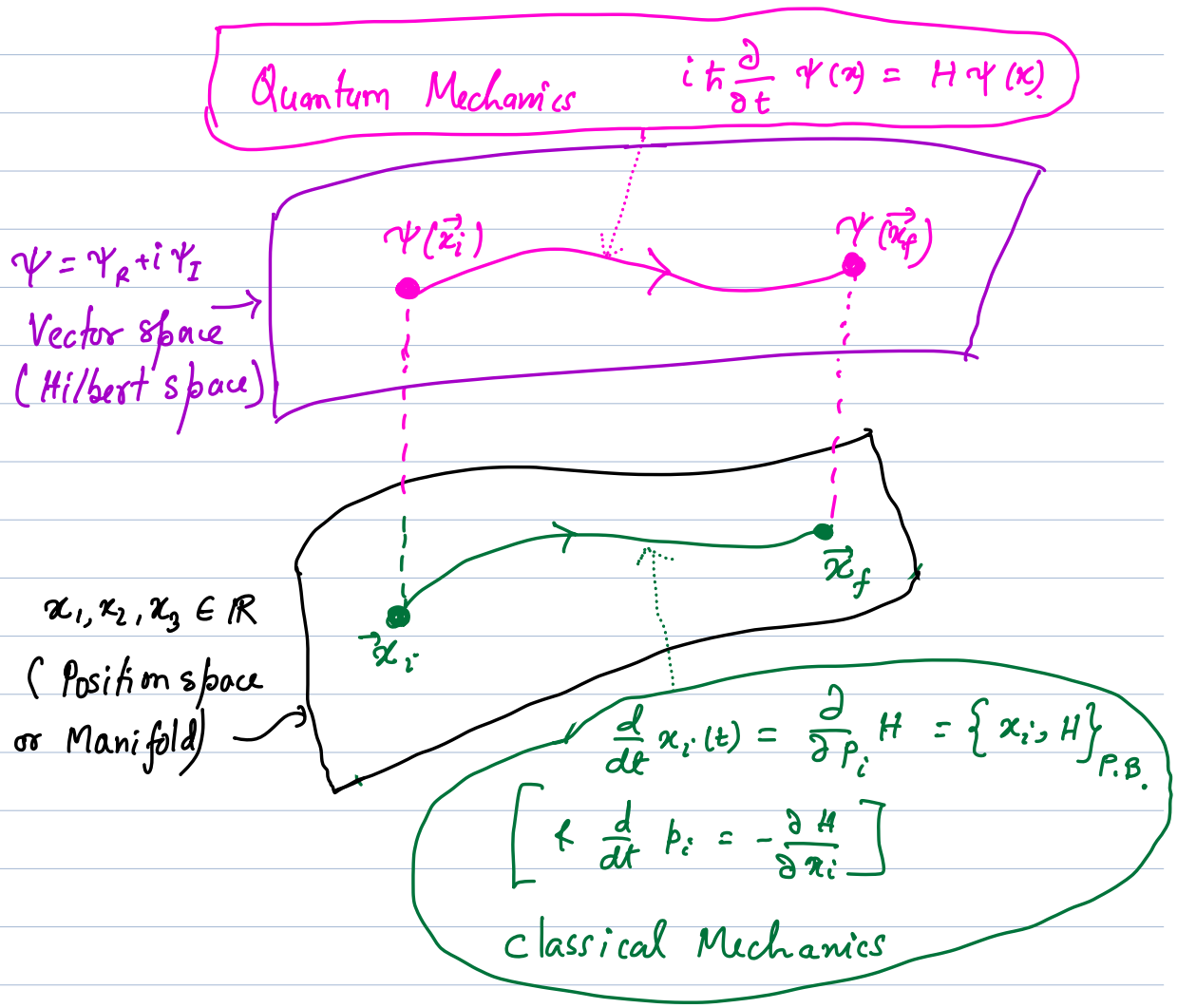
PH203: Quantum Mechanics

Prerequisite: Linear Algebra.

Refs:
- Mary L. Boas - Math Methods in the Physical Sciences
- Gilbert Strang - Introduction to Linear Algebra
- K.F. Riley, M.P. Hobson & S.J. Bence - Math Methods for Physics & Engineering.
- George B. Arfken & Hans J. Weber - Math Methods for Physicists.
- A.W. Joshi - Matrices & Tensors in Physics.


Quantum Mechanics
$i\hbar \frac{\partial}{\partial t} \psi(x) = H\psi(x)$
$\psi = \psi_R + i\psi_I$
Vector space
(Hilbert space)
$\psi(\vec{x}_i)$
$\psi(\vec{x}_f)$
$\vec{x}_f$
$\vec{x}_i$
$x_1, x_2, x_3 \in \mathbb{R}$
(Position space
or Manifold)
$\frac{d}{dt} x_i(t) = \frac{\partial}{\partial p_i} H = \{x_i, H\}_{P.B.}$
$\left[\dot{p}_i = -\frac{\partial H}{\partial x_i} \right]$
Classical Mechanics

In classical mechanics, we deal with individual coordinates of each particles in spatial dimensions $\vec{x}(t)$ (and also its momentum as the dynamics happens in phase space). Then we have the equation of motion for $\vec{x}(t)$ governed by the Newtonian equation or equivalently by Poisson bracket with a Hamiltonian $H(\vec{p},\vec{x}) = T + V$ as

