis states:

$$S_z = \left(+\tfrac{1}{2}\right)|S_z+\rangle\langle S_z+| + \left(-\tfrac{1}{2}\right)|S_z-\rangle\langle S_z-|$$

Now suppose we want a matrix representation of this system, an acceptable choice would be

$$|S_z+\rangle \rightsquigarrow \begin{bmatrix}1\\0\end{bmatrix} \;;\; |S_z-\rangle \rightsquigarrow \begin{bmatrix}0\\1\end{bmatrix} \quad \text{then } S_z \rightsquigarrow \left(+\tfrac{1}{2}\right)\begin{bmatrix}1&0\\0&0\end{bmatrix} + \left(-\tfrac{1}{2}\right)\begin{bmatrix}0&0\\0&1\end{bmatrix}$$

$$S_z \rightsquigarrow \frac{1}{2}\begin{bmatrix}1&0\\0&-1\end{bmatrix}$$

We can easily check that this represents the system

$$\frac{1}{2}\begin{bmatrix}1&0\\0&-1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = +\frac{1}{2}\begin{bmatrix}1\\0\end{bmatrix} \quad \text{c.f. } S_z|S_z+\rangle = +\frac{1}{2}|S_z+\rangle$$

$$\frac{1}{2}\begin{bmatrix}1&0\\0&-1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = -\frac{1}{2}\begin{bmatrix}0\\1\end{bmatrix} \quad \text{c.f. } S_z|S_z-\rangle = -\frac{1}{2}|S_z-\rangle.$$

But be aware that this representation is not unique, say instead we chose

$$|S_z+\rangle \rightsquigarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \;;\; |S_z-\rangle \rightsquigarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$$

$$\text{then } S_z = \left(+\tfrac{1}{2}\right)\cdot\frac{1}{2}\begin{bmatrix}1&1\\1&1\end{bmatrix} + \left(-\tfrac{1}{2}\right)\frac{1}{2}\begin{bmatrix}1&-1\\-1&1\end{bmatrix} = \frac{1}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}.$$

Looks different, but it's still a perfectly good representation:

$$\frac{1}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} = \left(+\tfrac{1}{2}\right)\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \quad \text{cf. } S_z|S_z+\rangle = +\frac{1}{2}|S_z+\rangle$$

$$\frac{1}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} = \left(-\tfrac{1}{2}\right)\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} \quad \text{c.f. } S_z|S_z-\rangle = -\frac{1}{2}|S_z-\rangle$$

This second choice corresponds to selecting a different set of basis states. There are infinitely many possible choices.

(MEASUREMENTS)

We saw earlier in both the electron-slit experiment & the filtering expt that when we make a measurement of the state of a system that we get a definite answer (hole 1 or hole 2 say), but that if we repeat the measurement for multiple identical setups we find the measurements distributed probabilistically.

e.g. say we prepared an $|S+\rangle$ state using a $\left\{ \begin{smallmatrix} + \\ - \!\!\parallel \end{smallmatrix} \right\}$ filter

and let this state enter a T-apparatus. We know that the $|S+\rangle$ state is a linear superposition of the eigenstates of T:

$$|S+\rangle = |T+\rangle\langle T+|S+\rangle + |T-\rangle\langle T-|S+\rangle$$
$$= \cos\theta/_2 \, |T+\rangle - \sin\theta/_2 \, |T-\rangle .$$

The T-apparatus though will measure either a $|T+\rangle$ state or a $|T-\rangle$ state. Say in one particular case it measures $|T+\rangle$. Then the state is $|T+\rangle$ from then on and nothing else. A subsequent measurement by a T-apparatus will measure $|T+\rangle$ with 100% probability.

In more general terms we can always express an arbitrary state $|\alpha\rangle$ in terms of the eigenkets of an operator corresponding to a measurement we're about to make (call it A):

$$|\alpha\rangle = \sum_i |a_i\rangle\langle a_i|\alpha\rangle$$

Upon measurement by A, the state "collapses" into one of the $|a_i\rangle$

$$|\alpha\rangle \xrightarrow{\text{A meas.}} |a_i\rangle$$

If we immediately measure with A again, nothing changes

$$|a_i\rangle \xrightarrow{\text{A meas.}} |a_i\rangle$$

We already know from our earlier examples that the <u>probability</u> of measuring a_i & collapsing into the state $|a_i\rangle$ from a state $|\alpha\rangle$ is

$$P = |\langle a_i|\alpha\rangle|^2$$

(clearly then the probability to collapse from $|a_i\rangle$ to $|a_i\rangle$ is $|\langle a_i|a_i\rangle|^2 = 1$)

(also the probability to collapse from $|a_i\rangle$ to a different eigenstate $|a_j\rangle$ is $|\langle a_j|a_i\rangle|^2 = 0$)

If we setup a quantum system in a given state many, many times we can make a measurement each time & determine the probabilities of the various possible outcomes. We could also compute an 'average' value of the measurement. Such an object corresponds to the expectation value of the operator corresponding to the measurement:

$$\langle A \rangle \equiv \langle \alpha | A | \alpha \rangle$$

$$= \sum_{ij} \langle \alpha | a_i \rangle \langle a_i | A | a_j \rangle \langle a_j | \alpha \rangle = \sum_i a_i \, |\langle \alpha | a_i \rangle|^2$$

$$= \sum_i a_i \, P_i^{(\alpha)}$$

In our earlier study using S & T apparatus we found that if we measured the system to be in, say, an $|S+\rangle$ state, there was still a probability for it to be in either a $|T+\rangle$ or a $|T-\rangle$ state. We speak of S & T as being incompatible observables.

Let's consider again those apparatus, this time with specific orientations. The S-apparatus, which splits in the z-direction we'll call S_z. We'll orient a 'T'-apparatus so that it splits along y and call it S_y, and we'll orient a third apparatus so that it splits along x, labelling it S_x.

