Module - I Part 1

Foundations

Module 1

PH 534 QIC

1 BASICS OF QUANTUM MECHANICS

Quantum mechanics is based on two important objects :-

Wave functions and operators

↓ State of a quantum system ↓ VECTORS

↓ observables, measurements density operators ↓ LINEAR TRANSFORMATIONS

So the natural language of QM is linear algebra. Let us take a step back and quickly go through some basics of linear algebra.

A) LINEAR ALGEBRA

Linear algebra takes the notion of ordinary vectors to an abstract form. As such, the basic objects of linear algebra are vector spaces.

i) Vectors — A vector space consists of :

a set of abstract objects or vectors — $(|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots)$

and

a set of scalars taken from the field of complex numbers — $(a, b, c, \ldots)$

and is CLOSED under :

- Vector addition
- Scalar multiplication

- Vector addition :

Addition : $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$ (all are elements in the space)

Commutative : $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$

Associative : $|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$

Null vector : $|\alpha\rangle + 0 = |\alpha\rangle$

Inverse vector : $|\alpha\rangle + \underbrace{|-\alpha\rangle}_{\text{abstract}} = 0$

- Scalar multiplication :

Multiplication : $a|\alpha\rangle = |\gamma\rangle$ ($|\alpha\rangle$ and $|\gamma\rangle$ are elements in the space)

Distributive : $a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a|\beta\rangle$

$(a+b)|\alpha\rangle = a|\alpha\rangle + b|\alpha\rangle$

Associative : $a(b|\alpha\rangle) = (ab)|\alpha\rangle$

Null and identity : $0|\alpha\rangle = 0$ and $1|\alpha\rangle = |\alpha\rangle$

Also, $|-\alpha\rangle = (-1)|\alpha\rangle = -|\alpha\rangle$ (Inverse vector)

All of this is quite intuitive if one thinks of the usual vector analysis that most are used to. The same logic can be extended to the more abstract idea of vector space and linear algebra.

ii) Linear combination and basis vectors

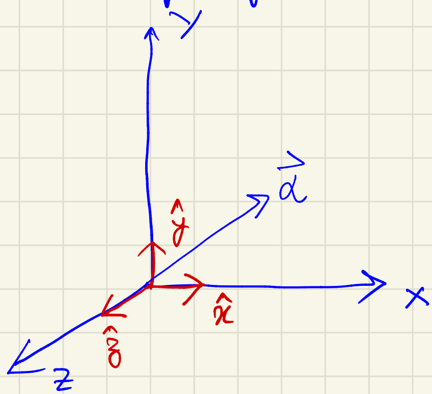
A linear combination of vectors is given by :

$$a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \dots$$

A set of vectors $\{|v_i\rangle\} = \{|v_1\rangle, |v_2\rangle, |v_3\rangle, \dots |v_n\rangle\}$ is said to span a vector space if all vectors in the space can be obtained by linear combination of the spanning set $\{|v_i\rangle\}$; i.e.,

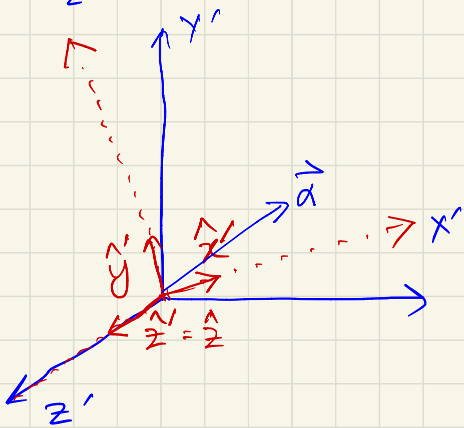
$$|\alpha\rangle = a_1|v_1\rangle + a_2|v_2\rangle + a_3|v_3\rangle + \dots + a_n|v_n\rangle$$

Take the example of the 3D Euclidean space :-



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

$\{\hat{x}, \hat{y}, \hat{z}\}$ span the space



$$\vec{\alpha} = x'\hat{x}' + y'\hat{y}' + z'\hat{z}'$$

$\{\hat{x}', \hat{y}', \hat{z}'\}$ span the space

The spanning set $\{|v_i\rangle\}$ is said to be linearly independent if its elements cannot be written as a linear combination of the remaining elements, i.e.,

$$a_1|v_1\rangle + a_2|v_2\rangle + \dots + a_n|v_n\rangle = 0, \forall\, a_i = 0$$

This implies that : $|v_k\rangle \neq \sum_{i\neq k} -a_i/a_k\,|v_k\rangle$

* Remember from the previous 3D example :-

$\{\hat{x}, \hat{y}, \hat{z}\}$ and $\{\hat{x}', \hat{y}', \hat{z}'\}$ both the span the basis

and also; $\hat{x} \neq y\hat{y} + z\hat{z}$ and $\hat{x}' \neq y'\hat{y}' + z'\hat{z}'$

but : $\hat{x} = y'\hat{y}' + z'\hat{z}'$ } linear independence only holds within the same spanning set.

Basis vectors :

Any spanning set $\{|v_i\rangle\}$ that is linearly independent forms a basis for the vector space. For any vector $|\alpha\rangle$:

$$|\alpha\rangle = a_1|v_1\rangle + a_2|v_2\rangle + a_3|v_3\rangle + \dots + a_n|v_n\rangle$$

$$= \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

} The column matrix gives us a more intuitive feel for the usual vector

Exercise : How would you represent the basis vectors in the notation ? Can you use this to work out the axioms of a vector space ?

iii) Inner products

The inner product is a generalisation of the notion of dot products to vector spaces.

$$\underbrace{(|\alpha\rangle, |\beta\rangle)}_{\text{two vectors from the space } V} = c \sim \text{complex numbers from the field } \mathbb{C}$$

One can also use the dual vector space $\{\langle\alpha|\}$, which is a vector space of all linear transformations from space $V \rightarrow \mathbb{C}$, together with vector addition and scalar multiplication.

$$\langle\alpha|(|\beta\rangle) \equiv \langle\alpha|\beta\rangle \equiv (|\alpha\rangle, |\beta\rangle)$$

We call $\langle\alpha|$ the dual vectors

- Properties of inner products

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$$

$$\langle\alpha|\alpha\rangle \geqslant 0 \text{ , with } \langle\alpha|\alpha\rangle = 0 \text{ iff } |\alpha\rangle = 0$$

and linearity in the original vector space

$$\langle\alpha|\left(b|\beta\rangle + c|\gamma\rangle\right) = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle$$

A vector space with an inner product is called an inner product space.