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \{x_i, P\} \quad \& \quad \dot{p}_i = -\frac{\partial H}{\partial x_i} = \{p_i, H\}_{P.B.}$$

In statistical mechanics and quantum mechanics (and also in electrodynamics), we do not solve the dynamics in the coordinate space. Rather we solve the dynamics or equation of motion in some special functional space $F(\vec{x},t)$. In statistical mechanics, the F-function is the density of particles $\rho(\vec{x},t)$, which is a simple, real number, function. In electrodynamics, we have fields $\vec{E}(\vec{x},t)$, $\vec{B}(\vec{x},t)$ which follow Maxwell's equations. In quantum mechanics, the F-function turns out to be some complex functions $\psi(\vec{x},t) = \psi_R(\vec{x},t) + i\,\psi_I(\vec{x},t)$. Most importly, $\psi(\vec{x},t)$ are not just simple complex variables/functions, They belong to something called the vector space or Hilbert space. These ψ belong to a "space" of functions which follows linear Algebra.

[Roughly, as we see for the case of vectors, all vectors in a d-dimensional space can be represented by d-linearly independent unit vectors with components $A_i(\vec{x},t)$ as

$$\vec{A}(\vec{x},t) = A_1(\vec{x},t)\,\hat{i}_1 + A_2(\vec{x},t)\,\hat{i}_2 + \cdots + A_d(\vec{x},t)\,\hat{i}_d.$$

And there are vector addition, multiplication rules. So, all these vectors form a vector space called tangent space.

The quantum mechanics is defined by a equation of motion in this vector space for how $\Psi(\vec{x},t)$ changes in space & time and its given by the Schrödinger equations

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{x},t) = H \Psi(\vec{x},t).$$

For a given Hamiltonian H, in a given spatial dimension $\vec{x}$, all possible solutions $\Psi(\vec{x},t)$ of this Schrödinger equation must belong to the same vector space and more strictly Hilbert space. The vector / Hilbert space is equipped with a fixed number of basis states, which are analogous to the unit vectors in the tangent space, such that all such wave functions $\Psi(\vec{x},t)$ can be expanded in this basis states $\phi_i(\vec{x},t)$, $i = 1, 2, \ldots, n$, where $n \neq d$.

Before we solve the schrödinger equation, we want to recap these imfootant concepts of the vector space & Hilbert space that you have learned in the Mathematical methods of Physics Course. Its part of something called the Linear Algebra.

Recap of Linear Algebra

- **(Linear) Vector space:** We first want to define the vector space of $\psi(\vec{x}, t)$, say $\mathbb{V}$. Mathematicians figured out that the axioms of a vector space $\mathbb{V}$ is independent of the position space $\vec{x}$, and can be formally defined without specifying the coordinates $\vec{x}, t$. This is called an abstract manifold. Without specifying $(\vec{x}, t)$, we denote such an abstract vector by

  $|\psi\rangle$, called Ket Vector.

  (We can always project our abstract vector $|\psi\rangle$ into the position or momentum or angular variable space or even to a matrix form as we will see below. This is called a representation and the key properties / axioms of the vector space remains independent of the choice of a representation).

→ **Formal definition:** "Space" is a set with a structure among its elements. A vector space $\mathbb{V}$ is a specific space with a structure that obey the following axioms (axioms make a structure). Their elements, denoted here by $|\psi\rangle \in \mathbb{V}$, are called Ket vector or vectors.

All vectors $|\psi\rangle$ following the below axioms form a vector space, denoted by $\mathbb{V}$. Then all ket vectors $|\psi\rangle \in \mathbb{V}$ must obey the following axioms:

(i) Closure under addition: $\forall\ |\psi\rangle, |\phi\rangle \in \mathbb{V}$

$$|\psi\rangle + |\phi\rangle = |\chi\rangle \in \mathbb{V}$$

(ii) Commutivity: $|\psi\rangle + |\phi\rangle = |\phi\rangle + |\psi\rangle$.

(iii) Associativity: $|\psi\rangle + (|\phi\rangle + |\chi\rangle) = (|\psi\rangle + |\phi\rangle) + |\chi\rangle$.

(iv) Null vector: The vector space must include a null (under addition) vector $|0\rangle$, such that
$|\psi\rangle + |0\rangle = |\psi\rangle$.

(v) Inverse: The vector space must include an inverse vector (under addition) $|-\psi\rangle$ such that $|-\psi\rangle = -|\psi\rangle$,
$|\psi\rangle + |-\psi\rangle = 0$.

(vi) Scalar multiplication: (a) for $\alpha \in \mathbb{R}, \mathbb{C}$, a scalar (or field $\mathbb{F}$)
$\alpha \circ |\psi\rangle \in \mathbb{V}$ if $|\psi\rangle \in \mathbb{V}$.
$\alpha, \beta \in \mathbb{R}, \mathbb{C}$ (or $\mathbb{F}$)
$(\alpha \cdot \beta) \circ |\psi\rangle = \alpha \cdot (\beta \circ |\psi\rangle)$

where $\cdot$ is the scalar / field multiplication
$\circ$ is the multiplication between a scalar / field with the vector.

