

A pattern exists.....

Mathematics language \leftrightarrow Relationships

Relationships \leftrightarrow Correlations

Correlations \leftrightarrow Quantum Mechanics

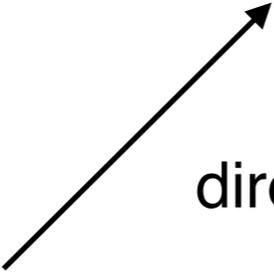
Quantum Mechanics \leftrightarrow Mathematics language

The reality of this pattern will become clear as we proceed through the class.

The Mathematics Of Quantum Mechanics - 1st Installment

**We must learn some mathematics BECAUSE it is language of QM.
We will not be able to explain and use the ideas of QM using WORDS!!**

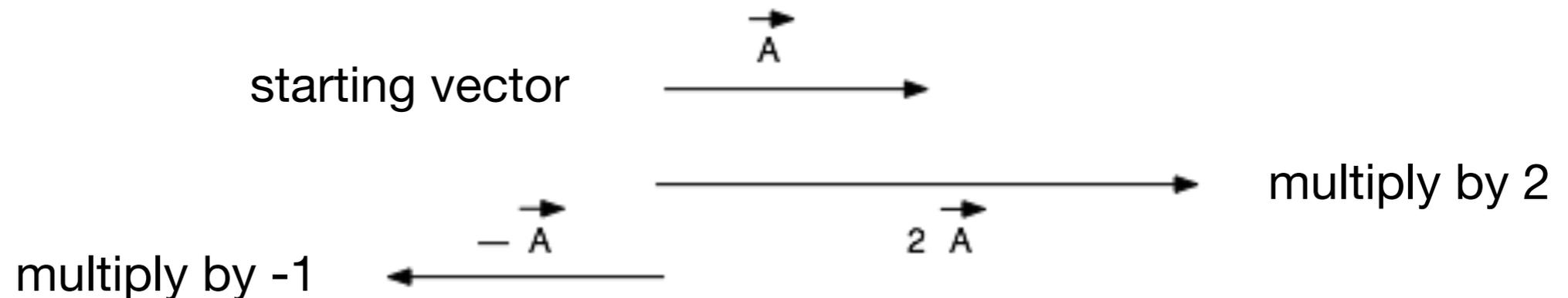
High School level Stuff...

Vector =  directed line segment

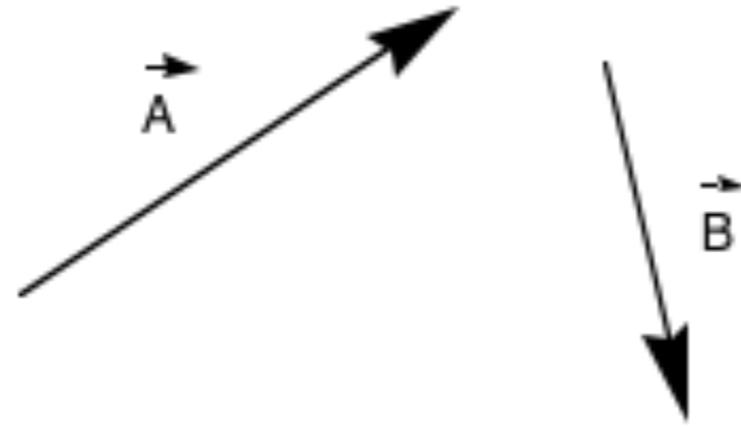
—-> 2 numbers (a,b) = number of dimensions (of plane)

or Vector —> 3 numbers (a,b,c) = number of dimensions in ordinary space

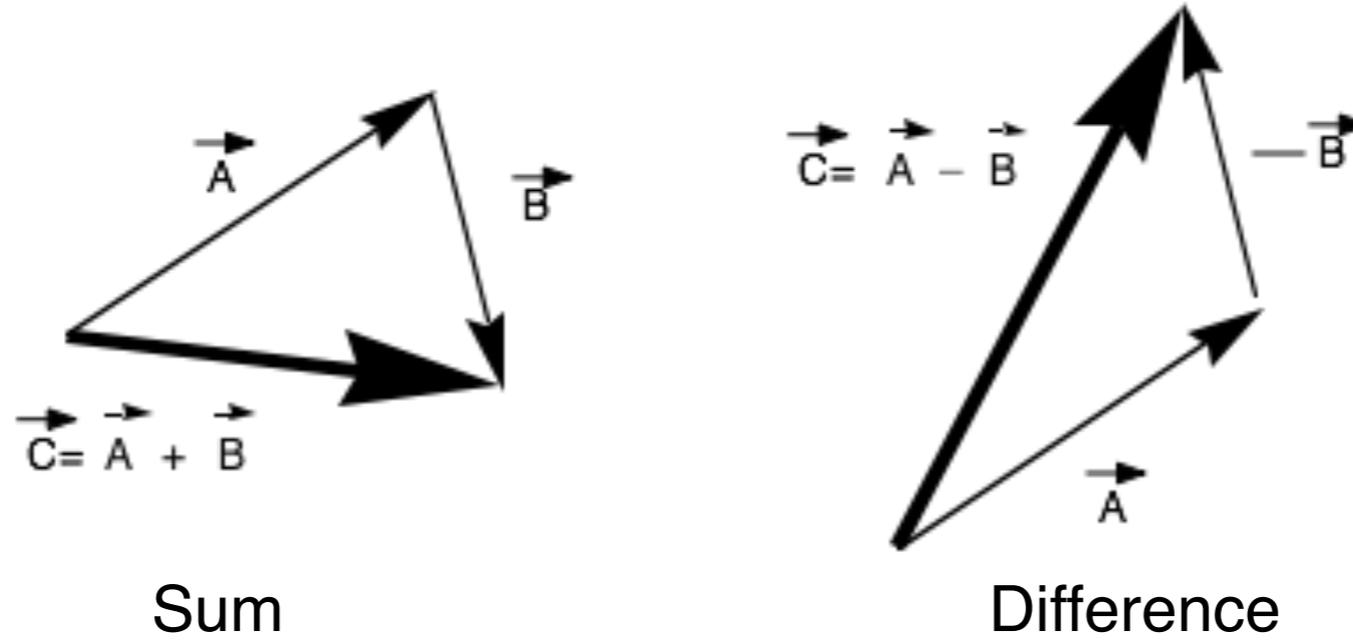
Multiplication by a scalar(a number)



Given two vectors



one can add/subtract them with geometric rules shown below



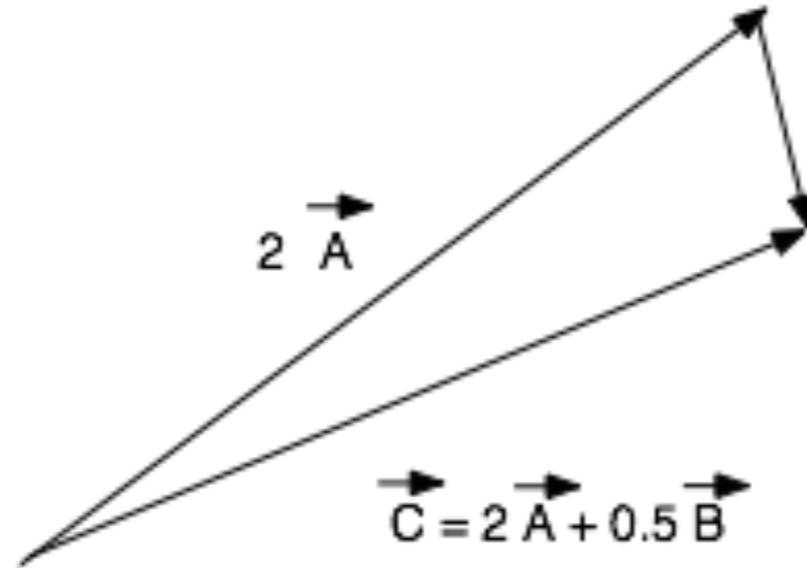
call the "tail to tip" rule

Now we generalize \rightarrow extend idea to a general linear combination(sum) of vectors

$$\vec{C} = \alpha \vec{A} + \beta \vec{B}$$

still a vector!

using $\alpha = 2$
 $\beta = 0.5$



adding parts \Rightarrow total

**I am drawing pictures in the real
3-dimensional world here!**

Here, I note that all coefficients are real numbers at this time.