We'll consider the details later, but for now I'll supply you with the following results:

The eigenstates of S_x $\left(S_x |S_x, \pm\rangle = \pm\frac{1}{2} |S_x, \pm\rangle \right)$ can be expressed in terms of the eigenstates of S_z $\left(S_z |S_z \pm\rangle = \pm\frac{1}{2} |S_z \pm\rangle \right)$ as follows:

$$|S_x; \pm\rangle = \frac{1}{\sqrt{2}} |S_z; +\rangle \pm \frac{1}{\sqrt{2}} |S_z; -\rangle$$

& for S_y:

$$|S_y; \pm\rangle = \frac{1}{\sqrt{2}} |S_z; +\rangle \pm \frac{i}{\sqrt{2}} |S_z; -\rangle$$

In this case the operators $S_{x,y,z}$ can be written in terms of the eigenstates of S_z as

$$S_x = \frac{1}{2}\Big(|+\rangle\langle -| + |-\rangle\langle +| \Big) \qquad \left(|\pm\rangle \equiv |S_z; \pm\rangle \text{ as a shorthand} \right)$$

$$S_y = -\frac{i}{2}\Big(|+\rangle\langle -| - |-\rangle\langle +| \Big)$$

$$S_z = \frac{1}{2}\Big(|+\rangle\langle +| - |-\rangle\langle -| \Big)$$

We can also express these in a matrix representation:

$|+\rangle \rightsquigarrow \begin{bmatrix}1\\0\end{bmatrix}$; $|-\rangle \rightsquigarrow \begin{bmatrix}0\\1\end{bmatrix}$

$|S_x;\pm\rangle \rightsquigarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ \pm 1\end{bmatrix}$; $|S_y;\pm\rangle \rightsquigarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ \pm i\end{bmatrix}$

$S_x \rightsquigarrow \frac{1}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$; $S_y \rightsquigarrow \frac{1}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$; $S_z \rightsquigarrow \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$

It is interesting to examine the commutator of two of these operators:

$$[S_x, S_y] \equiv S_xS_y - S_yS_x$$

using the bra-ket representation & the orthonormality of the $|\pm\rangle$ states: $\left(\begin{matrix}\langle +|-\rangle = 0\\ \langle +|+\rangle = 1\end{matrix}\right)$

$$[S_x, S_y] = -\tfrac{i}{4}\big(|+\rangle\langle -| + |-\rangle\langle +|\big)\big(|+\rangle\langle -| - |-\rangle\langle +|\big)$$
$$+ \tfrac{i}{4}\big(|+\rangle\langle -| - |-\rangle\langle +|\big)\big(|+\rangle\langle -| + |-\rangle\langle +|\big)$$

$$= \tfrac{i}{4}\big(|+\rangle\langle +| - |-\rangle\langle -| + |+\rangle\langle +| - |-\rangle\langle -|\big)$$
$$= \tfrac{i}{2}\big(|+\rangle\langle +| - |-\rangle\langle -|\big) = i\,S_z$$

$\underline{[S_x, S_y] = iS_z}$ so applying S_x then S_y is not the same as applying S_y then S_x.

Note that we can cook-up a fourth operator that we call $S^2 = \frac{3}{4}\big(|+\rangle\langle +| + |-\rangle\langle -|\big)$ $\left(S^2 \rightsquigarrow \frac{3}{4}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\right)$ which does commute with any of the S_i:

$$[S^2, S_z] \rightsquigarrow \frac{3}{8}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} - \frac{3}{8}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = 0 \qquad \underline{[S^2, S_z] = 0}$$

The commutator of two operators is important in quantum mechanics because two operators with commute ($[A,B]=0$) are <u>"compatible observables"</u>. That is if one takes a measurement of A, collapsing the system into an eigenstate of A and follows this with a measurement of B - the state <u>does not change</u> under the measurement of B.

Put another way, the eigenstates of B are the same as the eigenstates of A.

This is easy to check by considering the matrix element of $[A,B]$ between eigenkets of A:

$$0 = \langle a_j | [A,B] | a_i \rangle = \langle a_j | AB - BA | a_i \rangle = \langle a_j | a_j B - B a_i | a_i \rangle$$
$$= (a_j - a_i) \langle a_j | B | a_i \rangle$$

now assuming $a_j \neq a_i \Rightarrow \langle a_j | B | a_i \rangle = 0$ for $i \neq j$

$$\langle a_j | B | a_i \rangle = \langle a_i | B | a_i \rangle \delta_{ij}$$

hence $$B|a_k\rangle = \sum_{ij} |a_j\rangle \underbrace{\langle a_j | B | a_i \rangle}_{\langle a_i|B|a_i\rangle \delta_{ij}} \underbrace{\langle a_i | a_k \rangle}_{\delta_{ik}} = \underbrace{\langle a_k | B | a_k \rangle}_{\substack{\text{just a number} \\ = \text{eigenvalue}}} |a_k\rangle$$

$\Rightarrow B|a_k\rangle = b_k |a_k\rangle \quad \Rightarrow |a_k\rangle$ is an eigenket of B as well as A
- we can label the state by the eigenvalues of both compatible observables:

$$|a_i, b_i\rangle \quad : \quad A|a_i, b_i\rangle = a_i |a_i, b_i\rangle$$
$$B|a_i, b_i\rangle = b_i |a_i, b_i\rangle$$

The above proof is not relevant in the case that two or more eigenkets have the same eigenvalue. We call this situation a degeneracy. In this all linear combination of the degenerate eigenkets have the same eigenvalue and there is hence no unique choice.
In the case that there is a compatible observable like B, we can use the eigenvalues of B to label a unique set (provided that the kets are not also degenerate under B)

As an example consider the S^2 & S_z operators in the matrix representation:

$S^2 \to \frac{3}{4}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ has two degenerate eigenstates with eigenvalue $3/4$.

We could choose $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, but $\frac{a}{\sqrt{a^2+b^2}}\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{b}{\sqrt{a^2+b^2}}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

would do just as well.