Typically, these are simple multiplications as we see for scalar & matrices.

(vii) Distribution: $\alpha(|\psi\rangle + |\phi\rangle) = \alpha|\psi\rangle + \alpha|\phi\rangle$.
& $(\alpha + \beta)|\psi\rangle = \alpha|\psi\rangle + \beta|\psi\rangle$.

(viii) Identity: There must exist a scalar / field 1. such that $1 \circ |\psi\rangle = |\psi\rangle$, which leaves the ket vector unchanged.

Basis vectors: For a given vector space V, that follows the above axioms, one can prove that a vector space is equipped with 'n' linearly independent basis vectors, denoted by $|e_i\rangle$, $i = 1, 2, \cdots, n$. 'n' is called the dimension of this vector space. 'n' depends on the type of Hamiltonian H we are going to solve and also on the spatial dimension 'd', but $n \neq d$. (Mathematically we call it the span of the vector space $\text{Span}\{|e_i\rangle\}$, which is a subset of the vector space $\{|e_i\rangle\} \subset V$ or one denotes $|e_i\rangle \in V$, i.e., $|e_i\rangle$ is an element of V.

(i) **Linearly independent:** The linearly independent basis vectors imply that there n sets of basis are the minimum number of vectors one need in this vector space to span / expand / write all vectors $|\psi\rangle \in V$.

There is no unique choice of the set of the basis vectors $\{|e_i\rangle\}$. One can do a transformation (called unitary or orthogonal transformation) from one set of basis vectors to another linearly independent basis vectors. This is analogous to the coordinate transformation in ordinary vectors.

The set of basis vectors that spans a vector space must be linearly independent. Mathematically, it's defined as

$$\text{If, } \sum_{i=1}^{n} a_i |e_i\rangle = |0\rangle = \text{null vector.}$$

then $a_i = 0$ for all i if $|e_i\rangle$ are linearly independent.

These basis vectors need not be orthogonal to each other, per say, however, any set of linearly independent vectors can be made orthogonal by Gram-Schmidt Orthogonalization method.

(ii) spanning or expansion : All vectors $|\psi\rangle \in V$, can be spanned or expanded in the set of basis vectors as

$$|\psi\rangle = \sum_{i=1}^{n} a_i |e_i\rangle,$$

where $a_i \in \mathbb{R}$ or $\mathbb{C}$ (or sometimes called fields) which are scalar numbers, called expansion coefficients, defined as $a_i = \langle e_i | \psi \rangle$, where this angular bracket $\langle\ \rangle$, will be defined later.

e.g: (i) Matrix representation: Let's consider a $n=2$ dimensional vector $|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$, where $\psi_1, \psi_2 \in \mathbb{C}$. We can choose the basis vectors as

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |e_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Then the spanning or expansion of $|\psi\rangle$ in $\{e_i\}$ yields

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \psi_1 |e_1\rangle + \psi_2 |e_2\rangle = \psi_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

- Now, choose another basis

$$|e_1'\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |e_2'\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Show that $|e_i'\rangle$ are linearly independent.
Expand $|\psi\rangle$ in the $\{|e_i'\rangle\}$ basis and obtain the coefficients $a_i = \langle e_i' | \psi \rangle$.

(ii) The Fourier transformation from position to momentum space or time to frequency space and vice versa is a basis transformation or expansion of a function in position space to that in the momentum space.

$$|\phi(b)\rangle = \sum_{\{x\}} \langle \psi(x) | \phi(b) \rangle |\psi(x)\rangle$$

where $\langle \psi(x) | \phi(b) \rangle = \frac{e^{i \vec{p} \cdot \vec{x}}}{\sqrt{V}}$ and $\sum_{\{x\}} \sim \int d^3x$.

Hilbert space: It turns out the wavefunctions $|\psi\rangle$ in quantum mechanics have a more stringent criterion on the vector space, i.e., a subset of a vector space with two additional properties, inner product and completeness. Such a vector space is called the Hilbert space $\mathcal{H} \subset V$. This is sometimes called the complete inner product space.

To define the inner product, we need an additional vector space, called the dual space $\overline{V}$, whose elements are denoted by $\langle\psi|$, called "bra" vector or dual vector corresponding to each ket vector $|\psi\rangle \in V$. Operationally, this is defined by the adjoint or Hermitian operation which consists of transpose (T) + Complex conjugation ($*$) $= \dagger$.

$$\begin{array}{lccc} \text{Dual vector} & |\psi\rangle & \longrightarrow & \langle\psi| \\ \text{wave function} & \psi(x) & \rightarrow & \psi^\dagger(x) = \left(\psi^*(x)\right)^T. \end{array}$$

(i) Under this dual space, an inner product or scalar product is defined by

$$\langle\psi|\phi\rangle = \alpha \in \mathbb{C} \quad (\text{scalar number})$$

$$\text{or,} \quad \langle\psi|\phi\rangle = \int \psi^*(x)\,\phi(x)\,d^3x = \alpha$$

See $\phi(x)$ & $\psi^*(x)$ are defined at the same location x, i.e., locally.