A complete vector space $\longrightarrow$ Banach space
A complete inner product space $\longrightarrow$ Hilbert space
((with a NORM !!))

iv) Orthonormal basis

The norm of a vector in the vector space V is given by the relation

$\|V\| \rightarrow \mathbb{R}$ (where $\mathbb{R}$ is the real scalar field)

* Note the scalar field associated with V can be complex in general.

For inner product spaces, the inner product naturally allows one to define a norm such that

$$\|\alpha\| = \sqrt{\langle\alpha|\alpha\rangle} \in \mathbb{R}, \because \langle\alpha|\alpha\rangle \geqslant 0$$

The norm generalises the notion of length. It is positive definite, homogenous and subadditive. Allows for the definition of a metric $\|\alpha - \beta\|$ between vectors.

- A vector $|\alpha\rangle$ with unit norm is "normalised"
- Two vectors that satisfy $\langle\alpha|\beta\rangle = 0$ are said to be "orthogonal"

"unit vector" "perpendicular"

Consider the basis $\{|v_i\rangle\}$ that satisfies $\langle v_i|v_j\rangle = \delta_{ij}$ and therefore forms an "orthonormal" basis.

Now if $|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$ and $|\beta\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \dots + a_n^* b_n$$

$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \ldots\ldots a_n^* b_n$ } Similar to dot product between two regular vectors

Also, $\langle\alpha| = (a_1^* \; a_2^* \ldots a_n^*)$ is the row vector whose components are the complex conjugate of $|\alpha\rangle$

Exercise: Show that, $\|\alpha\|^2 = \langle\alpha|\alpha\rangle = \sum_i |a_i|^2$

One can also generalize the notion of an angle through the relation;

$$\cos\theta = \frac{|\langle\alpha|\beta\rangle|}{\sqrt{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}}$$

Again, think of two regular vectors $\cos\theta = \frac{\vec{a}\cdot\vec{b}}{|\vec{a}|\cdot|\vec{b}|}$

* $\langle\alpha|\beta\rangle$ in general is a complex number

The absolute value of $\cos\theta$ is less than 1 as

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$$ (Cauchy-Schwarz Inequality)

Exercise: Suppose $\{|w_i\rangle\}$ is a basis set for an inner product space. Show that one can find an orthonormal basis $\{|v_i\rangle\}$ by the iterative method:

Set $|v_1\rangle = \frac{|w_1\rangle}{\sqrt{\langle w_1|w_1\rangle}} = \frac{|w_1\rangle}{\||w_1\rangle\|}$

For $1 \leq k \leq d-1$; $|v_{k+1}\rangle \equiv \frac{|w_{k+1}\rangle - \sum_{i=1}^{k}\langle v_i|w_{k+1}\rangle|v_i\rangle}{\left\||w_{k+1}\rangle - \sum_{i=1}^{k}\langle v_i|w_{k+1}\rangle|v_i\rangle\right\|}$

This is called the Gram-Schmidt procedure.

Prove that $\{|v_i\rangle\}$ is indeed orthonormal.

v) Linear operators and matrices

A linear operator takes every vector in a vector space and "transforms" into another vector, keeping the linear structure intact,

$$T : V \to W \quad \text{such that} \quad T(a|\alpha\rangle + b|\beta\rangle) = aT|\alpha\rangle + bT|\beta\rangle$$

Another example : $T|\alpha\rangle = T\left(\sum_i a_i |v_i\rangle\right) = \sum_i a_i \underbrace{T|v_i\rangle}_{\text{transformation of the orthonormal basis vectors}}$

$$\boxed{\begin{array}{c}\text{For instance the identity and null operator} \\ I|\alpha\rangle = |\alpha\rangle \;;\quad 0|\alpha\rangle = 0\end{array}}$$

Matrices provide the most convenient way to represent linear operators and can be easily integrated with the row and column matrices for the vector and dual-vector space.

Let $\{|v_i\rangle\}$ be the basis for V and $\{|w_i\rangle\}$ be the basis for W, and $T : V \to W$

$$T|v_1\rangle = \sum_{i=1}^{m} t_{i1} |w_i\rangle \Big\} \because \text{a vector in } W \text{ spanned by } \{|w_i\rangle\}$$

Similarly,

$$T|v_2\rangle = \sum_{i=1}^{m} t_{i2} |w_i\rangle \Big\} \quad ''$$

$$\vdots$$

$$T|v_n\rangle = \sum_{i=1}^{m} t_{in} |w_i\rangle \Big\} \quad ''$$

So, if $|\alpha\rangle = \sum_{j=1}^{n} a_j |v_j\rangle$; $T|\alpha\rangle = \sum_{j=1}^{n} a_j T|v_j\rangle$

$$T|\alpha\rangle = \sum_{j=1}^{n} a_j \sum_{i=1}^{m} t_{ij} |w_i\rangle = \sum_{i=1}^{m} \sum_{j=1}^{n} t_{ij} a_j |w_i\rangle$$

Therefore the linear operator T transforms the components

$$T|\alpha\rangle = |\beta\rangle; \quad |\beta\rangle = \sum_{i=1}^{m} b_i |w_i\rangle; \quad b_i = \sum_{j=1}^{n} t_{ij} a_j$$

and $T = \begin{pmatrix} t_{11} & t_{12} & t_{13} & \cdots & t_{1n} \\ t_{21} & t_{22} & t_{23} & \cdots & t_{2n} \\ \vdots & & & & \\ t_{m1} & t_{m2} & t_{m3} & \cdots & t_{mn} \end{pmatrix}$ } Operator matrix