This works perfectly for all macroworld vectors.

But must generalize further in order to deal with microworld vectors.

Let us see how.....

The Space of Physics

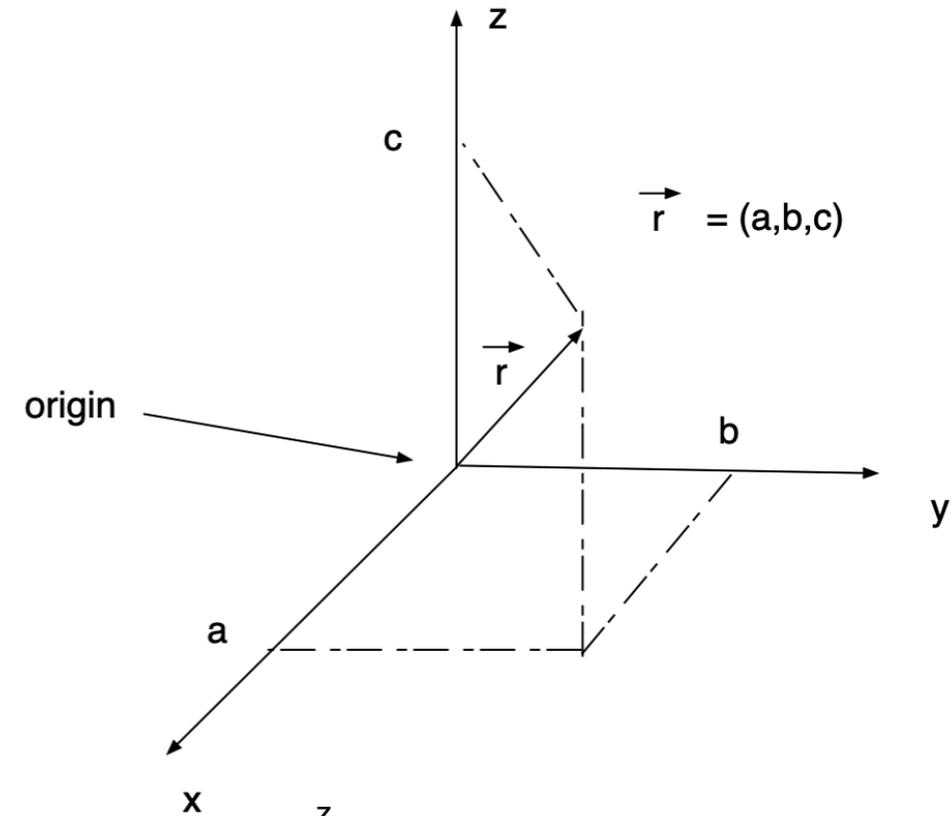
vector = 3 numbers (3 = dimension of our world)

Location in space (relative to an origin) = 3 numbers

use axis labels $(x = x_1, y = y_1, z = z_1)$

→ can define a position or radius vector

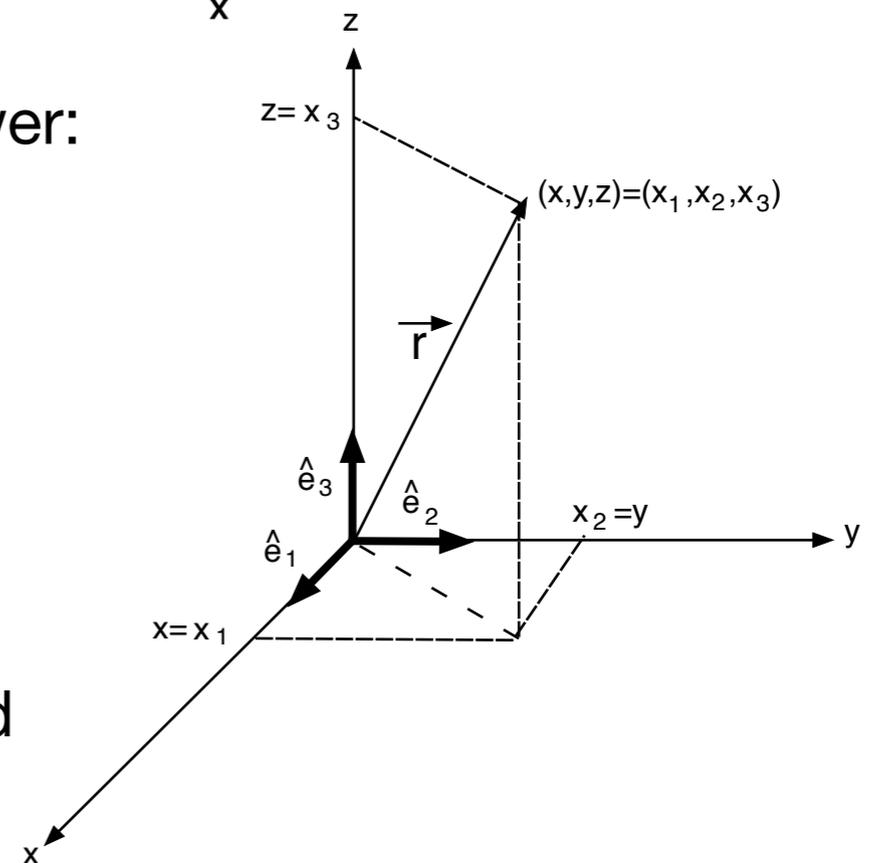
$$\vec{r} = (x, y, z) = (x_1, x_2, x_3) = (a, b, c)$$



Now to add more mathematics to increase descriptive power:

First - define 3 special vectors (called a **basis**) that will be used to construct all other vectors

$$\hat{e}_1, \hat{e}_2, \hat{e}_3 \text{ or } \hat{i}, \hat{j}, \hat{k} \text{ or } \hat{x}, \hat{y}, \hat{z}$$



They are unit vectors (length=1) and define a Right-Handed coordinate system as shown.

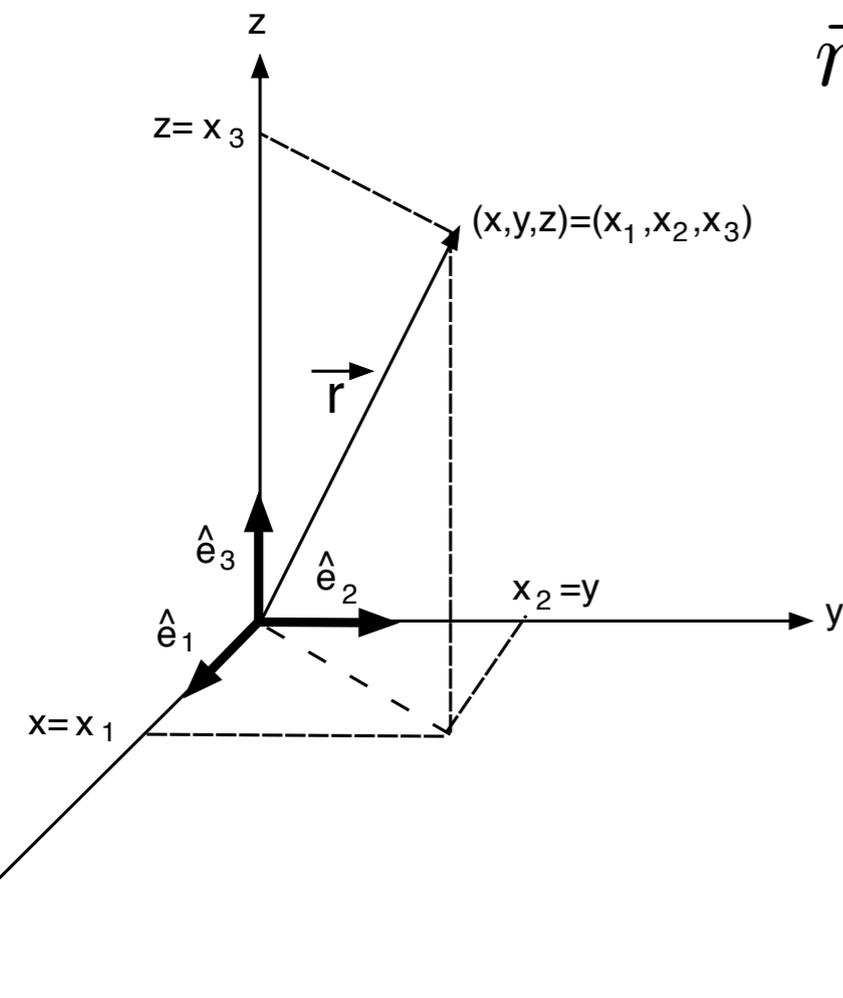
By using vector addition rules we have

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k} = x_1\hat{e}_1 + x_2\hat{e}_2 + x_3\hat{e}_3$$

$$= x\hat{x} + y\hat{y} + z\hat{z}$$

In words, $x_1=x$ =component of \vec{r} in 1-direction(x-direction), etc

$x_1\hat{e}_1$ is a vector in 1-direction of length x_1



\vec{r} is vector sum of three vectors $x_1\hat{e}_1, x_2\hat{e}_2, x_3\hat{e}_3$ draw it yourself