Since S^2 commutes with S_z ($[S^2, S_z] = 0$) we can have simultaneous eigenstates of both. In the matrix representation, the eigenstates of S_z are $\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ with eigenvalue $\pm\frac{1}{2}$. Hence we can label our states

$$|S^2 = 3/4, S_z = \pm\tfrac{1}{2}\rangle.$$

(THE UNCERTAINTY RELATION)

We can define something called the 'dispersion' of an operator:

$$\langle\alpha|\,(\Delta A)^2\,|\alpha\rangle \equiv \langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2.$$

You'll note that it looks rather like the 'variance' defined in statistics, so it is some sort of measure of 'spread'. As an example, in statistics you might have a variable x distributed continuously according to a probability $P(x)$. Say that probability is Gaussian:

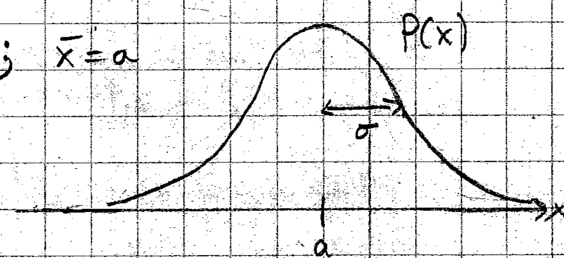
$$P(x) = \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left[-\frac{(x-a)^2}{2\sigma^2}\right]$$

then the mean value of x is $\bar{x} = \int_{-\infty}^{\infty} dx\; x\, P(x) = \frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty} dx\, x\, e^{-(x-a)^2/2\sigma^2} = \underline{\underline{a}}$

& the 'spread' or variance in the values of x is $(\Delta x)^2 = \overline{x^2} - \bar{x}^2$

$$\overline{x^2} = \frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty} dx\; x^2 e^{-\frac{(x-a)^2}{2\sigma^2}} = a^2+\sigma^2 \quad ; \quad \bar{x} = a$$

$$\Rightarrow (\Delta x)^2 = a^2+\sigma^2 - a^2 = \underline{\underline{\sigma^2}}$$



In quantum mechanics the dispersion indicates the 'fuzziness' of a certain measurement on a certain state.

e.g. say we have an eigenstate of S_z : $|S_z;+\rangle$, then a measurement of S_z should not be fuzzy at all since $S_z|S_z;+\rangle = +\tfrac{1}{2}|S_z;+\rangle$

$$\langle S_z;+|(\Delta S_z)^2|S_z;+\rangle = \langle S_z;+|S_z S_z|S_z;+\rangle - \left(\langle S_z;+|S_z|S_z;+\rangle\right)^2$$
$$= (+\tfrac{1}{2})(+\tfrac{1}{2})\langle S_z;+|S_z;+\rangle - \left((+\tfrac{1}{2})\langle S_z;+|S_z;+\rangle\right)^2$$
$$= \underline{0} \quad \text{no uncertainty or 'fuzziness'}$$

If we make a measurement of S_x on this state though, we know that we can get either $+\tfrac{1}{2}$ or $-\tfrac{1}{2}$ with certain probabilities, so there is a degree of 'fuzziness' to the measurement:

$$\langle S_z;+|(\Delta S_x)^2|S_z;+\rangle = \langle S_z;+|S_x S_x|S_z;+\rangle - \left(\langle S_z;+|S_x|S_z;+\rangle\right)^2$$

using the matrix representation:

$$\langle +|S_x S_x|+\rangle = [1,0]\frac{1}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\frac{1}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \frac{1}{4}[1,0]\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{4}[1,0]\begin{bmatrix}1\\0\end{bmatrix} = \underline{1/4}$$

$$\langle +|S_x|+\rangle = [1,0]\frac{1}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \underline{0} \qquad \Rightarrow \langle +|(\Delta S_x)^2|+\rangle = \underline{1/4}$$

The uncertainty relation is stated in terms of dispersions as

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} \left| \langle [A,B] \rangle \right|^2$$ (where A, B are Hermitian ops)

We'll prove this soon, but first notice that if $[A,B]=0$, and hence A & B are compatible observables, the product of the dispersions vanishes, that is, at least one of A & B is not fuzzy.

Now for the proof:

We need the Schwarz Identity which states: $\langle \alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (prove it!)

We also need that the expectation value of a Hermitian operator is real. (prove it!)

And that the expectation value of an anti-Hermitian operator ($C^\dagger = -C$) is imaginary. (prove it!)

We can treat $\Delta A \equiv A - \langle A\rangle$ as an operator, then suppose

$|\alpha\rangle = \Delta A|\gamma\rangle$ $\quad$ $|\beta\rangle = \Delta B|\gamma\rangle$

$\langle\alpha| = \langle\gamma|\Delta A$ $\quad$ $\langle\beta| = \langle\gamma|\Delta B$

} Schwarz $\rightarrow \langle\gamma|(\Delta A)^2|\gamma\rangle\langle\gamma|(\Delta B)^2|\gamma\rangle \geq \left|\langle\gamma|\Delta A\Delta B|\gamma\rangle\right|^2$

Write $\Delta A \Delta B = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\}$ $\quad$ ($\{X,Y\}$ = "anticommutator" $= XY + YX$)

$$\frac{1}{2}[A-\langle A\rangle, B-\langle B\rangle] = \frac{1}{2}[A,B]$$

$$([A,B])^\dagger = (AB-BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA - AB = -[A,B]$$

$\Rightarrow$ commutator is anti-Hermitian

$\{\Delta A, \Delta B\}$ is Hermitian

$$\langle \Delta A \Delta B\rangle = \frac{1}{2}\underbrace{\langle [A,B]\rangle}_{\text{imag} = iz_1} + \frac{1}{2}\underbrace{\langle\{\Delta A, \Delta B\}\rangle}_{\text{real} = z_2}$$

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \left|\frac{1}{2}(iz_1 + z_2)\right|^2 = \frac{1}{4}(z_1^2 + z_2^2) \geq \frac{1}{4}z_1^2$$

$$\Rightarrow \langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}\left|\langle[A,B]\rangle\right|^2$$

MATRIX EIGENSYSTEM

Suppose we have a matrix representation of an operator B in a representation that is not the eigensystem of B. In other words we know

$$\langle a_j | B | a_i \rangle$$

& we want to find the eigenvalues & eigenkets in $B|b_i\rangle = b_i |b_i\rangle$

The matrix representation furnishes the mathematical technique

$$B|b_i\rangle = b_i |b_i\rangle \Rightarrow \sum_{a_k} \langle a_j | B | a_k \rangle \langle a_k | b_i \rangle = b_i \langle a_k | b_i \rangle$$

$$\rightsquigarrow \begin{bmatrix} B_{11} & B_{12} & B_{13} & \cdots \\ B_{21} & B_{22} & B_{23} & \\ B_{31} & B_{32} & B_{33} & \\ \vdots & & & \ddots \end{bmatrix} \begin{bmatrix} C_1^{(i)} \\ C_2^{(i)} \\ C_3^{(i)} \\ \vdots \end{bmatrix} = b^{(i)} \begin{bmatrix} C_1^{(i)} \\ C_2^{(i)} \\ C_3^{(i)} \\ \vdots \end{bmatrix}$$

Conventional linear algebra tells us how to solve this problem.