One can use the relations of inner products and linear operators to represent T using the "outer product"

Let's say again $T: V \to W$ such that $T|\alpha\rangle = |\beta\rangle$

Define, $T = |\beta\rangle\langle\alpha|$, such that

$$T|\alpha'\rangle = |\beta\rangle\langle\alpha|\alpha'\rangle = \underbrace{\langle\alpha|\alpha'\rangle}_{\text{scalar}}|\beta\rangle$$

For the above example and if $\{|w_i\rangle\}$ and $\{|v_j\rangle\}$ are both orthonormal, then

$$T = \sum_{ij} t_{ij} |w_i\rangle\langle v_j|; \quad t_{ij} = \langle w_i|T|v_j\rangle.$$

An important result that comes up is the "completeness relation" for orthonormal vectors. Let $\{|v_i\rangle\}$ be an orthonormal basis set; $|v\rangle = \sum_i a_i |v_i\rangle$

such that $\langle v_i|v\rangle = a_i$, which then gives us

$$|v\rangle = \sum_i |v_i\rangle\langle v_i|v\rangle = \left(\sum_i |v_i\rangle\langle v_i|\right)|v\rangle$$

where, $\sum_i |v_i\rangle\langle v_i| = \mathbb{I}$ (identity)

vi) Some properties of linear operators and matrices.

It is now quite evident that the study of linear operators simply reduce to the study of matrices.

So, if you have two linear operators A and B, then the sum

$$\underbrace{(A + B)}_{A_{ij} + B_{ij}} |\alpha\rangle = A|\alpha\rangle + B|\alpha\rangle$$

the product :

$$A\,(B|\alpha\rangle) = \underbrace{AB}_{U_{ij} = \sum_j A_{ik} B_{kj}} |\alpha\rangle$$

Similarly : $|\alpha'\rangle = A|\alpha\rangle$, $\quad a'_i = \sum_j A_{ij} a_j$

- Transpose of an operator A^T, interchanges the rows and columns. A column vector becomes a row vector
- For a symmetric operator : $A = A^T$
- The complex conjugate of an operator A^*, is when all elements are replaced by their complex conjugates.
- The Hermitian conjugate or adjoint $A^\dagger$ is defined

$$A^\dagger = (A^*)^T$$

- A square matrix is Hermitian if $A^\dagger = A$.

EXERCISE : Show that every real symmetric operator is also Hermitian.

Note that all the above operations are also applicable to the column matrix, $|\alpha\rangle$.

- Matrix multiplication is not commutative in general

Commutator $[A, B] = AB - BA$

Anti-commutator $\{A, B\} = AB + BA$

- $(AB)^T = B^T A^T$ and $(AB)^\dagger = B^\dagger A^\dagger$

- $A^{-1} A = A A^{-1} = \mathbb{I}$, for a square, non-singular matrix A

- A matrix is non-singular if and only if $\underline{\det(A) \neq 0}$.

- A matrix is <u>unitary</u> if its inverse is equal to its adjoint

$A^{-1} = A^\dagger$: $AA^\dagger = A^\dagger A = \mathbb{I}$

Exercise: Find the properties of the determinant and trace of a matrix

vii) Changing the basis of the space

Now we know that a vector space can be spanned by multiple basis states. Let us consider $\{|v_i\rangle\}$ and $\{|w_i\rangle\}$.

$$|v_1\rangle = S_{11}|w_1\rangle + S_{21}|w_2\rangle + \cdots + S_{n1}|w_n\rangle$$

all vectors in the space can be expanded using a basis

these form a basis

$$\therefore |v_j\rangle = \sum_i S_{ij}|w_i\rangle$$

$$\text{Now, } |\alpha\rangle = \sum_i \bar{a}_i |w_i\rangle = \sum_j a_j |v_j\rangle = \sum_j a_j \sum_i S_{ij}|w_i\rangle$$

$$= \sum_i \Big(\sum_j S_{ij} a_j\Big)|w_i\rangle$$

$$\boxed{\begin{aligned} \therefore \quad \bar{a}_i &= \textstyle\sum_j S_{ij} a_j \\ |\alpha\rangle_{\{|w_i\rangle\}} &= S\,|\alpha\rangle_{\{|v_i\rangle\}} \\ \Rightarrow |\bar{\alpha}\rangle &= S\,|\alpha\rangle \end{aligned}}$$

* Note $|\bar{\alpha}\rangle$ and $|\alpha\rangle$ are the same vector but written in different bases.

So, how does an arbitrary linear operator (T) change due to the basis change.

$|\beta\rangle = T|\alpha\rangle$, where both $|\beta\rangle$ and $|\alpha\rangle$ use basis $\{|v_i\rangle\}$

Now, for the change of basis from $\{|v_i\rangle\}$ to $\{|w_i\rangle\}$ we have

$|\bar{\alpha}\rangle = S|\alpha\rangle$, where the tilde refers to use of basis $\{|w_i\rangle\}$

So, we have $|\alpha\rangle = S^{-1}|\bar{\alpha}\rangle$.

$$S|\beta\rangle = ST|\alpha\rangle \Rightarrow |\bar{\beta}\rangle = STS^{-1}|\bar{\alpha}\rangle \Rightarrow |\bar{\beta}\rangle = \bar{T}|\bar{\alpha}\rangle$$

Hence, we have the basis transformation for a linear operator

$$\bar{T} = STS^{-1}$$

Two matrices T_1 and T_2 are similar if $T_1 = ST_2S^{-1}$, for any non singular matrix S.

viii) Eigenvector and eigenvalues

An eigenvector of operator $\hat{A}$ — $\hat{A}|v\rangle = v|v\rangle : |v\rangle \neq 0$

Eigenvectors $|v\rangle$ and eigenvalues v are obtained by solving the characteristic function —

$$c(\lambda) = \det|A - \lambda I| = 0,$$ with solutions being the eigenvalues

The collection of all eigenvalues is called the spectrum.