$\hat{e}_1, \hat{e}_2, \hat{e}_3$ or $\hat{i}, \hat{j}, \hat{k}$ or $\hat{x}, \hat{y}, \hat{z}$ called a basis set

Important
 → any vector can be written in terms of a basis

length $r = |\vec{r}| = \sqrt{x^2 + y^2 + z^2}$

using Pythagorean theorem

Go to 2 dimensions (for simplicity)

$\hat{e}_x = \text{unit}(\text{length} = 1)$ vector in x – direction

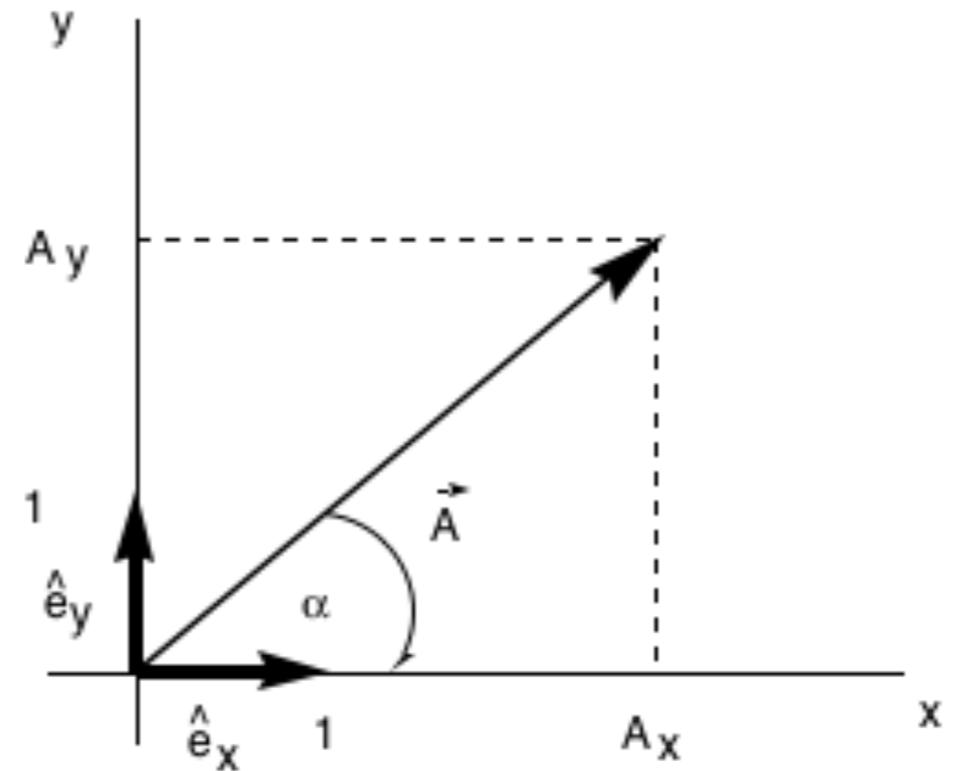
$\hat{e}_y = \text{unit}(\text{length} = 1)$ vector in y – direction

multiply by a scalar

$A_x \hat{e}_x = \text{vector of length } A_x \text{ in the } x \text{ – direction}$

$A_y \hat{e}_y = \text{vector of length } A_y \text{ in the } y \text{ – direction}$

$$\vec{A} = A_x \hat{e}_x + A_y \hat{e}_y \quad \text{by addition rule for vectors}$$



Now

$$A_x = A \cos \alpha \quad , \quad A_y = A \sin \alpha$$

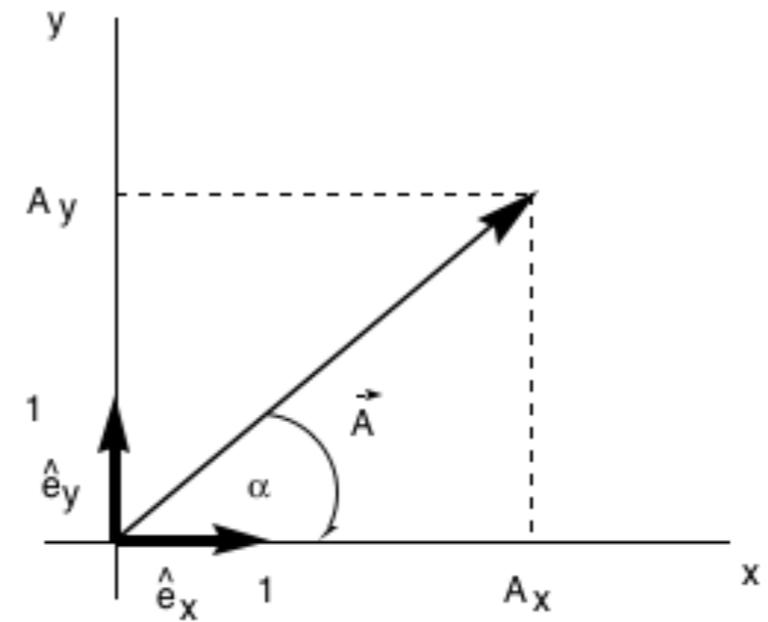
trigonometry \rightarrow **components**

For two vectors we now have

$$\vec{A} = A_x \hat{e}_x + A_y \hat{e}_y \quad , \quad \vec{B} = B_x \hat{e}_x + B_y \hat{e}_y$$

$$\vec{A} + \vec{B} = (A_x + B_x) \hat{e}_x + (A_y + B_y) \hat{e}_y$$

$$\vec{A} - \vec{B} = (A_x - B_x) \hat{e}_x + (A_y - B_y) \hat{e}_y$$



old tip-to-tail idea

eliminated in favor of adding and subtracting components; tip-to-tail idea cannot be extended to more complicated situations such as in microword!

More Generalization - Thinking about vectors

old $\vec{V} = v_1 \hat{e}_1 + v_2 \hat{e}_2$ or $|V\rangle = (v_1, v_2)$

Start of Dirac language

change of “notation” removes unit vectors

new \rightarrow Dirac **Ket** vector is the **first** element in new language

\longrightarrow $|A\rangle = (A_x, A_y)$

Your only job is to learn the new terminology; I will do the manipulations in class

addition

If $|V_1\rangle = (7, -2)$ and $|V_2\rangle = (-5, 3)$

then the sum $|V\rangle = |V_1\rangle + |V_2\rangle = (7 + (-5), (-2) + 3) = (2, 1)$

adding components as before!

difference

If $|V_1\rangle = (7, -2)$ and $|V_2\rangle = (-5, 3)$

then the difference $|V\rangle = |V_1\rangle - |V_2\rangle = (7 - (-5), (-2) - 3) = (12, -5)$

subtracting components as before!

length

If $|V\rangle = (v_1, v_2)$ then length $V = \sqrt{v_1^2 + v_2^2}$

Now we have language element that will allow of to extend ideas so they are useful in the microword:

A new operation and the generalized length

$$\text{If } |V\rangle = (v_1, v_2) \quad , \quad |U\rangle = (u_1, u_2) ,$$

$$\text{then } \langle V | U \rangle = v_1 u_1 + v_2 u_2 \quad \quad \quad \mathbf{\text{definition}}$$

we are using real-valued components \rightarrow called Euclidean vectors

symbol $\langle \dots | \dots \rangle$

\rightarrow Dirac bra-c-ket or **braket** symbol \rightarrow another element in Dirac language

Then

$$\langle V | V \rangle = v_1 v_1 + v_2 v_2 = v_1^2 + v_2^2 = (\text{length})^2$$

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{v_1^2 + v_2^2}$$

$$\mathbf{\rightarrow} \quad \langle V | V \rangle \geq 0$$

The formalism easily extends to more dimensions.....