Non-trivial solutions only exist if $\det(\underline{\underline{B}} - b\underline{\underline{I}}) = 0$ can be solved. The roots of this equation being the eigenvalues $b^{(i)}$.
With the eigenvalues in hand one can solve for the eigenvectors $\underline{C}^{(i)}$.

We often talk of this as "diagonalising" the matrix $\underline{\underline{B}}$. This is because we can build a matrix out of the eigenvectors

$$\underline{\underline{C}} = \begin{bmatrix} C_1^{(1)} & C_1^{(2)} & C_1^{(3)} & \cdots \\ C_2^{(1)} & C_2^{(2)} & C_2^{(3)} & \\ C_3^{(1)} & C_3^{(2)} & C_3^{(3)} & \\ \vdots & \vdots & \vdots & \end{bmatrix}$$

which when used as a similarity transform on $\underline{\underline{B}}$, yields a diagonal matrix with the eigenvalues of $\underline{\underline{B}}$ along the diagonal

$$\underline{\underline{C}}^\dagger \underline{\underline{B}}\, \underline{\underline{C}} = \underline{\underline{B}}_{\text{diag}} = \begin{bmatrix} b_1 & 0 & 0 & \cdots \\ 0 & b_2 & 0 & \\ 0 & 0 & b_3 & \\ \vdots & & & \ddots \end{bmatrix}$$

The matrix $\underline{\underline{C}}$ is the unitary transform from the $|a_i\rangle$ basis to the $|b_i\rangle$ basis

$$C_j^{(i)} = \langle a_j | b_i \rangle \qquad (C^\dagger C)_{ij} = \sum_k \langle b_i | a_k \rangle \langle a_k | b_j \rangle = \langle b_i | b_j \rangle = \delta_{ij}$$

$$\underline{\underline{C}}^\dagger \underline{\underline{C}} = \underline{\underline{I}} \Rightarrow \underline{\underline{C}}^\dagger = \underline{\underline{C}}^{-1} \quad \text{'unitary' matrix.}$$

[CONTINUOUS SPECTRA]

We will have to consider observables which do not take one of a finite number of discrete values, but rather can have any continuous value. An example would be the momentum p of a particle moving in one-dimension which can take on any real value from $-\infty$ to $+\infty$.

We won't go into the full mathematics required to understand continuous vector spaces, but rather just present the result by analogy to the finite case.

eigensystem : $(A|a_i\rangle = a_i|a_i\rangle)$ $\rightarrow \hat{x}|x\rangle = x|x\rangle$

$\hat{x}$ is an operator (I'll probably start to forget the hats soon)
$|x\rangle$ is the eigenket
x is the eigenvalue.

orthonormality : $(\langle a_j|a_i\rangle = \delta_{ij})$

$\rightarrow \langle x|x'\rangle = \delta(x-x')$ $\delta(x-x')$ is the Dirac delta function

completeness : $\left(\sum_i |a_i\rangle\langle a_i| = 1\right)$

$\rightarrow \int dx\, |x\rangle\langle x| = 1$

projection : $\left(|\alpha\rangle = \sum_i |a_i\rangle\langle a_i|\alpha\rangle\right)$

$\rightarrow |\alpha\rangle = \int dx\, |x\rangle\langle x|\alpha\rangle$

diagonal operator : $(\langle a_j|A|a_i\rangle = a_i\delta_{ij})$

$\rightarrow \langle x|\hat{x}|x'\rangle = x'\delta(x-x')$

An aside on the Dirac delta function:

Mathematicians quite rightly get shifty about this, because it isn't really a function. It only has true meaning under an integral, but you can think loosely of $\delta(x-a)$ as being zero everywhere except $x=a$ where it is ∞.
More rigourously $\int dx\, f(x)\delta(x-a) = f(a)$ for any function $f(x)$*

If explicit representations of $\delta(x-a)$ are required they can be obtained as the limits of certain functions peaked at $x=a$, e.g.

$$\lim_{\sigma\to 0} \frac{1}{\sigma\sqrt{\pi}} e^{-(x-a)^2/\sigma^2} \rightarrow \delta(x-a)$$

*smooth near $x=a$

POSITION AS AN OBSERVABLE

Suppose we can write an operator representing the position in one dimension. It will have an eigensystem:

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

x is just a number with dimensions of length. We can imagine expressing the quantum state of a single particle $|\alpha\rangle$ in the position eigenket basis:

$$|\alpha\rangle = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x|\alpha\rangle$$

The interpretation of this is very similar to before - the probability that a quantum state described by $|\alpha\rangle$ will be measured to be in the quantum state described by $|x\rangle$ (which is "located at x") is $|\langle x|\alpha\rangle|^2$.

Actually this isn't quite right - the probability to be located in a region of infinitesimal size dx around x is $|\langle x|\alpha\rangle|^2 dx$.

Now the probability that the particle is located 'somewhere' had better be one, so

$$\int dx\, |\langle x|\alpha\rangle|^2 = 1 = \int dx \langle\alpha|x\rangle\langle x|\alpha\rangle = \langle\alpha|\alpha\rangle$$

We can extend this to three-dimensions by assuming that the three-components of the position vector are compatible observables, ie. $[\hat{x}_i, \hat{x}_j] = 0$.