If the eigenvectors span the space they can form a basis and in this basis the operator $\hat{A}$ is a diagonal matrix with eigenvalues as the diagonal elements.

For transformations from an arbitrary to the eigenbasis, the similarity transformation (S) is constructed by using the eigenvectors $\{|v\rangle\}$ as the columns of S^{-1}

So, if A has a basis of eigenvectors $\{|v_i\rangle\}$, there exists a similarity transformation $(S^{-1})_{ij} = (|v_j\rangle)_i$ such that

$$\underbrace{A^{diag}}_{\text{where the diagonal elements are the eigenvalues } \{v_i\}} = S A S^{-1}$$

- Every normal matrix : $A^+A = AA^+$ is diagonalizable
- Diagonal representation : $A = \sum_i \lambda_i |i\rangle\langle i|$ $\Big\}$ $\langle i|j\rangle = \delta_{ij}$, λ_i are the eigenvalues.
- Any two matrix A and B that commute can be diagonalized with the same $\underbrace{\text{similarity transformation}}_{A \text{ and } B \text{ can be simultaneously diagonalized}}$.

- Adjoint operators — The Hermitian adjoint of a linear operator A is defined by the following

$$\langle A^+\alpha | \beta\rangle = \langle \alpha | A\beta\rangle \;\forall\; |\alpha\rangle, |\beta\rangle \text{ in } V$$

In the language of dual vectorspace we see –

$$\langle \alpha | A\beta\rangle = \underbrace{a^+}_{\text{Adjoint corresponds to vector in the dual space}} A b = (A^+a)^+ b = \langle A^+\alpha | \beta$$

- Properties of Hermitian operators, i.e., $A^+ = A$

Exercise : 1) Show that A has real eigenvalues

2) The eigenvectors of A with distinct eigenvalues are orthogonal

3) Eigenvectors of A spans the space and is therefore diagonalizable.

ix) Tensor product

A tensor product is a general way for creating larger vector spaces from smaller constituent vector spaces. These are important in understanding different aspects of quantum mechanics ranging from entanglement to strongly correlated many body quantum systems.

Say, V and W are vector spaces of dimension m and n, then

$V \otimes W$ is a vector space of dimension $m \times n$

If $\{|v_i\rangle\}_{i=1}^{m}$ and $\{|w_j\rangle\}_{j=1}^{n}$ are the orthonormal basis, then the new vector space is spanned by the basis

$$\{|z_k\rangle\}_{k=1}^{mn} = \{|v_i\rangle\}_{i=1}^{m} \otimes \{|w_j\rangle\}_{j=1}^{n}$$

Consider the famous Bell state or the singlet:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\{|01\rangle - |10\rangle\} = \frac{1}{\sqrt{2}}\{|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B\}$$

$$\{|0\rangle, |1\rangle\} \in V \quad \text{and} \quad |\psi\rangle \in V \otimes V$$

* Properties of tensor product states

1) $z(|v\rangle \otimes |w\rangle) = z|v\rangle \otimes |w\rangle = |v\rangle \otimes z|w\rangle$
2) $(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$
3) $(\underbrace{A \otimes B}_{\text{Linear operators}})(|v\rangle \otimes |w\rangle) = A|v\rangle \otimes B|w\rangle$

Some examples of tensor product :

Let $|v\rangle \in V$ and $|w\rangle \in W$, such that

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \quad \text{and} \quad |w\rangle = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$|v\rangle \otimes |w\rangle = \begin{pmatrix} v_1 \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \\ v_2 \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} v_1 w_1 \\ v_1 w_2 \\ v_2 w_1 \\ v_2 w_2 \end{pmatrix}$$

Again, let A and B to linear operators acting on V and W respectively, such that

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$A \otimes B = \begin{pmatrix} a_{11} B & a_{12} B \\ a_{21} B & a_{22} B \end{pmatrix} = \begin{pmatrix} a_{11} b_{11} & a_{11} b_{12} & a_{12} b_{11} & a_{12} b_{12} \\ a_{11} b_{21} & a_{11} b_{22} & a_{12} b_{21} & a_{12} b_{22} \\ a_{21} b_{11} & a_{21} b_{12} & a_{22} b_{11} & a_{22} b_{12} \\ a_{21} b_{21} & a_{21} b_{22} & a_{22} b_{21} & a_{22} b_{22} \end{pmatrix}$$

Similarly, tensor products can be applied to higher dimensional vector spaces.

B) QUANTUM STATE, EVOLUTION AND MEASUREMENTS

In previous lectures, we motivated that

QM states and operators $\longrightarrow$ vector space (some kind)

What are the specific properties of a quantum system?

1) Axioms or postulates that define a quantum state, observables, evolution and measurement

- The state space of an isolated quantum system is associated with a Hilbert space and the state of a system is given by a unit vector in this Hilbert space.

HILBERT SPACE $\rightarrow$ Complex vector space, Inner product, Normed and complete #

We assume the relevant Hilbert space is finite dimensional!!

A quantum state; $|\psi\rangle \in \mathcal{H}$ is a vector (actually a ray!!)#

$$\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^* \in \mathbb{C} \quad \text{(inner product)}$$

$$\| |\psi\rangle \| = \sqrt{\langle \psi | \psi \rangle} = 1 \quad \text{(unit norm)}$$

"Superposition": $a|\psi\rangle + b e^{i\phi} |\phi\rangle$

"Dual vector space": $\langle \phi | : |\psi\rangle \in \mathcal{H} \rightarrow \langle \phi | \psi \rangle \in \mathbb{C}$

Global phases leave the state unchanged. So, a state $|\psi\rangle$ is actually a set of vectors $\{|\psi\rangle\} \equiv e^{i\chi}|\psi\rangle \ \forall \chi$, which is called a ray.