3 dimensions

$$|V\rangle = (v_1, v_2, v_3) \quad , \quad |U\rangle = (u_1, u_2, u_3)$$

Definition:

**summation
symbol**

$$\sum_{j=1}^5 A_j = A_1 + A_2 + A_3 + A_4 + A_5$$

then

$$\langle V | U \rangle = v_1 u_1 + v_2 u_2 + v_3 u_3 = \sum_{k=1}^3 v_k u_k$$

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{v_1 v_1 + v_2 v_2 + v_3 v_3} = \sqrt{\sum_{k=1}^3 v_k^2}$$

More than 3 dimensions (not in Kansas anymore, Toto)

can no longer easily visualize(draw on paper)

$$|V\rangle = (v_1, v_2, \dots, v_n) \quad , \quad |U\rangle = (u_1, u_2, \dots, u_n)$$

$$\langle V | U \rangle = v_1 u_1 + v_2 u_2 + \dots + v_n u_n = \sum_{k=1}^n v_k u_k \quad \text{extended definition}$$

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{v_1 v_1 + v_2 v_2 + \dots + v_n v_n} = \sqrt{\sum_{k=1}^n v_k^2}$$

braket = scalar or inner product(or “dot” product)

Now we need to generalize the idea of “components”

Up to now “components” = “real” numbers and vectors were “Euclidean vectors”

Generalization → complex components

Digression on complex numbers

$i^2 = -1$, $i^3 = -i$, $i^4 = +1$, $i^5 = i$, $i^6 = -1$, and so on **definition of i**

$z = a + bi$ **definition of complex number** $a = \text{real part}$ $b = \text{imaginary part}$

$$(7 + 4i) + (-2 + 9i) = 5 + 13i$$

definition of addition

add real part and
imaginary parts
separately

$$\begin{aligned}(7 + 4i)(-2 + 9i) &= (7)(-2) + (7)(9i) + (4i)(-2) + (4i)(9i) \\ &= -14 + 63i - 8i - 36 = -50 + 55i\end{aligned}$$

definition of multiplication

using $i^2 = -1$

definition complex conjugate $z^* = a - bi$

$$|z|^2 = z^* z = (a - bi)(a + bi) = a^2 + b^2$$

$$|z| = \sqrt{a^2 + b^2}$$

absolute value

Note that z is real is $z^* = z$

braket becomes

$$\langle V | U \rangle = v_1^* u_1 + v_2^* u_2 + \cdots + v_n^* u_n = \sum_{k=1}^n v_k^* u_k$$

(same as before if components real, i.e., $v_i^* = v_i$)

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{\sum_{k=1}^n v_k^* v_k} = \sqrt{\sum_{k=1}^n |v_k|^2}$$

Vectors in QM = Euclidean vectors with complex components in Hilbert space

Now to extend idea of Basis vectors

$$|1\rangle = (1, 0) \leftrightarrow \hat{e}_x \quad , \quad |2\rangle = (0, 1) \leftrightarrow \hat{e}_y \quad \text{new representation for old unit basis vectors}$$

2 dimensions

$$|1\rangle = (1, 0, 0) \quad , \quad |2\rangle = (0, 1, 0) \quad , \quad |3\rangle = (0, 0, 1) \quad \text{called n-tuples}$$

3 dimensions

Clearly length = 1 (unit vectors) and they are perpendicular or orthogonal (by definition) and as we will prove shortly

Definition: Vector Space = collection of vectors such that

if add two vectors together \Rightarrow another vector in collection;

and have a **scalar product(bracket)** defined

Can write any vector in terms of basis \longleftrightarrow orthonormal set, i.e.,

$$|v_1, v_2\rangle = v_1(1, 0) + v_2(0, 1) = (v_1, 0) + (0, v_2) = (v_1, v_2)$$

$$|v_1, v_2\rangle = v_1(1, 0) + v_2(0, 1) = v_1 |1\rangle + v_2 |2\rangle$$

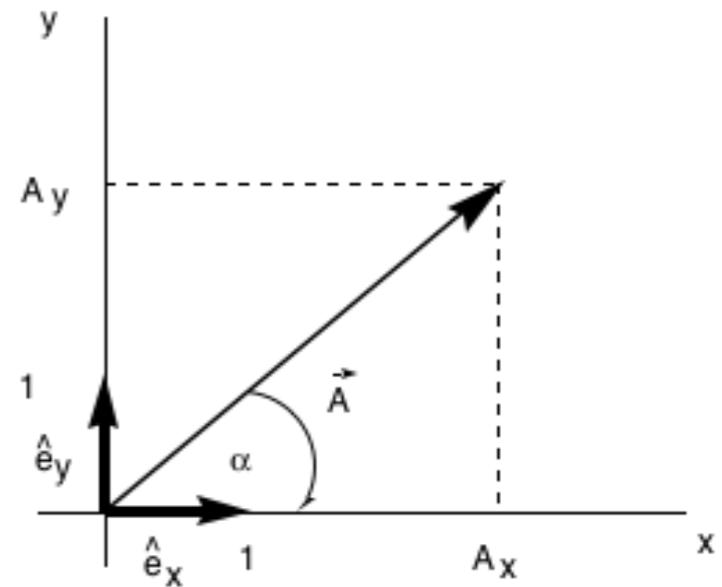
v_1 = component of vector in 1-direction, etc

Similarly for 3 dimensions

$$|U\rangle = (u_1, u_2, u_3) = u_1(1, 0, 0) + u_2(0, 1, 0) + u_3(0, 0, 1) = u_1 |1\rangle + u_2 |2\rangle + u_3 |3\rangle$$

and so on

\rightarrow **Hilbert space in microworld**



no longer a valid picture when components are complex;
just suggestive!!

Using earlier rule for evaluating the scalar product (sum of component products)

$$\langle 1 | 1 \rangle = (1, 0) \cdot (1, 0) = (1)(1) + (0)(0) = 1 \quad \langle 1 | 2 \rangle = (1, 0) \cdot (0, 1) = (1)(0) + (0)(1) = 0$$

$$\langle 2 | 1 \rangle = (0, 1) \cdot (1, 0) = (0)(1) + (1)(0) = 0 \quad \langle 2 | 2 \rangle = (0, 1) \cdot (0, 1) = (0)(0) + (1)(1) = 1$$

$$\langle 1 | V \rangle = v_1 \overset{=1}{\langle 1 | 1 \rangle} + v_2 \overset{=0}{\langle 1 | 2 \rangle} \quad \langle 2 | V \rangle = v_1 \overset{=0}{\langle 2 | 1 \rangle} + v_2 \overset{=1}{\langle 2 | 2 \rangle}$$

$$\longrightarrow \langle 1 | V \rangle = v_1 \quad \langle 2 | V \rangle = v_2 \quad \text{in new language}$$

—> The component of vector in particular direction(along basis vector) given by scalar product(bracket) of vector with corresponding basis vector.

Remember component = projection on vector in old real world!

But now, in Hilbert space, it is a “braket”.