Then we have
$$\hat{x}_1 = \hat{x} \qquad \hat{x}\,|x,y,z\rangle = x\,|x,y,z\rangle$$
$$\hat{x}_2 = \hat{y} \qquad \hat{y}\,|x,y,z\rangle = y\,|x,y,z\rangle$$
$$\& \ \hat{x}_3 = \hat{z} \qquad \hat{z}\,|x,y,z\rangle = z\,|x,y,z\rangle$$

A useful shorthand is $|\vec{x}\rangle = |x,y,z\rangle$.

Consider an operator that takes a state localised at $|\vec{x}\rangle$ and translates it to a state localised at $|\vec{x}+d\vec{x}\rangle$. For now just consider translation by an infinitesimal vector $d\vec{x}$.

$$T(d\vec{x})\,|\vec{x}\rangle = |\vec{x}+d\vec{x}\rangle$$

What properties should we demand of this operator?

1. It shouldn't break conservation of probability, ie.
$$\langle\alpha|\alpha\rangle = \langle\alpha|T^\dagger(d\vec{x})\,T(d\vec{x})|\alpha\rangle \quad \Rightarrow \quad T^\dagger(d\vec{x})\,T(d\vec{x}) = 1 \ \ \& \ T(d\vec{x}) \text{ is unitary}$$
2. Translating by $d\vec{x}$ then $d\vec{x}'$ should be the same as translating by $d\vec{x}+d\vec{x}'$
$$T(d\vec{x}')\,T(d\vec{x}) = T(d\vec{x}'+d\vec{x})$$
3. Translating by $-d\vec{x}$ after $d\vec{x}$ should be the same as the inverse after the operator, ie
$$T(-d\vec{x})\,T(d\vec{x}) = T^{-1}(d\vec{x})\,T(d\vec{x}) \quad \Rightarrow \quad T(-d\vec{x}) = T^{-1}(d\vec{x})$$
4. As the translation distance approaches zero the operator should approach 1
$$\lim_{d\vec{x}\to 0} T(d\vec{x}) \to 1.$$

A suitable realisation is $T(d\vec{x}) = 1 - i\,\hat{\vec{p}}\cdot d\vec{x}/\hbar$ where the components of $\hat{\vec{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ are Hermitian operators and $\hbar$ is a convenient normalisation.

1. $\rightarrow$ $T^\dagger(d\vec{x})T(d\vec{x}) = (1 + i\hat{\vec{p}}\cdot d\vec{x}/\hbar)(1 - i\hat{\vec{p}}\cdot d\vec{x}/\hbar) = 1 + O(d\vec{x}^2)$

2. $\rightarrow$ $T(d\vec{x}')T(d\vec{x}) = (1 - i\hat{\vec{p}}\cdot d\vec{x}'/\hbar)(1 - i\hat{\vec{p}}\cdot d\vec{x}/\hbar) = 1 - i\hat{\vec{p}}\cdot(d\vec{x}' + d\vec{x})/\hbar + O(d\vec{x}^2)$
$= T(d\vec{x}' + d\vec{x})$

3. $\rightarrow$ $T(-d\vec{x})T(d\vec{x}) = 1 = (1 + i\hat{\vec{p}}\cdot d\vec{x}/\hbar)(1 - i\hat{\vec{p}}\cdot d\vec{x}/\hbar) = 1 + O(d\vec{x}^2)$

4. $\rightarrow$ $\lim_{d\vec{x}\to 0} T(d\vec{x}) \longrightarrow 1$ ✓

Now, consider translating a state & then measuring its position:
$$\hat{\vec{x}}\,T(d\vec{x})|\vec{x}\rangle = \hat{\vec{x}}|\vec{x}+d\vec{x}\rangle = (\vec{x}+d\vec{x})|\vec{x}+d\vec{x}\rangle$$
and consider first measuring the position, then translating:
$$T(d\vec{x})\,\hat{\vec{x}}|\vec{x}\rangle = T(d\vec{x})\,\vec{x}|\vec{x}\rangle = \vec{x}\,T(d\vec{x})|\vec{x}\rangle = \vec{x}|\vec{x}+d\vec{x}\rangle$$

So then $[\hat{\vec{x}}, T(d\vec{x})]\,|\vec{x}\rangle = d\vec{x}\,|\vec{x}+d\vec{x}\rangle = d\vec{x}\,|\vec{x}\rangle$ to lowest order in $d\vec{x}$.
& since this is an arbitrary position state it must be true for the operators:

$$[\hat{\vec{x}}, T(dx)] = d\vec{x} \quad \Rightarrow \quad [\hat{\vec{x}}, 1 - i\hat{\vec{p}}\cdot d\vec{x}/\hbar] = d\vec{x}$$

$$-i/\hbar\,(\hat{\vec{x}}\,\hat{\vec{p}}\cdot d\vec{x} - \hat{\vec{p}}\cdot d\vec{x}\,\hat{\vec{x}}) = d\vec{x}$$

Choose $d\vec{x}$ pointing in the x-direction $\rightarrow$ $-i/\hbar\,(\hat{\vec{x}}\,\hat{p}_1 - \hat{p}_1\hat{\vec{x}}) = d\vec{x}$

$\rightarrow$ $-i/\hbar\,(\hat{x}_1\hat{p}_1 - \hat{p}_1\hat{x}_1) = 1$
& $-i/\hbar\,(\hat{x}_2\hat{p}_1 - \hat{p}_1\hat{x}_2) = 0$
& $-i/\hbar\,(\hat{x}_3\hat{p}_1 - \hat{p}_1\hat{x}_3) = 0$

repeating this for y & z directions
$$\Rightarrow \quad \underline{[\hat{x}_i, \hat{p}_j] = i\hbar\,\delta_{ij}} \quad \text{(A)}$$

You might recall that in classical mechanics, the generator of spatial translations is the momentum. Here also we can identify $\hat{\vec{p}}$ as the operator corresponding to momentum.

The result (A) tells us that the x-position of a particle and its x-component of momentum are incompatible observables - it is impossible to find simultaneous eigenkets of x & p_x. "We cannot simultaneously know where something is & how fast it is going".