- How does this compare to the known quantum state $\psi(x)$?

$$|\psi\rangle \longrightarrow \psi(x)$$ { functions are the vectors in $\mathcal{H}$

$$\langle\phi|\psi\rangle \longrightarrow \int \phi^*(x)\,\psi(x)\,dx$$
$$\langle\psi|\phi\rangle \longrightarrow \int \phi(x)\,\psi^*(x)\,dx$$
} inner product

"for infinite dimensional space, we assume the space is complete."

$$\||\psi\rangle\| = 1 \longrightarrow \int |\psi(x)|^2 dx = 1 \quad \text{(normalized)}$$

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \longrightarrow \psi(x) = \sum_n c_n \phi_n(x)$$

- All observables are self adjoint or Hermitian operators on the Hilbert space.

Adjoint of quantum operator A is A^+

$$\langle\phi|A\psi\rangle = \langle A^+\phi|\psi\rangle \quad \#$$

Now, $$\underbrace{\langle\psi|A\psi\rangle}_{\text{expectation value of } A} \to \int \psi^*(x)\, A\, \psi(x)\, dx$$ } which should be real as A is an observable

$$\langle\psi|A\psi\rangle = \langle\psi|A\psi\rangle^* \longleftarrow$$
$$= \langle A\psi|\psi\rangle$$

Using relation #, we have $A^+ = A$ for all observable A, which is therefore a self adjoint or Hermitian operator.

Diagonalizable : $$A = \sum a_n |\phi_n\rangle\langle\phi_n|$$

Hermitian operators have a discrete spectrum, with real eigenvalues.

$$A = \sum_n \underbrace{a_n}_{\text{real eigenvalues}} \underbrace{|\phi_n\rangle\langle\phi_n|}$$

orthonormal eigenbasis $\{|\phi_n\rangle\}$
$\langle\phi_i|\phi_j\rangle = \delta_{ij}$

$|\phi_k\rangle\langle\phi_k|$ project any state to the eigenspace $|\phi_k\rangle$.

- Quantum measurements are perfomed by a set of linear operators $\{M_i\}$, each corresponding to a set of outcomes $\{m_i\}$

For an initial state $|\psi\rangle$, probability of obtaining outcome m_i is given by

$$p(m_i) = \langle\psi| M_i^\dagger M_i |\psi\rangle, \text{ with}$$

$$|\psi_f\rangle = \frac{M_i|\psi\rangle}{\sqrt{\langle\psi|M_i^\dagger M_i|\psi\rangle}}, \text{ being the state after the measurement}$$

The measurement operators satisfy the completeness relation

$$\sum_i M_i^\dagger M_i = \mathbb{I}$$

Example: $|\psi\rangle = a|0\rangle + b|1\rangle$, $M_0 = |0\rangle\langle 0|$ and $M_1 = |1\rangle\langle 1|$

$\therefore\ M_0^\dagger M_0 + M_1^\dagger M_1 = \mathbb{I}$

$$\left.\begin{aligned} p(m_0 = 0) &= \langle\psi| M_0^\dagger M_0|\psi\rangle = \langle\psi|0\rangle\langle 0|\psi\rangle = |a|^2 \\ p(m_1 = 1) &= \langle\psi|M_1^\dagger M_1|\psi\rangle = \langle\psi|1\rangle\langle 1|\psi\rangle = |b|^2 \end{aligned}\right\} \text{Born's rule}$$

EXERCISE: i) Prove that $\sum_i M_i^\dagger M_i = \mathbb{I}$

ii) Calculate the post-measurement states in the example.

- The time evolution of a closed quantum system is determined by a unitary operator.

Initial state: $|\psi_i\rangle \rightarrow \underbrace{U}_{\text{unitary operator, } U^\dagger U = UU^\dagger = \mathbb{I}}|\psi_i\rangle = |\psi_f\rangle$, final state

Again, QM does not tell us at this point which U describes the actual dynamics.

Restatement: Time evolution of a closed system is determined by the Schrödinger equation.

$$\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle$$

Here, H is the Hamiltonian of the system and in general can be time-dependent. Importantly, H is a Hermitian operator.

For infinitesimal time, the evolution proceeds via a series of unitary operators:

$$|\psi(t+\Delta t)\rangle = (\mathbb{I} - iH(t)\Delta t)|\psi(t)\rangle = \underbrace{e^{-iH(t)\Delta t}}_{U(t+\Delta t,\, t)}|\psi(t)\rangle$$

unitary linear transformation of the state $|\psi(t)\rangle$ from t to $t+\Delta t$.

Importantly, the evolution of the closed system is a linear transformation in the Hilbert space, $\mathcal{H}$, which contains the states of the physical system — complexity in the system lies in its complex description.

The Hamiltonian has a spectral decomposition : $H = \sum_n \varepsilon_n |\varepsilon_n\rangle\langle\varepsilon_n|$,

where ε_n and $|\varepsilon_n\rangle$ are the energy eigenstates and eigenvectors.

In the energy eigenstates any state : $|\psi\rangle = \sum_n c_n(t)|\varepsilon_n\rangle$

$$\begin{aligned} \therefore \; |\psi(t+\Delta t)\rangle &= e^{-iH\Delta t}|\psi(t)\rangle \\ &= e^{-iH\Delta t}\sum_n c_n(t)|\varepsilon_n\rangle \\ &= \sum_n e^{-i\varepsilon_n\Delta t} c_n(t)\, |\varepsilon_n\rangle \end{aligned}$$

Assuming H is constant for Δt $\because$ H is Hermitian

For Hermitian H, $e^{-iH\Delta t}|\varepsilon_n\rangle = e^{-i\varepsilon_n\Delta t}|\varepsilon_n\rangle$ $\because$ $H|\varepsilon_n\rangle = \varepsilon_n|\varepsilon_n\rangle$

- The Hilbert space of composite system is the tensor product

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

If $|\psi_A\rangle \in \mathcal{H}_A$ and $|\psi_B\rangle \in \mathcal{H}_B$, then the orthonormal basis describing any composite system is given by :-

$$\{ \underbrace{|i_A\rangle}_{\text{orthonormal basis for } \mathcal{H}_A} \otimes \underbrace{|j_B\rangle}_{\text{orthonormal basis for } \mathcal{H}_B} \}$$