The inner product must satisfy

(a) Linear in the second argument, i.e. $|\phi\rangle \to c|\phi\rangle$,

$$\langle\psi|\phi\rangle \to c\langle\psi|\phi\rangle \quad , c \in \mathbb{C}.$$

(b) Conjugate symmetric

$$\left(\langle\psi|\phi\rangle\right)^* = \langle\phi|\psi\rangle = \alpha^*.$$

(c) Positive definite, i.e. $\langle\psi|\psi\rangle \geq 0$, with equality holds iff $|\psi\rangle = 0$.

The norm of the vector $|\psi\rangle$ is defined as

$$\||\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle}$$

This norm has the interpretation of the quantum probability density of the particle to be at the position $\vec{x}$.

(ii) The set of basis vectors $\{|e_i\rangle\}$, must be complete, such that the spanning / expansion of any vector $|\psi\rangle$ in this basis set converges and keep the vector within the vector space V. The mathematical definition of completeness is

$$\sum_{i=1}^{n} |e_i\rangle\langle e_i| = \mathbb{I}.$$

- Physically, completeness means the basis states spans the entire space. This means any vector $|\psi\rangle \in V$ can be expressed as a linear combination of the basis vectors. If we apply the above sum $\sum_{i=1}^{n} |e_i\rangle\langle e_i| = \mathbb{I}$ to any state $|\psi\rangle$, we get back the same state. No part of $|\psi\rangle$ lies outside the space of $\{|e_i\rangle\}$.

(*) Example of inner product:

→ Finite dimensional case (vector in $\mathbb{C}^n$)

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix}$$

then $$\langle\psi|\psi\rangle = \sum_{i=1}^{n} \psi_i^* \psi_i = \||\psi\|\|^2$$

and $\rho_i = \psi_i^* \psi_i$ is the probability density of the state $|\psi\rangle$ to be in the i^{th} basis state.

→ Infinite dimensional case (vector in $L^2(\mathbb{R})$)

$\psi(x) \in L^2(\mathbb{R})$:

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \underbrace{\psi^*(x)\psi(x)}_{\rho(x)}\, dx.$$

$$= \||\psi\|\|^2.$$

e.g.: If $|\psi\rangle = \sum_{i=1}^{n} \alpha_i |e_i\rangle$

Then $\langle\psi| = \sum_{i=1}^{n} \alpha_i^* \langle e_i|$

- Now with Gram-Schmidt orthogonalization condition, we achieve the basis vectors to be orthogonal and normalized such that

$$\langle e_i | e_j \rangle = \delta_{ij}$$

Then we have $\langle\psi|\psi\rangle = ||\psi||^2 = \sum_{i=1}^{n} |\alpha_i|^2$.

Here $\alpha_i = \langle e_i|\psi\rangle \in \mathbb{F}$ can be interpreted as the probability amplitude of the vector or state $|\psi\rangle$ to be in the $|e_i\rangle$ basis state, where $|\alpha_i|^2$ is the corresponding probability.

- So, sometimes the Hilbert space is defined as a vector space of square integrable function (ei, inner product), denoted by L^2. For example, e^x is a growing function in x and hence its not square integrable.

H.W. Diagonalize all the eigenvectors of the Pauli-matrices and show they for 2-dimensional Hilbert space.

Cauchy - Schwarz Inequality :

For any two vectors $|\psi\rangle, |\phi\rangle \in V$, their inner product is always less than or equal to the product of length to two vectors. Mathematically :

$$|\langle\psi|\phi\rangle|^2 \leq |\langle\psi|\psi\rangle|\,|\langle\phi|\phi\rangle|.$$

[This inequality is analogous to the triangular inequality of vectors.

$$|\vec{A}\cdot\vec{B}|^2 \leq |\vec{A}|\,|\vec{B}|.$$

as $|A\cdot B| = |A||B|\cos\theta$ and $0 \leq (\cos\theta)^2 \leq 1$.]

[In probability theory, there is an equivalent called covariance inequality. Let X, Y be two random variables. The covariance between them is always less than or equal to the product of their variances :

$$\mathrm{Cov}(X,Y)^2 \leq \Delta X\,\Delta Y$$

The equality holds when X & Y are completely uncorrelated!]

This inequality governs the uncertainty principle between any two quantum operators $\hat{X}, \hat{Y}$. If they are uncorrelated, i.e, they commute, then they can be precisely measured simultaneously, otherwise not. Then uncertainty is given by ΔX.

Proof: Lets consider the projection operator along the direction of the $|\psi\rangle$ vector. The unit vector is

$$|e_\psi\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$$

Then we define

$$|\phi\rangle = \frac{\langle\psi|\phi\rangle}{\sqrt{\langle\psi|\psi\rangle}}|e_\psi\rangle + \left(|\phi\rangle - \frac{\langle\psi|\phi\rangle}{\sqrt{\langle\psi|\psi\rangle}}|e_\psi\rangle\right)$$

Now define a new vector $|\chi\rangle \in V$, as

$$|\chi\rangle = |\phi\rangle - \frac{\langle\psi|\phi\rangle}{\sqrt{\langle\psi|\psi\rangle}}|e_\psi\rangle$$

Then $\langle\chi|\chi\rangle = \langle\phi|\phi\rangle - \frac{\langle\psi|\phi\rangle\langle\phi|\psi\rangle}{\langle\psi|\psi\rangle}$ (after the algebra)

Since $\langle\chi|\chi\rangle \geq 0$, so,

$$|\langle\psi|\phi\rangle|^2 \geq \langle\psi|\psi\rangle\langle\phi|\phi\rangle$$

- Gram - Schmidt Orthogonalization : Revise yourselves.