We can derive a special case of the uncertainty principle derived earlier:

$$\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p})^2\rangle \geq \frac{1}{4}\left|\langle[\hat{x},\hat{p}]\rangle\right|^2$$
$$\geq \hbar^2/4$$

more usually written in short-hand as $\Delta x\,\Delta p \geq \hbar/2$ "Heisenberg's Uncertainty Relation"

Suppose we wish to translate not by an infinitesimal amount $d\vec{x}$ but by a finite amount $\Delta\vec{x}$. We can achieve this by compounding small translations of $d\vec{x}$.

$$|\vec{x}+\Delta x\hat{i}\rangle = T(\Delta x\hat{i})|\vec{x}\rangle = \lim_{N\to\infty}\left[1-\frac{i\hat{p}_x}{\hbar}\left(\frac{\Delta x}{N}\right)\right]^N|\vec{x}\rangle$$

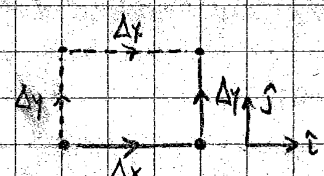
$$\boxed{\left(1+\frac{a}{N}\right)^N = 1+N\left(\frac{a}{N}\right)+\frac{N(N-1)}{2!}\left(\frac{a}{N}\right)^2+\dots \xrightarrow{N\to\infty} 1+a+a^2/2!+a^3/3!+\dots \longrightarrow e^a}$$

$$= \exp\left[-i\frac{\hat{p}_x}{\hbar}\Delta x\right]|\vec{x}\rangle$$

so $T(\Delta x\hat{i}) = e^{-i\hat{p}_x\Delta x/\hbar}$. This is a function of the operator $\hat{p}_x$, whose action can be defined by a power series:

$$e^{\hat{x}} = 1+\hat{x}+\frac{1}{2!}\hat{x}\hat{x}+\frac{1}{3!}\hat{x}\hat{x}\hat{x}+\dots$$

A property we demand of translations is that travelling to the right by 1m then up by 2m is the same as travelling up by 2m then to the right by 1m



$$\left.\begin{aligned} T(\Delta y\hat{j})T(\Delta x\hat{i}) &= T(\Delta x\hat{i}+\Delta y\hat{j}) \\ T(\Delta x\hat{i})T(\Delta y\hat{j}) &= T(\Delta x\hat{i}+\Delta y\hat{j}) \end{aligned}\right\} [T(\Delta x\hat{i}), T(\Delta y\hat{j})] = 0$$

$\Rightarrow$ expanding the exponential:

$$0 = \left[\left(1-\frac{i}{\hbar}\hat{p}_x\Delta x - \frac{1}{2\hbar^2}\hat{p}_x^2\Delta x^2+\dots\right), \left(1-\frac{i}{\hbar}\hat{p}_y\Delta y - \frac{1}{2\hbar^2}\hat{p}_y^2\Delta y^2\right)\right]$$

$$= -\frac{1}{\hbar}\Delta x\Delta y[\hat{p}_x,\hat{p}_y]+\dots \quad\Rightarrow\quad \underline{[\hat{p}_x,\hat{p}_y]=0}$$

in general the components of momentum commute: $[\hat{p}_i,\hat{p}_j]=0$ & there are eigenkets

$$|\vec{p}\rangle = |p_x\, p_y\, p_z\rangle$$

We call the overlap of a state $|\alpha\rangle$ with the position eigenbra $\langle x|$, the "wavefunction"

$$\psi_\alpha(x) \equiv \langle x|\alpha\rangle$$

for any state α, this object is simply a complex function of the variable x.

The inner product between two states can be expressed in terms of an overlap integral:

$$\langle\beta|\alpha\rangle = \int dx \langle\beta|x\rangle\langle x|\alpha\rangle = \int dx\, \psi_\beta^*(x)\psi_\alpha(x)$$

Suppose we have a basis of state $|a_i\rangle$, then we know we can express an arbitrary state $|\alpha\rangle$ by

$$|\alpha\rangle = \sum_i |a_i\rangle\langle a_i|\alpha\rangle, \qquad \left(A|a_i\rangle = a_i|a_i\rangle\right)$$

expressed in the position basis this becomes

$$\langle x|\alpha\rangle = \sum_i \langle x|a_i\rangle\langle a_i|\alpha\rangle$$

$$\psi_\alpha(x) = \sum_i C_{a_i}^{(\alpha)}\, \phi_{a_i}(x)$$

where $\phi_{a_i}(x)$ is an <u>eigenfunction</u> of the operator A expressed in the position basis

$$A|a_i\rangle = a_i|a_i\rangle \Rightarrow \int dx\, \langle x'|A|x\rangle\langle x|a_i\rangle = a_i\langle x'|a_i\rangle$$

$$\int dx\, \langle x'|A|x\rangle\, \phi_{a_i}(x) = a_i\phi_{a_i}(x')$$

if $\langle x'|A|x\rangle$ is local $= A(x)\delta(x'-x)$

$$\Rightarrow A(x)\,\phi_{a_i}(x) = a_i\phi_{a_i}(x)$$

we'll see that this may not be entirely trivial since $A(x)$ may contain differential operators

Expectation values become space-integrals:

$$\langle\beta|A|\alpha\rangle = \int dx dx' \langle\beta|x'\rangle\langle x'|A|x\rangle\langle x|\alpha\rangle = \int dx dx'\, \psi_\beta^*(x')\langle x'|A|x\rangle\psi_\alpha(x)$$

$$= \int dx dx'\, \psi_\beta^*(x') A(x',x)\psi_\alpha(x)$$

a simplification occurs if A is a function of only the position operator $\hat{x}$,

e.g. $A = \hat{x}^2$ then $\langle x'|\hat{x}^2|x\rangle = \langle x'|x^2|x\rangle = x^2\langle x'|x\rangle = x^2\delta(x'-x)$

$$\& \quad \langle\beta|\hat{x}^2|\alpha\rangle = \int dx dx'\, \psi_\beta^*(x')\, x^2\, \delta(x'-x)\psi_\alpha(x) = \int dx\, \psi_\beta^*(x)\, x^2\, \psi_\alpha(x)$$

or more generally $\langle\beta|f(\hat{x})|\alpha\rangle = \int dx\, \psi_\beta^*(x) f(x)\psi_\alpha(x)$

Suppose we've chosen to work in the position basis but we want to consider the effect of the momentum operator on a state. We need to know how the momentum operator is represented in the position basis.