Dimension of the composite system $= d_A \times d_B$

Example :- If $\mathcal{H}_A$ is spanned by $\{|0_A\rangle, |1_B\rangle\}$ and $\mathcal{H}_B$ is spanned by $\{|0_B\rangle, |1_B\rangle, |2_B\rangle\}$, then the joint system is spanned by $\{|00\rangle, |01\rangle, |02\rangle, |10\rangle, |11\rangle, |12\rangle\}$ and the joint dimension is $d = 2 \times 3 = 6$.

ii) Measurements — Projective vs POVM

In our discussion of the axioms / postulates we focussed on a very general form of measurement :

Operators $\{M_i\}$ with outcomes $\{m_i\}$

$$p(m_i) = \langle\psi|M_i^{\dagger}M_i|\psi\rangle \quad \text{and} \quad |\psi_f\rangle = \frac{M_i|\psi\rangle}{\sqrt{p(m_i)}}$$

Most discussions in QM focuses on what are called as "projective measurements"

Let us think of an observable P (Hermitian operator) with real eigenvalues $\{p_i\}$ and eigenbasis $\{|P_i\rangle\}$

$$P = \sum_i p_i |P_i\rangle\langle P_i| \quad \text{(spectral representation)}$$

For projective measurement; $\{M_i\} = \{|P_i\rangle\langle P_i|\}$ with outcome $\{p_i\}$, with probability $|\langle\psi|P_i\rangle|^2$.

The final post measurement state : $|P_i\rangle$

Expectation / average values of an observable :

$$E(P) = \sum_i m_i\, p(m_i) \quad \Big\} \text{ average of the outcome with probability}$$

$$= \sum_i m_i \langle\psi|P_i\rangle\langle P_i|\psi\rangle$$

$$= \langle\psi|\sum_i m_i |P_i\rangle\langle P_i|\psi\rangle$$

$$= \langle\psi|P|\psi\rangle$$

Exercise : Calculate the standard-deviation of P.

Example of a projective measurement : $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\{m_i\}$

with eigenvalues $\{-1, 1\}$ and projectors $\{|1\rangle\langle 1|, |0\rangle\langle 0|\}$

For a quantum state : $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ $\{M_i\}$

The outcomes $\{-1, 1\}$ occur with prob. $\{|\beta|^2, |\alpha|^2\}$ $\{p(m_i)\}$

Expectation value of σ_z is : $1|\alpha|^2 - 1|\beta|^2 = |\alpha|^2 - |\beta|^2$

or equivalently : $(\alpha^* \quad \beta^*) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

$$= \begin{pmatrix} \alpha^* & 0 \\ 0 & -\beta^* \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = |\alpha|^2 - |\beta|^2$$

NOTE : It is quite common to associate projective measurements with simply an orthonormal basis $\{|P_i\rangle\}$ and not any observable.

In several instances in QIC, especially in experiments the restriction to observables or an orthonormal basis can be limiting*. In principle one can extend the notion of measurements to any "general" "positive valued" operator.

Operators : $\{M_i\}$ with outcomes $\{m_i\}$ $\forall \sum_i M_i^\dagger M_i = \mathbb{1}$

One can define a positive semidefinite operator, $E_i = M_i^\dagger M_i$.

The set of operators $\{E_i\}$ is called a POVM (positive operator valued measurement)

with outcome probability : $p(m_i) = \langle\psi| E_i |\psi\rangle$; $\sum_i E_i = \mathbb{I}$

* Note that a POVM does not really give you a well defined post measurement state.

iii) Distinguishing quantum states

Say there are two parties: Alice and Bob

ALICE $\longrightarrow$ $|\psi_i\rangle$ $\longrightarrow$ BOB

$\{|\psi_i\rangle\}_{i=1}^{N}$

uses $\{M_i = |\psi_i\rangle\langle\psi_i|\}$

and $M_0 = \mathbb{1} - \sum_i M_i$

If $\{|\psi_i\rangle\}$ is an orthonormal set then Bob can get $p_i = \langle\psi_i|M_i^\dagger M_i|\psi\rangle = 1$, and therefore can reliably distinguish the state $|\psi_i\rangle$.

But, what happens if $\{|\psi_i\rangle\}$ is not orthonormal. For simplicity let's assume Alice sends either $|\psi_1\rangle$ or $|\psi_2\rangle$, where $\langle\psi_1|\psi_2\rangle \neq 0$, i.e.,

$$|\psi_2\rangle = \alpha|\psi_1\rangle + \beta|\varphi\rangle, \; |\alpha|^2 + |\beta|^2 = 1 \text{ and } |\beta| < 1 \left\} \begin{array}{l} \langle\psi_1|\varphi\rangle = 0 \\ \langle\psi_1|\psi_2\rangle \neq 0 \end{array}\right.$$

Let us assume Bob has a measure such that

$$\langle\psi_1|M_1^\dagger M_1|\psi_1\rangle = 1 \text{ and } \langle\psi_2|M_2^\dagger M_2|\psi_2\rangle = 1 \quad \#$$

Now, $\sum_i \langle\psi_1|M_i^\dagger M_i|\psi_1\rangle = 1$ as $\sum_i M_i^\dagger M_i = \mathbb{I}$, which implies that $\langle\psi_1|M_2^\dagger M_2|\psi_1\rangle = 0$ and $\therefore M_2|\psi_1\rangle = 0$

$$M_2|\psi_2\rangle = \alpha \cancelto{0}{M_2|\psi_1\rangle} + \beta M_2|\varphi\rangle = \beta M_2|\varphi\rangle$$

$$\therefore \langle\psi_2|M_2^\dagger M_2|\psi_2\rangle = |\beta|^2 \underbrace{\langle\varphi|M_2^\dagger M_2|\varphi\rangle}_{\langle\varphi|M_2^\dagger M_2|\varphi\rangle \leq \sum_i \langle\varphi|M_i^\dagger M_i|\varphi\rangle = 1} < 1 \quad \star$$

$\sum_i M_i^\dagger M_i = \mathbb{I}$

So the statement # and ☆ contradict each other.

What can be done if Bob chooses to use a POVM?