Operators: An operator $\hat{O}$ is a map (or rule) that acts on a vector space $|\psi\rangle$ and produces a new vector $|\phi\rangle$. It is written as

$$\hat{O}|\psi\rangle = |\hat{O}\psi\rangle = |\phi\rangle.$$

- Typically, for sure in quantum mechanics, we want the operators that keeps the new vector $|\phi\rangle$ in the same H as $|\psi\rangle$
- The corresponding dual vector $\langle\phi| = \langle\hat{O}\psi| = \langle\psi|\hat{O}^{\dagger}$.
- In the cartoon on the first page, we showed $\psi(t_i)$, $\psi(t_f)$ and $\psi(t)$ in general have to remain in the same Hilbert space. The operator that produces the time-evolution (which turn out to be the Hamiltonian) must not project a state out of this Hilbert space. The same in position space also that $\psi(x_i, t) \to \psi(x_f, t)$ must always remain in the same Hilbert space. If this does not happen, then we have an unphysical system.

Mathematical Definition: operators also belong to a space, called operator space. It is, as usual, a set of points (numbers, fields) with a specific structure for addition, multiplication, and scalar multiplication.

- The most common operators used in quantum mechanics are Linear, Hermitian, and unitary.

Linear: An operator $\hat{O}$ is linear if it preserves the superposition principle. Mathematically.

$$\hat{O}(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha\,\hat{O}|\psi\rangle + \beta\,\hat{O}|\phi\rangle, \text{ where } \alpha, \beta \in \mathbb{C}.$$

Hermitian: An operator $\hat{H}$ is Hermitian if its expectation value is equal to the expectation value of its adjoint operator $\hat{H}^\dagger$ (also called Hermitian conjugate or transpose and complex conjugation).

Mathematically,

$$\langle \psi | H\phi \rangle = \langle H\psi | \phi \rangle, \quad \forall \ |\psi\rangle, |\phi\rangle \in \mathcal{H}.$$

This identity is also written as

$\langle \psi | H | \phi \rangle = \langle \psi | H^\dagger | \phi \rangle$, as the expectation values of H & $H^\dagger$.

- The self-adjoint operators $H = H^\dagger$ always obey Hermitian condition. The reverse is not necessarily true. In quantum mechanics, we only deal with self-adjoint operators and these are referred as Hermitian operators.

- The important property of the Hermitian operators is that all its expectation values and eigenvalues are real. Therefore, all physically measurable quantities are denoted by Hermitian operators in Quantum mechanics.

H. W. Prove that Hermitian operators have real expectation values & real eigenvalues.

- **Unitary operator**: An operator $\hat{U}$ is unitary if it satisfies

$$U^\dagger U = U U^\dagger = \mathbb{I}. \quad (\text{identity operator}).$$

Properties: (i) If U is unitary, then $U^{-1} = U^\dagger$.

(ii) The eigenvalues of unitary operator is unimodular or pure phase. (H.W.)

(iii) Under the unitary evolution of a vector, the norm of the vector remains unchanged.

$$|\psi\rangle \to |\psi'\rangle = |U\psi\rangle = U|\psi\rangle$$

Then $\langle \psi'|\psi'\rangle = \langle U\psi|U\psi\rangle = \langle \psi|U^\dagger U|\psi\rangle$

$= \langle\psi|\psi\rangle$ as $U^\dagger U = \mathbb{I}$.

(The definition of identity operator is

$$\mathbb{I}|\psi\rangle = |\psi\rangle \quad , \forall\, |\psi\rangle.$$

)

- In quantum mechanics, any physical (measurable) quantity, such as position, momentum and energy are defined by linear, Hermitian operators. The evolutions/rotations of the states in time, space are done with unitary operators, such that the norm of the state remains invariant. Unitary operator rotates an orthonormal set of basis to another orthonormal basis set. So, the basis states of a Hilbert space is arbitrary by an (fixed, not space, time dependent) unitary transformation.

Matrix elements, Expectation value and Eigenvalue of operators.

For every observable, ie, the one we can measure, there exists an operator, rather an Hermitian operator, whose expectation value is what we measure. In quantum mechanics we also have to specify in which state or ket vector the observation is to be made.

Let $|\psi\rangle \in \mathcal{H}$ defines a general vector, and $\hat{O}$ be a linear operator in the same Hilbert space. Let $|\phi\rangle = \hat{O}|\psi\rangle \in \mathcal{H}$ be a vector obtained by operating $\hat{O}$ on $|\psi\rangle$. Then the following three definitions arises.

(i) Transition probability from state $|\psi\rangle$ to $|\chi\rangle$ by the operator $\hat{O}$ is

$$T = \langle \chi | \hat{O} | \psi \rangle \in \mathbb{C}.$$

(ii) Expectation value of $\hat{O}$ in state $|\psi\rangle$ is

$$\lambda = \langle \psi | \hat{O} | \psi \rangle \in \mathbb{R} \quad \text{— (1)}$$

(Prove that λ is real). if $\hat{O}$ is hermitian.