Let's begin with the definition of linear momentum as the generator of spatial translation. For an infinitesimal translation Δx:

$$\left(1 - \tfrac{i}{\hbar}\hat{p}\Delta x\right)|\alpha\rangle = \int dx\; T(\Delta x)|x\rangle\langle x|\alpha\rangle = \int dx\; |x+\Delta x\rangle\langle x|\alpha\rangle$$

changing the integration variable $(x' = x+\Delta x)$

$$= \int dx'\; |x'\rangle\langle x'-\Delta x|\alpha\rangle = \int dx\; |x\rangle\langle x-\Delta x|\alpha\rangle$$

Taylor expanding

$$= \int dx\; |x\rangle\left(\langle x|\alpha\rangle - \Delta x\frac{\partial}{\partial x}\langle x|\alpha\rangle + O(\Delta x^2)\right)$$

$$= |\alpha\rangle - \Delta x\int dx\; |x\rangle\frac{\partial}{\partial x}\langle x|\alpha\rangle + \ldots$$

$$\Rightarrow \quad \tfrac{i}{\hbar}\hat{p}\,|\alpha\rangle = \int dx\,|x\rangle\frac{\partial}{\partial x}\langle x|\alpha\rangle$$

$\times\langle x'|$

$$\langle x'|\hat{p}|\alpha\rangle = -i\hbar\int dx\;\langle x'|x\rangle\frac{\partial}{\partial x}\langle x|\alpha\rangle = -i\hbar\int dx\;\delta(x'-x)\frac{\partial}{\partial x}\langle x|\alpha\rangle$$

$$= -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$$

Suppose that the state $|\alpha\rangle$ happens to be the position eigenstate $|x\rangle$

$$\underline{\langle x'|\hat{p}|x\rangle = -i\hbar\frac{\partial}{\partial x'}\delta(x'-x)}$$

which is the representation of $\hat{p}$ in the position basis

Thus $\langle\beta|\hat{p}|\alpha\rangle = \int dx\,dx'\;\langle\beta|x'\rangle\langle x'|\hat{p}|x\rangle\langle x|\alpha\rangle = \int dx'\,dx\;\psi_\beta^*(x')\left[-i\hbar\frac{\partial}{\partial x'}\delta(x'-x)\right]\psi_\alpha(x)$

$$= \underline{\int dx\;\psi_\beta^*(x)\left[-i\hbar\frac{\partial}{\partial x}\right]\psi_\alpha(x)}$$

It should be clear from the abstract ket notation that we've been following, that there is nothing special about position-space wavefunctions. Position-space just happens to be a handy representation in certain cases. In other cases, other representations will be more useful - let's consider momentum-space wavefunctions.

basis eigenkets $\hat{p}|p\rangle = p|p\rangle$ $\qquad\qquad \langle p'|p\rangle = \delta(p'-p)$

$$|\alpha\rangle = \int dp\, |p\rangle\langle p|\alpha\rangle$$

& the probability that the state $|\alpha\rangle$ is measured to have a momentum in an interval dp around p is $|\langle p|\alpha\rangle|^2 dp$.

We call $\langle p|\alpha\rangle$ the momentum-space wavefunction $\quad \langle p|\alpha\rangle = \varphi_\alpha(p)$

normalisation: $\langle\alpha|\alpha\rangle = 1 = \int dp\, \langle\alpha|p\rangle\langle p|\alpha\rangle = \int dp\, |\varphi_\alpha(p)|^2 = 1.$

We might find ourselves in the situation where we have either the position or momentum space wave functions & we want the other. We should find the 'transformation' function, which in our general bra-ket formalism should be given by $\langle x|p\rangle$.

Consider $\langle x|\hat{p}|p\rangle = -i\hbar \frac{\partial}{\partial x}\langle x|p\rangle$

$\qquad = p\langle x|p\rangle$

So there is a first-order differential eqn $\quad -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle$

which is solved by $\langle x|p\rangle = N e^{ipx/\hbar}$ with N = normalisation constant

$$\langle x'|x\rangle = \delta(x'-x) = \int dp\, \langle x'|p\rangle\langle p|x\rangle = \int dp\, |N|^2 e^{ipx'/\hbar} e^{-ipx/\hbar}$$

$$= |N|^2 \int dp\, e^{ip(x'-x)/\hbar}$$

$$= |N|^2 \hbar 2\pi \cdot \left[\frac{1}{2\pi}\int dk\, e^{ik(x'-x)}\right] = |N|^2 2\pi\hbar\, \delta(x'-x)$$

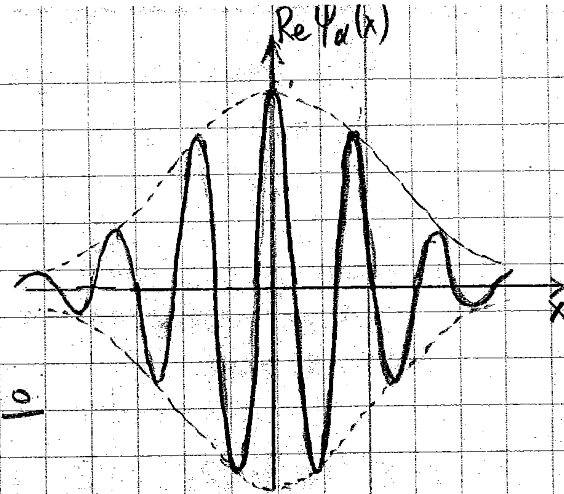
$$\Rightarrow \quad \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

Then $\psi_\alpha(x) = \langle x|\alpha\rangle = \int dp\, \langle x|p\rangle\langle p|\alpha\rangle = \int dp\, \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\varphi_\alpha(p)$

& $\varphi_\alpha(p) = \langle p|\alpha\rangle = \int dx\, \langle p|x\rangle\langle x|\alpha\rangle = \int dx\, \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}\psi_\alpha(x)$