Let us assume Alice sends : $|\psi_1\rangle = |0\rangle$ and $|\psi_2\rangle = \frac{1}{\sqrt{2}}\{|0\rangle + |1\rangle\}$

In this instance Bob uses : $E_1 \equiv \frac{\sqrt{2}}{1+\sqrt{2}} |1\rangle\langle 1|$

$$E_2 = \frac{\sqrt{2}}{1+\sqrt{2}} \cdot \frac{1}{2}\{|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|\}$$

$$E_3 = \mathbb{I} - E_1 - E_2$$

Now if Alice sends the state $|\psi_1\rangle = |0\rangle$ and Bob measures $\{E_1, E_2, E_3\}$.

$$\langle\psi_1|E_1|\psi_1\rangle = 0 \Big\} \therefore \text{ if } E_1 \neq 0,\ |\psi_2\rangle \text{ is detected}$$

Similarly $E_2 \neq 0$ implies that the state is $|\psi_1\rangle$.

For other outcomes Bob is unable to given an answer.

Importantly, Bob does not make a mistake using POVM.

iv) Measurement in a composite system

From the axiom on composite system we know that the combined state space is given by the tensor product :

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

((Quantum states))

$$|i\rangle_{AB} = |i\rangle_A \otimes |j\rangle_B$$

$$|\psi\rangle_{AB} = \sum_i \alpha_i |i\rangle_{AB}$$

Quantum operators

$$(M_A \otimes M_B)|\psi\rangle_{AB}$$

Consider a quantum system Q and we want to use measurement operators $\{M_i\}$. We consider an "ancilla" system M with an orthonormal basis $\{|m_i\rangle\}$ that corresponds to the possible outcomes of M.

Let us define a operator $\mathcal{U}$ that gives us:

$$\mathcal{U}\,|\psi\rangle \otimes |0\rangle \equiv \sum_i M_i|\psi\rangle \otimes |m_i\rangle$$

$$\langle\varphi|\langle 0|\underbrace{\mathcal{U}^\dagger \mathcal{U}}_{\mathcal{U}^\dagger\mathcal{U} = \mathbb{I}}|\psi\rangle|0\rangle = \sum_{i,i'} \langle\varphi|M_{i'}^\dagger M_i|\psi\rangle\langle m_{i'}|m_i\rangle$$

preserves inner product and can be generalized to a unitary

$$= \sum_i \langle\varphi|M_i^\dagger M_i|\psi\rangle = \langle\varphi|\psi\rangle$$

Make a joint projective measurement $\{P_i\}$

$$P_i = \mathbb{I}_Q \otimes |m_i\rangle\langle m_i|$$

$$p(m_i) = \langle\psi|\langle 0|\mathcal{U}^\dagger(\mathbb{I}_Q \otimes |m_i\rangle\langle m_i|)\mathcal{U}|\psi\rangle|0\rangle$$

$$= \sum_{j,j'} \langle\psi|M_j^\dagger\langle m_j|m_i\rangle\langle m_i|m_{j'}\rangle M_{j'}|\psi\rangle$$

$$= \langle\psi|M_i^\dagger M_i|\psi\rangle$$

Joint quantum state of the system after P_i:

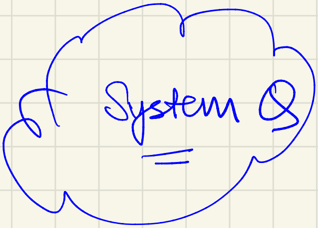
$$(\mathbb{I}_Q \otimes |m_i\rangle\langle m_i|)\,\mathcal{U}|\psi\rangle|0\rangle / \sqrt{p(m_i)}$$

$$= (\mathbb{I}_Q \otimes |m_i\rangle\langle m_i|)\sum_j M_j|\psi\rangle|m_j\rangle / \sqrt{p(m_i)}$$

$$= M_i|\psi\rangle|m_i\rangle / \langle\psi|M_i^\dagger M_i|\psi\rangle$$

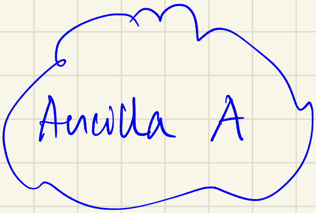
So, POVM is an operator $\mathcal{U}$ and projective measurement in a composite system

- Understanding POVM as projective measurement on a larger Hilbert space



← Measure the state $|\psi\rangle$ in system Q with POVM $\{E_i\}$ $\forall$ $E_i = M_i^\dagger M_i$ } $\{M_i\}$ is a set of linear operators in Q

+



← We couple Q with an ancilla A. Think of this as a measuring apparatus coupled to Q. The ancilla A has an orthonormal basis $\{|m_i\rangle\}$

So, how does POVM work ?

$\{E_i = M_i^\dagger M_i\}$ acts on Q $\longrightarrow$ Probability: $p(m_i) = \langle\psi| E_i |\psi\rangle$

Now think of the composite state in Q + A, say the state is $|\psi\rangle \otimes |0\rangle$; where $|0\rangle$ is some fixed state in A and the POVM, $\{E_i\} = \{M_i^\dagger M_i\}$ acts on Q.

We can always find an operator, $\mathcal{U} = \sum_i M_i \otimes |m_i\rangle\langle 0|$

$$\mathcal{U}\, |\psi\rangle \otimes |0\rangle = \sum_i M_i |\psi\rangle \otimes |m_i\rangle = \sum_i M_i |\psi\rangle |m_i\rangle$$

$$U|\psi\rangle|0\rangle = \sum_i \underbrace{M_i|\psi\rangle}_{\text{lives in } Q}\underbrace{|m_i\rangle}_{\text{lives in } A}$$

$$\langle 0|\langle\psi|U^\dagger U|\psi\rangle|0\rangle = \sum_{i,i'} \langle m_i|\langle\psi| M_i^\dagger M_{i'}|\psi\rangle|m_{i'}\rangle$$

$$= \sum_{i,i'} \underbrace{\langle\psi|M_i^\dagger M_{i'}|\psi\rangle}_{\text{lives in } Q}\underbrace{\langle m_i|m_{i'}\rangle}_{\substack{\text{lives in } A \\ \delta_{ii'}}}$$

$$U^\dagger U = \mathbb{I}$$

$$= \sum_i \langle\psi|M_i^\dagger M_i|\psi\rangle$$

Exercise: U can be extended to be a unitary i.e $UU^\dagger = \mathbb{I}$

$$= \sum_i \langle\psi|E_i|\psi\rangle$$

$$= \langle\psi|\mathbb{I}|\psi\rangle \quad \underbrace{\because \sum_i E_i = \mathbb{I}}_{\text{property of POVM}}$$