Thus, we can always write

$$|V\rangle = \langle 1 | V \rangle |1\rangle + \langle 2 | V \rangle |2\rangle \quad \text{general definition in new language}$$

Orthogonality

First way - remember High School - use old language

$$\vec{V} = (7, 4) \quad \hat{x} = (1, 0) \quad , \quad \hat{y} = (0, 1)$$

$$\longrightarrow \vec{V} = 7\hat{x} + 4\hat{y} \quad \text{using old notation}$$

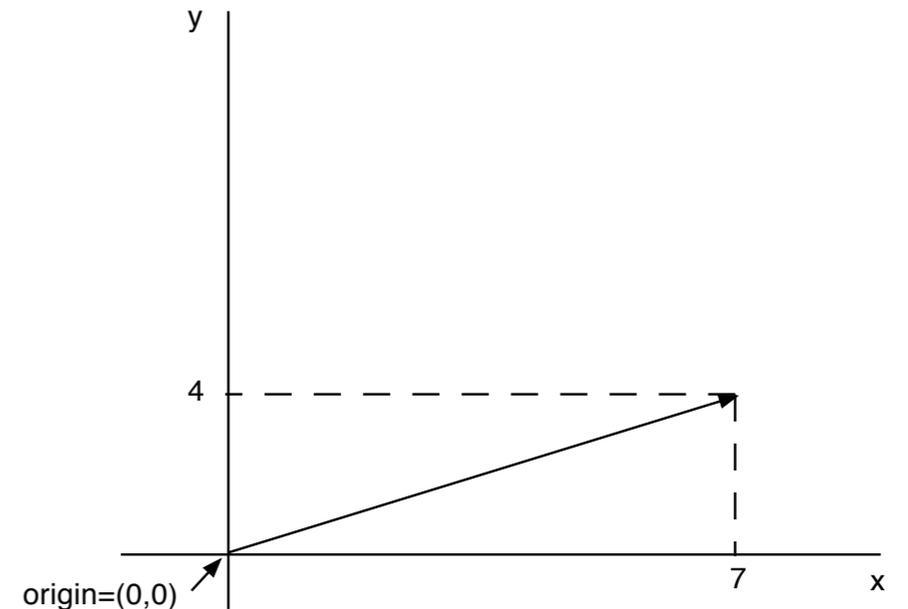
Define “dot” product:

$$\vec{A} \cdot \vec{B} = A_x B_x + A_y B_y = \langle A | B \rangle \quad \text{as is easy to check -> old/new related}$$

components

$$7 = v_x = \hat{x} \cdot \vec{V} \quad , \quad 4 = v_y = \hat{y} \cdot \vec{V}$$

$$\sqrt{v_x^2 + v_y^2} = \sqrt{65} \quad \text{length}$$



Now we can always write (in peculiar way)

$$7 = v_x = \hat{x} \cdot \vec{V} = \text{length}(\hat{x}) \times \text{length}(\vec{V}) \times \frac{v_x}{\text{length}(\vec{V})}$$

**whole mess just multiplies by 1
can you see?**

Now

$$\frac{v_x}{\text{length}(\vec{V})} = \text{cosine of angle between } \vec{V} \text{ and } \hat{x} \quad \text{—> definition of cosine}$$

so

$$\vec{A} \cdot \vec{B} = \text{length}(\vec{A}) \times \text{length}(\vec{B}) \times \cos(\text{angle between } \vec{A} \text{ and } \vec{B})$$

—————> $\vec{A} \cdot \vec{B} = AB \cos \theta$
generalize

Important special cases:

$$\hat{x} \cdot \hat{x} = \text{length}(\hat{x}) \times \text{length}(\hat{x}) \cos(0^\circ) = 1 \quad \hat{x} \cdot \hat{y} = \text{length}(\hat{x}) \times \text{length}(\hat{y}) \cos(90^\circ) = 0$$

—> Basis vectors are orthonormal!

As I have been assuming!

= orthogonal + normalized to 1 (length=1)

—> orthonormal

Generalize further (add new notation) by defining in a vector space

$$\langle A | B \rangle = AB \cos(\theta_{AB}) \quad \text{orthonormality clear!}$$

no simple geometric picture possible (as with real components); angle not geometric angle but just a parameter now!

To explore further we need the **definition of a Kronecker Delta.**

$$\langle n | m \rangle = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases} \quad \text{for basis vectors}$$

then

$$\langle 1 | 1 \rangle = \delta_{11} = 1 \quad \text{--> length = 1}$$

$$\langle 1 | 2 \rangle = \delta_{12} = 0 \quad \text{--> orthogonal}$$

$$\langle 2 | 1 \rangle = \delta_{21} = 0 \quad \text{--> orthogonal}$$

$$\langle 2 | 2 \rangle = \delta_{22} = 1 \quad \text{--> length = 1}$$

Using Kronecker delta to do algebra -> very powerful tool

$$\sum_{k=1}^3 A_k \delta_{k2} = A_1 \delta_{12} + A_2 \delta_{22} + A_3 \delta_{32} = A_1(0) + A_2(1) + A_3(0) = A_2$$

$$\sum_{k=1}^n A_k \delta_{km} = A_m \quad m \leq n$$

In order to complete our mathematic necessary to describe the microworld we need one last mathematical object is needed —> completely new —> a **Matrix**

m × n matrix is **m × n array(m rows and n columns)** of numbers(**matrix elements**)

with a well-defined set of associated mathematical rules.

For example, see sample matrices shown below

$$\begin{pmatrix} 2 \\ 5 \end{pmatrix} \quad 2 \text{ elements}$$

2 × 1 matrix (column vector)

$$(2 \quad 5) \quad 2 \text{ elements}$$

1 × 2 matrix (row vector)

$$\begin{pmatrix} 2 & 5 \\ -3 & 10 \end{pmatrix} \quad 4 \text{ elements}$$

2 × 2 matrix

$$\begin{pmatrix} 2 & 5 & -1 \\ -3 & 10 & 5 \end{pmatrix}$$

2 × 3 matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \quad \text{using row-column labels}$$

diagonal elements
off-diagonal elements

Consider two matrices

$$\mathbf{A} = \begin{pmatrix} 2 & 5 \\ -3 & 10 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} -8 & 15 \\ 7 & 4 \end{pmatrix}$$

→ 2
2 × 2 matrices (note boldface)

addition => add elements

$$\mathbf{A} + \mathbf{B} = \begin{pmatrix} (2) + (-8) & (5) + (15) \\ (-3) + (7) & (10) + (4) \end{pmatrix} = \begin{pmatrix} -6 & 20 \\ 4 & 14 \end{pmatrix}$$

matrix multiplication

$$\mathbf{AB} = \begin{pmatrix} 2 & 5 \\ -3 & 10 \end{pmatrix} \begin{pmatrix} -8 & 15 \\ 7 & 4 \end{pmatrix} = \begin{pmatrix} (2)(-8) + (5)(7) & (2)(15) + (5)(4) \\ (-3)(-8) + (10)(7) & (-3)(15) + (10)(4) \end{pmatrix} = \begin{pmatrix} 19 & 50 \\ 94 & -5 \end{pmatrix}$$

I just followed the general rule

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \quad \text{using row-column labels}$$

$$\mathbf{AB} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}$$

special cases:

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \textit{identity matrix} \quad \rightarrow \quad \mathbf{IA} = \mathbf{AI} = \mathbf{A}$$

$$\det \mathbf{A} = a_{11}a_{22} - a_{12}a_{21} = \textit{determinant of A}$$

$$\mathbf{A}^{-1} = \frac{1}{\det \mathbf{A}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix} = \textit{inverse matrix} \quad \rightarrow \quad \mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

$$A = \begin{pmatrix} 1 & 4i \\ -4i & 7 \end{pmatrix} \quad A^{-1} = \frac{1}{2 - 12i} \begin{pmatrix} 2 & -4i \\ -3 & 1 \end{pmatrix} \quad \rightarrow \quad AA^{-1} = I$$

$$\mathbf{A}^{\mathbf{T}} = \begin{pmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{pmatrix} = \textit{transpose matrix} \quad \mathbf{A}^{\dagger} = \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix} = \textit{Hermitian conjugate matrix}$$

If $\mathbf{A}^{\dagger} = \mathbf{A}$ matrix = Hermitian

$$A = \begin{pmatrix} 1 & 4i \\ -4i & 7 \end{pmatrix}$$

If $\mathbf{A}^{\dagger} = \mathbf{A}^{-1}$ matrix = Unitary

$$A = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}$$

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

$$\textit{Tr}(\mathbf{A}) = a_{11} + a_{22}$$

sum over diagonal elements

Trace

Start to pull it all together for QM

Filling out Dirac language for QM

$$|V\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \text{"ket" vector} \qquad \langle V| = (v_1^* \quad v_2^*) = \text{"bra" vector}$$

Every Ket vector has a corresponding Bra vector

$$\langle V|U\rangle = (v_1^* \quad v_2^*) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = v_1^* u_1 + v_2^* u_2 = \text{"braket"}$$

—> rule is just matrix multiplication

From now on we assume that all ket vectors are unit vectors

Thinking about Operators

Operator is mathematical object which acts on vector in vector space and **results** in another vector in same vector space.