(iii) Eigenvalue: $|\psi\rangle$ is called an eigenvector of $\hat{O}$ if it satisfies

$$\hat{O}|\psi\rangle = \beta|\psi\rangle \quad \cdots (2)$$

where β is called the eigenvalue or proper value of $\hat{O}$.

- All eigenvalues are also the expectation values, but the reverse is not true.
  → Show that if $|\psi\rangle$ is an eigenvalue of $\hat{O}$, then it's also an eigenvalue of all its power $\hat{O}^n$ and also $e^{\hat{O}}$, with the eigenvalues
  $$\hat{O}^n|\psi\rangle = \beta^n|\psi\rangle \; ; \; e^{\hat{O}}|\psi\rangle = e^{\beta}|\psi\rangle.$$

- We will show below that in a N-dimensional Hilbert space, the operator $\hat{O}$ has N- eigenvalues and N-eigenvectors. (Otherwise it's called a defective or unphysical operator). Moreover, the N-eigenvectors of any Hermitian matrix form an orthonormal basis states.

⊛ Commutator and Uncertainty Relation

Two successive operations, say by operators A & B, do not commute (in the matrix representation of operators, we will see that its equivalent to saying the matrix multiplication is not commutative).

$$\text{i.e.} \quad AB|\psi\rangle \neq BA|\psi\rangle.$$

This is quite intuitive. B acting on $|\psi\rangle$ gives a state, say, $|\phi\rangle = B|\psi\rangle$, and on the L.H.S A is acting on $|\phi\rangle$. On the other hand, on the R.H.S, A is acting on $|\psi\rangle$, giving, say, $|\chi\rangle = A|\psi\rangle$. Here B is acting on $|\chi\rangle$. So, the result is expected to be different.

This prompts us to define two quantities, the commutator, and anti-commutator between A & B:

$$\text{Commutator}: [A, B] = AB - BA$$
$$\text{Anti-commutator}: \{A, B\} = AB + BA.$$

The commutator, and anti-commutator are anti-symmetric and symmetric under the exchange between A & B. So, we can write

$$AB = \frac{1}{2}[A, B] + \frac{1}{2}\{A, B\}. \quad -(1)$$

- Next we are interested in deriving the uncertainty principle between two operators. The expectation value of an operator is $\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$. Its standard deviation / variance of the operator A around its expectation value (like the mean value) is

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2} = \sqrt{(A - \langle A \rangle)^2}.$$

This is equivalent to looking at the expectation value of of the square of $\delta A = A - \langle A \rangle$, the fluctuation around its mean value. We also denote $\delta B = B - \langle B \rangle$. Then we define

$$|\phi\rangle = (\delta A)|\psi\rangle \quad \& \quad |\chi\rangle = (\delta B)|\psi\rangle.$$

Then using Cauchy-Schwarz inequality we get

$$|\langle \phi | \chi \rangle|^2 \leq \langle \phi | \phi \rangle \langle \chi | \chi \rangle$$

we get

$$\langle \psi | (\delta A)(\delta B) | \psi \rangle \leq \langle \psi | (\delta A)^2 | \psi \rangle \langle \psi | (\delta B)^2 | \psi \rangle$$

$$|\langle \delta A \, \delta B \rangle|^2 \leq (\Delta A)^2 (\Delta B)^2 \quad \text{(from definition)}$$

(Recall the equivalent expression in classical prob. theory that the covariance is less than equal to product of variances.

Now, using eq ①:

$$\delta A \, \delta B = \frac{1}{2}[\delta A, \delta B] + \frac{1}{2}\{\delta A, \delta B\}$$

↑ purely imag ↑ purely real

we have

$$|\langle \delta A \, \delta B \rangle|^2 = \frac{1}{4}|\langle [\delta A, \delta B] \rangle|^2 + \frac{1}{4}|\langle \{\delta A, \delta B\} \rangle|^2.$$

Then we get

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

(This is the Robertson-Schrödinger uncertainty principle)

If the anticommutator vanishes or ignored, then we get

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [A,B] \rangle|.$$

- For most practical purposes, if the Hilbert space is finite dimensional, the operators can be written in matrix form.

Suppose we have a Hilbert space of N-dimension. This means, we have some N-basis states $\{|\varphi_n\rangle \mid n = 1, 2, \cdots N\}$. We expand $|\psi\rangle$ in this basis states as

$$|\psi\rangle = \sum_{n=1}^{N} \alpha_n |\varphi_n\rangle, \quad \text{where } \alpha_n = \langle \varphi_n | \psi \rangle \in \mathbb{C}.$$

Now, the expectation value of an operator $\hat{O}$ in this basis state reads as

$$\lambda = \langle \psi | \hat{O} | \psi \rangle = \left(\sum_n \alpha_n^* \langle \varphi_n | \right) \hat{O} \left(\sum_m \alpha_m |\varphi_m\rangle \right)$$

$$= \sum_n \sum_m \alpha_n^* \alpha_m \underbrace{\langle \varphi_n | \hat{O} | \varphi_m \rangle}_{O_{mn}}$$

$$= \sum_n \sum_m \alpha_n^* \alpha_m O_{nm}. \qquad \text{— (3)}$$

O_{nm} is the element of an $N \times N$ matrix defined in this basis state, hence the name matrix element.