So the joint state in $Q + A$ is $|\varphi\rangle = U|\psi\rangle|0\rangle$ and we use the projective measurement $\{\mathbb{I}_A \otimes |m_i\rangle\langle m_i|\}$

Probability: $p(m_i) = \langle\varphi|\mathbb{I}_A \otimes |m_i\rangle\langle m_i|\varphi\rangle$

$$\Rightarrow \langle 0|\langle\psi|U^\dagger(\mathbb{I}_A \otimes |m_i\rangle\langle m_i|)U|\psi\rangle|0\rangle$$

$$= \sum_{j,j'} \langle m_j|\langle\psi| M_j^\dagger(\mathbb{I}_A \otimes |m_i\rangle\langle m_i|)M_{j'}|\psi\rangle|m_{j'}\rangle$$

$$= \sum_{j,j'} \underbrace{\langle\psi|M_j^\dagger \mathbb{I}_A M_{j'}|\psi\rangle}_{\text{lives in } Q} \otimes \underbrace{\overset{\delta_{ij}}{\langle m_j|m_i\rangle}\overset{\delta_{ij'}}{\langle m_i|m_{j'}\rangle}}_{\text{lives in } A}$$

$$= \langle\psi|M_i^\dagger M_i|\psi\rangle$$

$$= \langle\psi|E_i|\psi\rangle$$ (which is the same as that for POVM !!)

So all POVMs can be thought of as a unitary/isometry and projective measurement on a larger Hilbert space!

iv) A quantum bit (Qubit)

The analogous to a classical computational bit is the qubit (a quantum bit).

What is a qubit ? State in a 2D Hilbert space

$$\{ |0\rangle, |1\rangle \} \longleftrightarrow \{ |\uparrow\rangle, |\downarrow\rangle \} \longleftrightarrow \{ |H\rangle, |V\rangle \}$$

Linear operators in the qubit space are spanned by the Pauli operators and the identity :

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \ \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}; \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

So, a qubit state in the σ_z -basis : $|\psi\rangle = a|0\rangle + b|1\rangle$

If we measure in the projective basis of σ_z we get

$$p(|0\rangle) = |a|^2 ; \ p(|1\rangle) = |b|^2 ; \ |a|^2 + |b|^2 = 1$$

But a qubit is more than just probabilities of getting $|0\rangle$ and $|1\rangle$ (or heads and tails in a classical coin) !!

The qubit state $|\psi\rangle$ also has information about all the other observables in the qubit space.

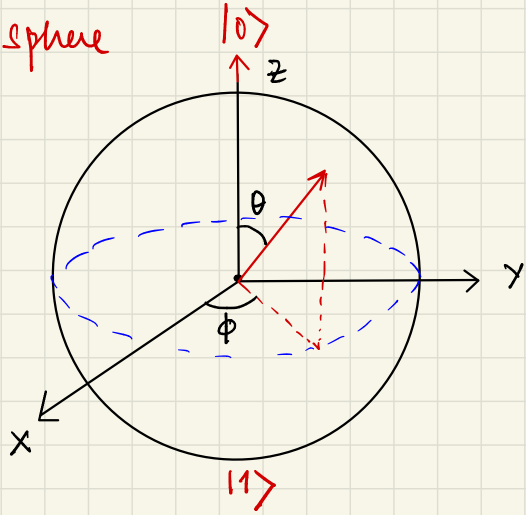
We can write the qubit as: $|\psi\rangle = \cos\theta/_2 |0\rangle + e^{i\phi} \sin\theta/_2 |1\rangle$

where $\theta = [0, \pi]$ and $\phi = [0, 2\pi]$ (two parameter space)*

This form of the qubit has a nice visualization in a 3D sphere with unit radius — Bloch sphere

* We can reduce to two real parameters due to the constraint on normalisation and the additional condition that we ignore the global phase.

Bloch sphere



$\theta = 0, \pi$

$|\psi\rangle = |0\rangle, |1\rangle$

(in the σ_z basis)

$\phi = 0, \theta = \pi/2$

$|\psi\rangle = \frac{1}{\sqrt{2}}\{|0\rangle + |1\rangle\}$

$$|\psi(\theta, \phi)\rangle = \cos\theta/2\,|0\rangle + e^{i\phi}\sin\theta/2\,|1\rangle$$

$$\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \rightarrow \{x, y, z\}$$

Any operator in this space : $\hat{n}\cdot\vec{\sigma} = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3$

$$\hat{n}\cdot\vec{\sigma}\,|\psi(\theta,\phi)\rangle = |\psi(\theta,\phi)\rangle$$

So, even if we get two outcomes when we measure the state in the σ_z-basis, there will always exist a operator where $|\psi(\theta,\phi)\rangle$ is an eigenstate.

For example : $|\psi(\theta = \pi/2, \phi = 0)\rangle = \frac{1}{\sqrt{2}}\{|0\rangle + |1\rangle\} = |+\rangle$

In σ_z-basis ; we get $p(|0\rangle) = 1/2$ and $p(|1\rangle) = 1/2$

But we have ; $\sigma_x|+\rangle = |+\rangle$; so in σ_x-basis $p(|+\rangle) = 1$

Exercise : i) Find the other eigenstate of σ_x.

ii) Calculate $\langle\sigma_x\rangle, \langle\sigma_y\rangle$ and $\langle\sigma_z\rangle$ for a qubit $|\psi(\theta,\phi)\rangle$.