Similar to a function with numbers $y=f(x)$.

Example

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad |V\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

$$\mathbf{A} |V\rangle = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} a_{11}v_1 + a_{12}v_2 \\ a_{21}v_1 + a_{22}v_2 \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = |U\rangle$$

Therefore

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \text{an operator} \quad \rightarrow \text{matrices are operators in QM}$$

Operators very important because

observables or measurable quantities are represented in QM by Hermitian operators(matrices)

and

transformations or physical changes of vectors are represented in QM by Unitary operators (matrices).

Properties of operators - $\hat{\mathbf{O}}$ (note boldface + hat)

Matrix representation

Definition: Matrix element (nm)=(row,column)

$$o_{nm} = \langle n | \hat{\mathbf{O}} | m \rangle$$

$$\text{--> } \mathbf{O} = \begin{pmatrix} \langle 1 | \hat{\mathbf{O}} | 1 \rangle & \langle 1 | \hat{\mathbf{O}} | 2 \rangle \\ \langle 2 | \hat{\mathbf{O}} | 1 \rangle & \langle 2 | \hat{\mathbf{O}} | 2 \rangle \end{pmatrix} = \begin{pmatrix} o_{11} & o_{12} \\ o_{21} & o_{22} \end{pmatrix}$$

Assume that $\hat{\mathbf{O}} |1\rangle = |q\rangle$, $\hat{\mathbf{O}} |2\rangle = |r\rangle$ that is what operator do!

then
$$o_{11} = \langle 1 | \hat{\mathbf{O}} | 1 \rangle = \langle 1 | q \rangle$$

$$o_{12} = \langle 1 | \hat{\mathbf{O}} | 2 \rangle = \langle 1 | r \rangle$$

$$o_{21} = \langle 2 | \hat{\mathbf{O}} | 1 \rangle = \langle 2 | q \rangle$$

$$o_{22} = \langle 2 | \hat{\mathbf{O}} | 2 \rangle = \langle 2 | r \rangle$$

--> Matrix elements are just brackets = numbers!!

Most important special case:

If $\hat{A} |V\rangle = a |V\rangle$ (i.e., we get same vector back) then

$|V\rangle$ called an **eigenvector** of operator \hat{A} with **eigenvalue** a .

For Hermitian operators, used for observables in QM, the set of eigenvectors **always** forms an orthonormal basis - called **complete set** and the eigenvalues are all real. Very useful!

If basis used to calculate matrix representing an operator

is set of eigenvectors of operator, i.e., if

$$\hat{O} |1\rangle = o_1 |1\rangle \quad , \quad \hat{O} |2\rangle = o_2 |2\rangle \quad \{o_1, o_2\} \quad = \text{eigenvalues}$$

then

$$o_{11} = \langle 1 | \hat{O} | 1 \rangle = o_1 \langle 1 | 1 \rangle = o_1 \quad o_{21} = \langle 2 | \hat{O} | 1 \rangle = o_1 \langle 2 | 1 \rangle = 0$$

$$o_{12} = \langle 1 | \hat{O} | 2 \rangle = o_2 \langle 1 | 2 \rangle = 0 \quad o_{22} = \langle 2 | \hat{O} | 2 \rangle = o_2 \langle 2 | 2 \rangle = o_2$$

$$\longrightarrow \mathbf{O} = \begin{pmatrix} \langle 1 | \hat{O} | 1 \rangle & \langle 1 | \hat{O} | 2 \rangle \\ \langle 2 | \hat{O} | 1 \rangle & \langle 2 | \hat{O} | 2 \rangle \end{pmatrix} = \begin{pmatrix} o_1 & 0 \\ 0 & o_2 \end{pmatrix}$$

Matrix representation with operator's eigenvectors is **diagonal** matrix

(nonzero elements (eigenvalues) on diagonal).

For general basis vectors(not eigenvectors),

matrix representation generally **not** diagonal.

An **alternate method** for defining operators uses the “ket” and “bra” vectors.

Consider the quantity

using our rules we get

$$\mathcal{P}_{fg} = |f\rangle \langle g| \quad \longrightarrow \quad \mathcal{P}_{fg} |V\rangle = (|f\rangle \langle g|) |V\rangle = \langle g | V\rangle |f\rangle = \textit{number} \times |f\rangle$$

Thus, the new object is an **operator!**

Called the “**ket-bra**”

If g=f, then we get

$$\mathcal{P}_f = |f\rangle \langle f| \quad = \textbf{projection operator i.e.,}$$

$$\mathcal{P}_f |V\rangle = (|f\rangle \langle f|) |V\rangle = \langle f | V\rangle |f\rangle$$

“projects” onto $|f\rangle$ final vector now in that direction

$$\langle f | V\rangle \quad \textbf{gives amount in direction} \quad |f\rangle$$

Notice we used the rule: $(\langle f|)(|f\rangle) = \langle f | f\rangle$

to simplify notion

Now consider set of orthonormal basis vectors:

$$\{|n\rangle\}, \quad n = 1, 2, 3, \dots, N$$

$$\longrightarrow \langle k | n\rangle = \delta_{kn}$$

We have (doing some algebra for practice):

$$(|k\rangle \langle k|)(|k\rangle \langle k|) = |k\rangle (\langle k | k\rangle) \langle k| = |k\rangle (1) \langle k| = |k\rangle \langle k|$$

$$\textbf{Another example:} \quad (|k\rangle \langle k|)(a |1\rangle + b |2\rangle) = |k\rangle (a \langle k | 1\rangle + b \langle k | 2\rangle) = (\textit{number}) \times |k\rangle$$

More details:

Now consider basis vectors: $\{|n\rangle\}, n = 1, 2, 3, \dots, N$ $\langle n | m \rangle = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$
{set} **→ orthonormal**

We have:

$$(|k\rangle \langle k|)(|k\rangle \langle k|) = |k\rangle \langle k | k \rangle \langle k| = |k\rangle \langle k| \quad \text{→ member of set}$$

$$\text{→} \quad \mathcal{P}_k^2 = \mathcal{P}_k$$

Now $\mathcal{P}_k |n\rangle = (|k\rangle \langle k|) |n\rangle = |k\rangle \langle k | n \rangle = \langle k | n \rangle |k\rangle$

Since $\langle k | n \rangle = 0 \quad k \neq n$ $\langle k | n \rangle = 1 \quad k = n$ **basis vectors**

Thus: $\mathcal{P}_k |n\rangle = \begin{cases} |k\rangle & n = k \\ 0 & n \neq k \end{cases} \quad \longrightarrow \quad \begin{aligned} \mathcal{P}_k |k\rangle &= +1 |k\rangle = |k\rangle \\ \mathcal{P}_k |n \neq k\rangle &= 0 |n \neq k\rangle = 0 \end{aligned}$

→ eigenvalues of \mathcal{P}_k are 0,1

Another way

$$\mathcal{P}_k^2 |n\rangle = \mathcal{P}_k |n\rangle$$

$$(\mathcal{P}_k - \mathcal{P}_k^2) |n\rangle = 0$$

$$\mathcal{P}_k(1 - \mathcal{P}_k) |n\rangle = 0 \quad \longrightarrow \quad \text{eigenvalues of } \mathcal{P}_k \text{ are 0,1}$$

Now for some useful properties needed for derivations and examples of use of new language.

Now for some useful properties for later derivations and examples of use of the language

Consider operator

$$\sum_{k=1}^n |k\rangle \langle k| \quad \rightarrow \text{sum of projection operators}$$

Remember from earlier that for any Ket vector, we can write (example in 2 dimensions)

$$|V\rangle = \langle 1 | V \rangle |1\rangle + \langle 2 | V \rangle |2\rangle$$

or in general

$$|V\rangle = \sum_{k=1}^2 \langle k | V \rangle |k\rangle$$

so in n dimensions we have(2 terms in sum --> n terms)

$$|V\rangle = \sum_{k=1}^n \langle k | V \rangle |k\rangle \quad \text{this is very powerful notation}$$

We have

$$\left(\sum_{k=1}^n |k\rangle \langle k| \right) |V\rangle = \sum_{k=1}^n \langle k | V \rangle |k\rangle = |V\rangle \quad \xrightarrow{\text{no change!!}} \quad \sum_{k=1}^n |k\rangle \langle k| = \hat{\mathbf{I}}$$

the identity operator

Will be very important!