- Special case, when $|\varphi_n\rangle$ are the eigenvectors of $\hat{O}$ with eigenvalue β_n,

$$\hat{O} |\varphi_n\rangle = \beta_n |\varphi_n\rangle, \quad n = 1, \cdots, N.$$

This eigenvalue equation is written alternatively as

$$\beta_n = \langle \varphi_n | \hat{O} | \varphi_n \rangle, \quad \langle \varphi_n | \varphi_m \rangle = \delta_{nm}, \quad \sum_n |\varphi_n\rangle\langle\varphi_n| = \mathbb{I}, \text{ as the}$$

eigenvectors of an Hermitian operator is orthonormal. This we can write in compact form as

$$\langle \phi_n | \hat{O} | \phi_m \rangle = \beta_n \delta_{nm}.$$

In other words, the operator $\hat{O}$ is diagonal with β_n being in the diagonal entries in its eigenbasis $|\phi_n\rangle$. Therefore, finding eigenvalue & eigenvector amounts to diagonalizing an operator.

Connection between the eigenvectors and unitary operator.

There is an interesting and powerful connection between the eigenvectors of an Hermitian operator and an unitary rotation that is often used in quantum mechanics, as well as in other branches of Physics.

Each eigenvectors $|\phi_n\rangle$ is $N \times 1$ vector or column vectors. Next, we construct a matrix U by placing each eigenvector at subsequent columns as

$$U = \left(|\phi_1\rangle \; |\phi_2\rangle \; \cdots \; |\phi_N\rangle \right)$$

Clearly U is a $N \times N$ matrix. Its adjoint is

$$U^\dagger = \begin{pmatrix} \langle \phi_1 | \\ \langle \phi_2 | \\ \vdots \\ \langle \phi_N | \end{pmatrix}$$

, where $\langle \phi_n |$ is a $1 \times N$ row vector.

Then we get $U^\dagger U = \sum_{nm} \langle \phi_n | \phi_m \rangle = \mathbb{I}$ as $|\phi_n\rangle$ are orthonormal.

We also get $U U^{\dagger} = \sum_n |\phi_n\rangle\langle\phi_n| = \mathbb{I}$ as $|\phi_n\rangle$ are complete.

- Therefore, the eigenvalue equation can be written as a unitary rotation/transformation to a diagonal matrix as

$$\hat{U}^{\dagger}\hat{O}\hat{U} = \hat{D}, \text{ where } D = \text{diag}(\beta_1, \beta_2 \cdots \beta_n)$$

& U consist of corresponding eigenvectors.

or, $\hat{O} = \hat{U}\hat{D}\hat{U}^{\dagger}$.

- ## Unitary rotation / transformation / evolution :

An important property of quantum mechanics is that under any unitary transformation (which is also referred as unitary rotation or evolution), the physics should not change. By physics we mean the observables or measurable quantities, which are denoted by expectation value and the norm of the state vectors of any Hermitian operator $\hat{O}$ in any state $|\psi\rangle$ must remain unchanged. Since operator and states are not observables, they are allowed to change with unitary rotation to the extent that the expectation value and the norm of the state remain unchanged.

Lets start with the expectation value :

$$\chi = \langle\psi|\hat{O}|\psi\rangle = \langle\psi|U^\dagger U \hat{O} U^\dagger U|\psi\rangle$$

$$= \langle\psi'|\hat{O}'|\psi'\rangle$$

First we insert $\mathbb{I} = U^\dagger U$ before the states. Next we define a new state $|\psi'\rangle = U|\psi\rangle$, and a new operator $\hat{O}' = U^\dagger \hat{O} U$, such that the expectation value remains invariant.

It is easy to prove that the norm of the state vector also remains invariant as $\langle\psi'|\psi'\rangle = \langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\mathbb{I}|\psi\rangle = \langle\psi|\psi\rangle$.

This is the beauty of Q. mechanics that the state vector and operators are not well defined, defined modulo a unitary transformation, but the expectation value, that we measure, must be invariant.

- The summary is, under unitary transformation, the things that changes are

  (i) State vector : $|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$

  (ii) Operator : $\hat{O}' \to \hat{O}' = U\hat{O}'U^\dagger$

  (iii) EOM: The equation of motion that governs the dynamics, such as Schrödinger equation, also changes under a unitary rotation.

Physical quantities remain invariant:

(i) Norm of state vector: $\langle\psi|\psi\rangle$.

(ii) Expectation values : $\langle\psi|\hat{O}|\psi\rangle$.

(iii) Eigenvalues of $\hat{O}$: $\hat{O}|\psi\rangle = \lambda|\psi\rangle$.

In short, any scalar quantity, that easily commute with the unitary operator, remains invariant.

Matrix Algebra

- An operator, when written in a specific basis, it becomes a matrix. Needless to say all properties of an operator, its matrix form naturally inherits.
- A matrix A is a set of real or complex numbers, which are arranged with two indices A_{ij}, $i = 1, \dots N$; $j = 1, \dots, M$, with a specific structure defined for matrix addition, multiplication and scalar multiplication. N & M are called the dimension of the matrix A, with total $N \times M$ elements present.