An example – the Gaussian wavepacket

$$\psi_\alpha(x) \equiv \langle x|\alpha\rangle = \frac{1}{\pi^{1/4}\sqrt{d}}\, e^{ikx - x^2/2d^2}$$



The 'average' position of this state $\langle x\rangle = \langle\alpha|\hat{x}|\alpha\rangle$

$$\langle x\rangle = \int dx\, \psi_\alpha^*(x)\cdot x\cdot\psi_\alpha(x) = \frac{1}{\sqrt{\pi}\,d}\int_{-\infty}^{\infty} dx\, x\, e^{-x^2/d^2} = \underline{0}$$

while

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

So the dispersion of x in this state is $\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = \underline{d^2/2}$

The 'average' momentum, $\langle p\rangle = \langle\alpha|\hat{p}|\alpha\rangle$ is

$$\langle p\rangle = \int dx\,dx'\, \langle\alpha|x'\rangle\langle x'|\hat{p}|x\rangle\langle x|\alpha\rangle = \int dx\,dx'\, \psi_\alpha^*(x')\left(-i\hbar\frac{\partial}{\partial x'}\delta(x'-x)\right)\psi_\alpha(x)$$

$$= \int dx\, \psi_\alpha^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_\alpha(x)$$

$$= -i\hbar\int dx\, \psi_\alpha^*(x)\left(ik - \frac{2x}{2d^2}\right)\psi_\alpha(x) = \hbar k\int dx\, \psi_\alpha^*(x)\psi_\alpha(x) = \hbar k$$

$$\underline{\langle p\rangle = \hbar k}$$

$$\langle p^2\rangle = \int dx\, \psi_\alpha^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)^2\psi_\alpha(x) = -\hbar^2\int dx\, \psi_\alpha^*(x)\frac{\partial}{\partial x}\left(\left(ik - \frac{x}{d^2}\right)\psi_\alpha(x)\right)$$

$$= -\hbar^2\int dx\, \psi_\alpha^*(x)\left(-\frac{1}{d^2} + \left(ik - \frac{x}{d^2}\right)^2\right)\psi_\alpha(x)$$

$$= -\hbar^2\left(-\frac{1}{d^2} - k^2 + \frac{1}{d^4}\int dx\, \psi_\alpha^*(x)\,x^2\,\psi_\alpha(x)\right) = -\hbar^2\left(-\frac{1}{d^2} - k^2 + \frac{1}{2d^2}\right)$$

$$= \hbar^2k^2 + \hbar^2/2d^2$$

$$\Rightarrow \langle(\Delta p)^2\rangle = \langle p^2\rangle - \langle p\rangle^2 = \underline{\hbar^2/2d^2}$$

What is the momentum space wavefunction for this state?

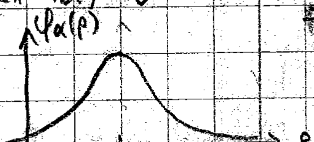
$$\varphi_\alpha(p) = \int dx\, \frac{1}{\sqrt{2\pi\hbar}}\, e^{-ipx/\hbar}\,\psi_\alpha(x)$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\cdot\frac{1}{\pi^{1/4}\sqrt{d}}\int dx\, e^{ix(k-\frac{p}{\hbar})}\, e^{-x^2/2d}$$

$$\left[ix\left(k-\tfrac{p}{\hbar}\right) - x^2/2d = -\frac{1}{2d^2}\left(x - id^2\left(k-\tfrac{p}{\hbar}\right)\right)^2 - \frac{d^2}{2}\left(k-\tfrac{p}{\hbar}\right)^2\right]$$

$$= \left(2\pi^{3/2}\hbar d\right)^{-1/2} e^{-d^2/2\hbar^2(\hbar k-p)^2}\int_{-\infty}^{\infty} dx\, \exp\left[-\frac{1}{2d^2}\left(x - id^2/\hbar\,(\hbar k-p)\right)^2\right] = \left(2\pi^{3/2}\hbar d\right)^{-1/2} e^{-\frac{d^2}{2\hbar^2}(\hbar k-p)^2}\sqrt{2}\,d\underbrace{\int_{-\infty}^{\infty} dy\, e^{-y^2}}_{\sqrt{\pi}}$$

$$= \frac{\sqrt{2\pi}\,d}{\sqrt{2\pi\hbar d}\,\pi^{1/4}}\exp\left[-\frac{d^2}{2\hbar^2}(p-\hbar k)^2\right] = \sqrt{\frac{d}{\hbar\sqrt{\pi}}}\,\exp\left[-\frac{d^2}{2\hbar^2}(p-\hbar k)^2\right]$$



POSITION & MOMENTUM IN THREE DIMENSIONS

Rather straightforward extension:

$$\hat{\vec{x}}|\vec{x}\rangle = \vec{x}|\vec{x}\rangle \qquad \hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle$$

$$\langle\vec{x}'|\vec{x}\rangle = \delta^{(3)}(\vec{x}'-\vec{x}) \qquad \langle\vec{p}'|\vec{p}\rangle = \delta^{(3)}(\vec{p}'-\vec{p})$$

$$= \delta(x'-x)\delta(y'-y)\delta(z'-z)$$

$$\int d^3\vec{x}\,|\vec{x}\rangle\langle\vec{x}| = 1 \qquad \int d^3\vec{p}\,|\vec{p}\rangle\langle\vec{p}| = 1$$

$$\psi_\alpha(\vec{x}) = \langle\vec{x}|\alpha\rangle \qquad \varphi_\beta(\vec{p}) = \langle\vec{p}|\alpha\rangle$$

$$\langle\beta|\hat{\vec{p}}|\alpha\rangle = \int d^3\vec{x}\;\psi_\beta^*(\vec{x})\left(-i\hbar\vec{\nabla}\right)\psi_\alpha(\vec{x})$$

$$\langle\vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\,e^{i\vec{p}\cdot\vec{x}/\hbar}$$

$$\psi_\alpha(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3\vec{p}\;e^{i\vec{p}\cdot\vec{x}/\hbar}\,\varphi_\alpha(\vec{p})$$

$$\varphi_\alpha(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3\vec{x}\;e^{-i\vec{p}\cdot\vec{x}/\hbar}\,\psi_\alpha(\vec{x})$$