Technical term: It is a representation of the identity

Expectation Value

$$\langle \hat{\mathbf{O}} \rangle = \langle V | \hat{\mathbf{O}} | V \rangle$$

Very important object!!

Will turn out(see later) to be the average value of an observable from a set of measurements on identical systems in state $|V\rangle$. Let us see how.

First, we need an **alternative representation** of an operator

(also some simple algebra practice for you to do)

$$\hat{\mathbf{B}} |b_k\rangle = b_k |b_k\rangle \quad k = 1, 2, 3, \dots, n \quad \text{eigenvector/eigenvalues equation}$$

if operator Hermitian \longrightarrow $|b_k\rangle$ are an orthonormal basis so that

$$\langle b_i | b_j \rangle = \delta_{ij} \quad b_k = \text{eigenvalues} \quad \text{and} \quad \sum_{k=1}^n |b_k\rangle \langle b_k| = \hat{\mathbf{I}}$$

Then

$$\hat{\mathbf{B}} = \hat{\mathbf{B}}\hat{\mathbf{I}} = \hat{\mathbf{B}} \sum_{k=1}^n |b_k\rangle \langle b_k|$$

identity operator does not change anything

$$= \sum_{k=1}^n \hat{\mathbf{B}} |b_k\rangle \langle b_k| = \sum_{k=1}^n b_k |b_k\rangle \langle b_k|$$

operator moves through summation
and operates on Ket vector

or

$$\hat{\mathbf{B}} = \sum_{k=1}^n b_k |b_k\rangle \langle b_k|$$

→ operator written in terms of eigenvalues/eigenvectors or projection operators

Algebra gives (see next slide for details)

$$\hat{\mathbf{B}}^2 = \sum_{k=1}^n b_k^2 |b_k\rangle \langle b_k|$$

$$\hat{\mathbf{B}}^3 = \sum_{k=1}^n b_k^3 |b_k\rangle \langle b_k|$$

$$\hat{\mathbf{B}}^n = \sum_{k=1}^n b_k^n |b_k\rangle \langle b_k|$$

Examples of algebra with useful end results: Let us step through algebra.....

$$\hat{\mathbf{B}}^2 = \left(\sum_{k=1}^n b_k |b_k\rangle \langle b_k| \right) \left(\sum_{m=1}^n b_m |b_m\rangle \langle b_m| \right)$$
$$= \sum_{k=1}^n \sum_{m=1}^n b_k b_m |b_k\rangle \langle b_k | b_m\rangle \langle b_m| = \sum_{k=1}^n \sum_{m=1}^n b_k b_m |b_k\rangle \langle b_m| \delta_{km}$$

$$= \sum_{k=1}^n b_k^2 |b_k\rangle \langle b_k| \quad \text{using} \quad \sum_k A_k \delta_{kn} = A_n$$

$$\longrightarrow \hat{\mathbf{B}}^3 = \sum_{k=1}^n b_k^3 |b_k\rangle \langle b_k| \quad \longrightarrow \hat{\mathbf{B}}^n = \sum_{k=1}^n b_k^n |b_k\rangle \langle b_k|$$

Definition: Power series representation of a function:

$$f(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \dots = \sum_{k=0}^{\infty} a_k x^k$$

Examples(the real definitions):

$$e^{\alpha x} = \sum_{k=0}^{\infty} \frac{1}{k!} \alpha^k x^k$$

$$\sin \alpha x = \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (-1)^k \alpha^{2k+1} x^{2k+1}$$

$$\cos \alpha x = \sum_{k=0}^{\infty} \frac{1}{(2k)!} (-1)^k \alpha^{2k} x^{2k}$$

Now consider

$$e^{\alpha x} = \sum_{k=0}^{\infty} \frac{1}{k!} \alpha^k x^k$$

$$\xrightarrow{x \rightarrow \hat{\mathbf{O}}}$$

$$e^{\alpha \hat{\mathbf{O}}} = \sum_{k=0}^{\infty} \frac{1}{k!} \alpha^k \hat{\mathbf{O}}^k$$

In special case where

$$\hat{\mathbf{O}}^2 = \hat{\mathbf{I}}$$

(algebra on next slide)

$$e^{i\alpha \hat{\mathbf{O}}} = \cos \alpha \hat{\mathbf{I}} + i \hat{\mathbf{O}} \sin \alpha$$

One of most powerful relations in QM

(original derivation for ordinary functions by Euler in 16th century)

$$e^{i\theta} = \cos \theta + i \sin \theta$$

$$\rightarrow e^{i\pi/2} = i, \quad e^{i\pi} = -1$$

real definition

$$e^{i\theta\hat{\mathbf{O}}} = \sum_{k=0}^{\infty} \frac{1}{k!} (i\theta)^k \hat{\mathbf{O}}^k = \sum_{k=0}^{\infty} \frac{1}{k!} (i)^k \theta^k \hat{\mathbf{O}}^k = \hat{\mathbf{I}} + i\theta\hat{\mathbf{O}} + \frac{1}{2!} i^2 \theta^2 \hat{\mathbf{O}}^2 + \frac{1}{3!} i^3 \theta^3 \hat{\mathbf{O}}^3 + \frac{1}{4!} i^4 \theta^4 \hat{\mathbf{O}}^4 + \dots$$

where have used $i^2 = -1, i^3 = -i, i^4 = +1, \dots$

$$= \hat{\mathbf{I}} + i\theta\hat{\mathbf{O}} - \frac{1}{2!} \theta^2 \hat{\mathbf{O}}^2 - i \frac{1}{3!} \theta^3 \hat{\mathbf{O}}^3 + \frac{1}{4!} \theta^4 \hat{\mathbf{O}}^4 + \dots$$

$$= \left(\hat{\mathbf{I}} - \frac{1}{2!} \theta^2 \hat{\mathbf{O}}^2 + \frac{1}{4!} \theta^4 \hat{\mathbf{O}}^4 + \dots \right) + i \left(\theta \hat{\mathbf{O}} - \frac{1}{3!} \theta^3 \hat{\mathbf{O}}^3 + \dots \right)$$

where have used

$$\hat{\mathbf{O}}^2 = \hat{\mathbf{O}}^4 = \hat{\mathbf{O}}^6 = \dots = \hat{\mathbf{I}}$$

$$\hat{\mathbf{O}} = \hat{\mathbf{O}}^3 = \hat{\mathbf{O}}^5 = \dots = \hat{\mathbf{O}}$$

$$= \left(\hat{\mathbf{I}} - \frac{1}{2!} \theta^2 \hat{\mathbf{I}} + \frac{1}{4!} \theta^4 \hat{\mathbf{I}} + \dots \right) + i \left(\theta \hat{\mathbf{O}} - \frac{1}{3!} \theta^3 \hat{\mathbf{O}} + \dots \right)$$

$$= \cos \theta \hat{\mathbf{I}} + i \hat{\mathbf{O}} \sin \theta$$

In general, if we need operator for an arbitrary function $f(x)$ we do the following:

if $\hat{B} |b_k\rangle = b_k |b_k\rangle \quad k = 1, 2, 3, \dots, n$ **then** $f(\hat{B}) = \sum_{k=1}^n f(b_k) |b_k\rangle \langle b_k|$

Definition

$$\text{commutator} = [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

ordinary numbers “commute”

operators may not “commute”

This is mathematical property behind Heisenberg uncertainty principle.

Remember these useful properties:

$$|V\rangle = v_1 |1\rangle + v_2 |2\rangle \quad , \quad |U\rangle = u_1 |1\rangle + u_2 |2\rangle$$

$$\langle V | U \rangle = v_1^* u_1 + v_2^* u_2$$

$$\langle U | V \rangle = u_1^* v_1 + u_2^* v_2 = \langle V | U \rangle^*$$

$$|V\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

$$\langle V| = (v_1^* \quad v_2^*) = |V\rangle^\dagger$$

I have an interesting thought....(this is how a theoretical physicist works.....)

$$\langle \hat{\mathbf{B}} \rangle = \langle V | \hat{\mathbf{B}} | V \rangle = \text{expectation value}$$

$\hat{\mathbf{B}}$ is Hermitian \rightarrow

$\hat{\mathbf{B}}$ eigenvectors are complete orthonormal set = basis \rightarrow make expansions

$$|V\rangle = \sum_{k=1}^n d_k |b_k\rangle, \quad d_k = \langle b_k | V \rangle$$

$$\langle V | = \sum_{k=1}^n d_k^* \langle b_k |$$

Can always do this with any basis set!!