(i) Addition and substration:

We can only add & subtract two matrices of same dimension. The addition & substraction happends for each elements as $A + B = C$ is defined as

$$A_{ij} + b_{ij} = c_{ij}, \quad \forall\ i, j.$$

Addition is commutative, distributive and associative.

(ii) Matrix multiplication: This has a special rule:

Suppose $C = A B$

Then $$c_{ij} = \sum_k A_{ik} B_{kj}, \quad \forall\ i = 1, \dots N,\ j = 1, \dots M,\ k = 1 \dots L.$$

The 1st index i of C must be same as the first index of the first matrix A, and 2nd index j is same for the 2nd index of the 2nd matrix B. The k-index in between is summed over. Therefore, the dimension of A & B donot necessarily be the same, however,

the number of columns of A must be same as the number of rows of the 2nd matrix B.

The matrix multiplication is non-commutative, which plays an important role in quantum mechanics.

$$AB \neq BA.$$

We often define a commutator

$$[AB - BA] = D.$$

So, if $D \neq 0$, A & B said to commute with each other, otherwise A & B commute if $D = 0$.

(iii) Scalar multiplication : If $\alpha A = B$, $\alpha \in \mathbb{C}$, then

$$\alpha A_{ij} = B_{ij}.$$

④ **Inverse Matrix** : The inverse only exists for square matrix whose $N = M$.

Let A be a square matrix, its inverse, denoted by A^{-1}, is defined as

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

We will not discuss here how an inverse is obtained, except that $A^{-1} \propto \frac{1}{\det(A)}$.

Therefore, if the $\det(A) = 0$, then its inverse does not exist. Such a matrix is called the singular matrix.

⑤ **Unitary matrix** : $U U^{\dagger} = U^{\dagger} U = \mathbb{I}$.

$\Rightarrow U^{\dagger} = U^{-1}$.

(If the entries of the matrix is real, then we don't need to take the complex conjugation. Then we have $U U^{T} = U^{T} U = \mathbb{I}$. This is called orthogonal matrix).

⑥ **Hermitian matrix** : $H^{\dagger} = H$. (For real matrix, it called symmetric matrix if $H^{T} = H$).

→ Trace of a matrix: $a = Tr(A) \in \mathbb{C}$

$= \sum_{i=1}^{N} A_{ii}$ only defined for square matrices.

$$Tr(AB) = \sum_{ij} A_{ij} B_{ji} = \sum_{ji} B_{ji} A_{ij} = Tr(BA)$$

Trace is cyclic.: $Tr(ABC) = Tr(CAB) = Tr(BCA)$

$\neq Tr(ACB)$

Theorem: Trace a matrix A is equal to the summation over its eigenvalues.

Proof: Since $A = U D U^{\dagger}$, where $D = diag(\lambda_1, \lambda_2, \ldots)$

λ_i are eigenvalues of A

U = eigenvectors of A

Then $Tr(A) = Tr(U D U^{\dagger})$

$= Tr(\underbrace{U^{\dagger} U}_{\mathbb{I}} D)$ since Tr is cyclic

$= Trace(D)$

$= \sum_{i=1}^{n} \lambda_i$.

→ Trace is preserved under a unitary transformation, i.e., Trace is a physically measurable quantity.

- **Determinant:** Determinant is another scalar quantity that defines for a matrix. The mathematical definition is a bit involved:

$$|A| = \det(A) = \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} A_{i,\sigma(i)}$$

where S_n = set of all permutations of $\{1, 2, \dots n\}$.
$\operatorname{sgn}(\sigma) = \pm 1$ if the permutation is even or odd,
$A_{i,\sigma(i)}$ are the matrix elements chosen according to the permutation

e.g. 1×1 matrix / scalar : $\det(A) = A$.

2×2 matrix : $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, $\det(A) = ad - bc$

3×3 matrix : $A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & 0 \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$.

- **Properties:** (i) $\det(AB) = \det(A)\det(B) = \det(B)\det(A) = \det(BA)$.

  (ii) $\det(A^T) = \det(A)$, $\det(A^\dagger) = (\det(A))^*$

  (iii) $\det(A^{-1}) = (\det(A))^{-1}$, if A is invertible.

  (iv) $\det(A) = \prod_i \lambda_i$, where λ_i eigenvalues of A.

- Invariance of $\det(A)$ under unitary transformation.

  Suppose $A \to A' = UAU^\dagger$. Then

  $\det(A') = \det(UAU^\dagger) = \det(U)\det(A)\det(U^\dagger)$

  $= \det(A)$ since $\det(U^\dagger) = \det(U^{-1}) = \frac{1}{\det(U)}$.

- $|\det(U)| = 1$ if U is unitary or orthogonal.

- **Geometric properties:** In $\mathbb{R}^n$, $|\det(A)|$ is the scaling factor for n-dim volume under linear transformation $\vec{x} \to A\vec{x}$.

  If $\det(A) > 1$, it's a proper transformation

  or $\det(A) < 1$, it's an improper transformation

  i.e., it flips orientation.

* **Application of determinant:** In eigenvalue solver, we use it as follows: If λ is an eigenvalue of A then it satisfies

$$\det(A - \lambda I) = 0.$$

This is called the secular equation.