More algebra gives:

$$\langle \hat{\mathbf{B}} \rangle = \sum_{k=1}^n b_k |d_k|^2$$

see algebra on next slide

$$\langle \hat{\mathbf{B}} \rangle = \left(\sum_{k=1}^n d_k^* \langle b_k | \right) \hat{\mathbf{B}} \left(\sum_{m=1}^n d_m | b_m \rangle \right) = \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m \langle b_k | \hat{\mathbf{B}} | b_m \rangle$$

$$= \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m \langle b_k | b_m | b_m \rangle = \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m b_m \langle b_k | b_m \rangle$$

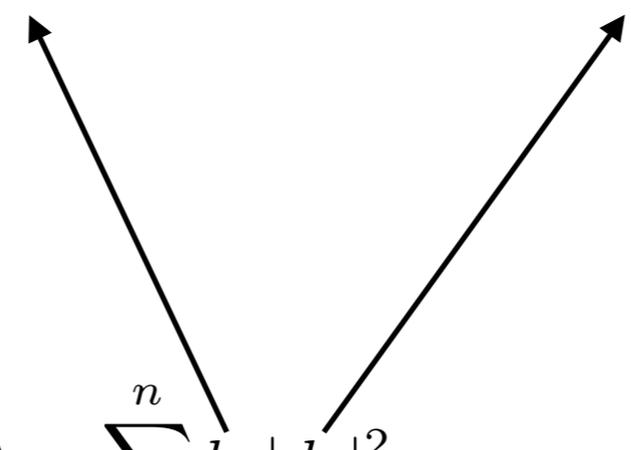
$$= \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m b_m \delta_{km} = \sum_{k=1}^n b_k d_k^* d_k = \sum_{k=1}^n b_k |d_k|^2$$

Now, in general, if expectation value = average value, then we must have

$$\langle \hat{\mathbf{B}} \rangle = \sum_{\text{allowed values}} (\text{allowed value of B}) \times (\text{Probability of that value})$$

which is just the **definition** of the average value!!

Now we just derived

$$\langle \hat{\mathbf{B}} \rangle = \sum_{k=1}^n b_k |d_k|^2$$


Comparing(see arrows) last two equations - we might guess

allowed values = eigenvalues

and

probability = square of component value

Now we can write

$$|d_k|^2 = d_k^* d_k = (\langle b_k | V \rangle)^* \langle b_k | V \rangle = |\langle b_k | V \rangle|^2 = \langle V | b_k \rangle \langle b_k | V \rangle$$

This says that

$$|\langle b_k | V \rangle|^2 = \text{probability of observing value } b_k \text{ when in state } |V\rangle$$

Also says

$$\langle V | b_k \rangle \langle b_k | V \rangle = |\langle b_k | V \rangle|^2 = |\text{component}|^2$$

$$= \text{probability of observing value } b_k \text{ in state } |V\rangle$$

$$= \text{expectation value of the projection operator}$$

Repeat of Time Evolution Derivation - it is clearly so important

Energy eigenvectors evolve in time with exponential factor $e^{-iEt/\hbar}$

—> for energy eigenvector $|E\rangle$ have $\hat{U}(t) |E\rangle = e^{-iEt/\hbar} |E\rangle$

Thus, if want to find time evolution of arbitrary state,

then follow procedure stated earlier:

1. Write arbitrary initial ($t = 0$) state $|\psi\rangle$ in terms of energy eigenvectors, i.e., use energy basis.

$$|\psi(0)\rangle = \sum_n a_n |E_n\rangle \quad \text{where } a_n = \langle E_n | \psi \rangle.$$

2. Operate with time development operator

$$|\psi(t)\rangle = \hat{U}(t) |\psi\rangle = \hat{U}(t) \sum_n a_n |E_n\rangle = \sum_n a_n \hat{U}(t) |E_n\rangle = \sum_n a_n e^{-iE_n t/\hbar} |E_n\rangle$$

3. Do measurement of observable, \hat{B}

—> must change basis to eigenvectors of \hat{B} (go to HOME space). Have

$$|E_n\rangle = \sum_k c_{kn} |b_k\rangle \quad \text{where } \hat{B} |b_k\rangle = b_k |b_k\rangle \quad \text{and} \quad c_{kn} = \langle b_k | E_n \rangle$$

4. Finally, probability amplitude for measuring b_k if in state $|\psi(t)\rangle$ given by

$$\langle b_k | \psi(t) \rangle = \sum_n a_n e^{-iE_n t/\hbar} \langle b_k | E_n \rangle = \sum_n a_n e^{-iE_n t/\hbar} c_{kn}$$

Have, formally, answered question,

although computation might be difficult.

Another way of thinking about time evolution

is to work directly with time-evolution operator $\hat{U}(t)$.

Makes above discussion more formal.

Most of operators we have been discussing correspond to observables.

In mathematics \rightarrow Hermitian operators.

Since their eigenvalues

are possible results of measurements of observables and eigenvalues

must be real numbers

\rightarrow always true for Hermitian operators.

Time-evolution operator representative of 2nd class of operators in quantum theory.

These operators do not represent observables,

but instead transform kets (states) into different kets (states).

Because coefficients of basis states in representation of arbitrary state

are related to probability amplitudes

and therefore sum of their absolute squares must equal 1,

these transformation-type operators, in mathematics \rightarrow unitary operators.

Unitary operators in mathematics have eigenvalues whose absolute value always equals 1.

From our study of complex numbers,

know that if $z = e^{i\alpha} = \cos \alpha + i \sin \alpha$, then $|z|^2 = \cos^2 \alpha + \sin^2 \alpha = 1$

or $|z| = 1$ always.

Thus, eigenvalues of any unitary operator

can always be represented by a complex exponential.

If eigenvectors/eigenvalues of $\hat{U}(t)$ represented by equation $\hat{U}(t) |\beta_n\rangle = e^{i\beta_n} |\beta_n\rangle$

then can write
$$\hat{U}(t) = \sum_n e^{i\beta_n} |\beta_n\rangle \langle \beta_n|$$

In many physical systems,

energy operator does not change with time.

In quantum theory

\rightarrow both energy operator

and time-evolution operator have same eigenvectors.

If have $\hat{H} |E_k\rangle = E_k |E_k\rangle$, then \rightarrow can write $\hat{U}(t) = \sum_n e^{-iE_n t/\hbar} |E_n\rangle \langle E_n|$

\rightarrow for energy eigenvector have

$$\hat{U}(t) |E_k\rangle = \left[\sum_n e^{-iE_n t/\hbar} |E_n\rangle \langle E_n| \right] |E_k\rangle = e^{iE_k t/\hbar} |E_k\rangle$$

i.e., only change by phase factor.

\rightarrow no probabilities changes during time evolution of these states
and called **stationary states**.

More importantly, property gives method for finding time evolution for arbitrary state \rightarrow

1. Write initial arbitrary state in energy basis $|\psi(0)\rangle = \sum_n a_n |E_n\rangle$ where $a_n = \langle E_n | \psi \rangle$

2. Operate with time development operator

$$|\psi(t)\rangle = \hat{U}(t) |\psi\rangle = \hat{U}(t) \sum_n a_n |E_n\rangle = \sum_n a_n \hat{U}(t) |E_n\rangle = \sum_n a_n e^{-iE_n t/\hbar} |E_n\rangle$$

3. and so on as before.....

If you wanted to do it, you are now able to to do QM calculations!!

These ideas will become postulates - that is what random thinking sometimes produces

That is all mathematics will need for QM - lots of repetition coming.....

As we worked through the mathematics

we have laid the ground work for the postulates of QM

(in some cases we have actually stated the postulate already).

We will not use any more mathematics than I have shown you already.

You will get better at using the mathematics as we will use it in class and you get used to the language.

If you cannot follow all the details of the mathematics,

then just follow along with the ideas that I present.

That will be sufficient to understand QM.