Chapter 1 – Mathematical Introduction

O says that this is an important chapter that we should not rush through at any cost.

Linear Vector Spaces –

△ **Def 1**: A linear vector space $\mathbb{V}$ is a collection of objects, $|1\rangle, |2\rangle, \ldots, |V\rangle, \ldots, |W\rangle, \ldots$ called vectors, for which $\exists$

1. A definite rule for forming the vector sum $|V\rangle + |W\rangle$
2. A definite rule for multiplication by scalars $a, b, \ldots$ denoted by $a|V\rangle$ with the following features

   (a) Closure: $|V\rangle + |W\rangle \in \mathbb{V}$

   (b) Distribution of scalar mult over vector add – $a(|V\rangle + |W\rangle) = a|V\rangle + a|W\rangle$

   (c) Distribution of scalar mult over scalar add: $(a+b)|V\rangle = a|V\rangle + b|V\rangle$

   (d) Commutative vec add: $|V\rangle + |W\rangle = |W\rangle + |V\rangle$

   (e) Associative vec add: $(|V\rangle) + (|W\rangle + |Z\rangle) = (|V\rangle + |W\rangle) + |Z\rangle$

   (f) Existence of additive identity: $|V\rangle + |0\rangle = |V\rangle$

   (g) $\forall\ |V\rangle\ \exists!$ an inverse $|-V\rangle$ s.t.,
   $$|V\rangle + |-V\rangle = |0\rangle$$

(*) Do what comes naturally – to remember these.

△ The numbers $a, b, \ldots$ over which the vector space is defined, is called a field.

→ If it is real, we call the vector space a "real vector space", and a "complex vec space" if it is complex.

We have some additional claims that we can make from these -

① $|0\rangle$ is unique

② $0|v\rangle = |0\rangle$

③ $|-v\rangle = -|v\rangle$

④ $|-v\rangle$ is unique for $|v\rangle$ as additive inv.

⊛ $|v\rangle$ is pronounced Ket v — it is Dirac's notation.

Δ The set of vectors is said to be linearly independent if the only such linear relation as

$$\sum_{i=1}^{n} a_i |i\rangle = |0\rangle$$

is the trivial one with all $a_i = 0$.

If the set of vectors are not linearly independent, we say that they are linearly dependent.

⊛ Will be skipping some of the material here in notes as it is too elementary.

- Dimension of vector space
- Basis of a vector space
- Coordinates of vector w.r.t a given basis (Components)
- $|v\rangle = \sum_i v_i |i\rangle \quad , \quad |w\rangle = \sum_i w_i |i\rangle$

  $|v\rangle + |w\rangle = \sum_i (v_i + w_i) |i\rangle$
- $a|v\rangle = a\sum_i v_i |i\rangle = \sum_i a v_i |i\rangle$

Inner Product Spaces →

We need a sensible analogue of the vector dot product for all vector spaces,

$$\vec{A}\cdot\vec{B} = |\vec{A}||\vec{B}|\cos\theta$$

Where we may define the length of $\vec{A}$ as,

$$\sqrt{|\vec{A}\cdot\vec{A}|}$$

and the angle b/w two vectors as,

$$\cos\theta = \frac{\vec{A}\cdot\vec{B}}{|\vec{A}||\vec{B}|}$$

We can do this, as the dot product has a second definition in terms of components →

$$\vec{A}\cdot\vec{B} = A_x B_x + A_y B_y + A_z B_z$$

We need to define a similar formula for the general case where we know a basis and the components of a vector w.r.t the basis.

Main features of the dot product –

1. $\vec{A}\cdot\vec{B} = \vec{B}\cdot\vec{A}$ (symmetric)
2. $\vec{A}\cdot\vec{A} \geq 0$ (positive semi-definite)
3. $\vec{A}\cdot(b\vec{B} + c\vec{C}) = b\vec{A}\cdot\vec{B} + c\vec{A}\cdot\vec{C}$ (linearity)

We wish to invent a generalisation called the dot product or the scalar product or inner product of two vectors $|V\rangle$ and $|W\rangle$ →

Denoted by symbol $\langle V|W\rangle$.

It follows the following axioms –

1. $\langle V|W\rangle = \langle W|V\rangle^*$ (Skew-symmetry)
2. $\langle V|V\rangle \geq 0$, $\langle V|V\rangle = 0$ iff $|V\rangle = |0\rangle$ (positive semi-definite)
3. $\langle V|(a|W\rangle + b|Z\rangle)\rangle \equiv \langle V|aW + bZ\rangle$
$= a\langle V|W\rangle + b\langle V|Z\rangle$

(Linearity in Ket)

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

(*) The first rule makes the inner product sensitive to order of the two factors — in real vector spaces, this just states symmetry
It also ensures that $\langle v|v\rangle$ is real.
(*) The positive semi-definiteness ensures that we can define the norm
(*) What if the first factor is a linear superposition?

$$\langle aw + bz | v\rangle = \langle v | aw + bz\rangle^*$$
$$= (a\langle v|w\rangle + b\langle v|z\rangle)^*$$
$$= a^*\langle v|w\rangle^* + b^*\langle v|z\rangle^*$$
$$= a^*\langle w|v\rangle + b^*\langle z|v\rangle$$

$\longrightarrow$ Anti-linearity of inner prod. w.r.t first factor.
(*) IMP assymmetry.

Δ We say that two vectors are orthogonal or perpendicular if their inner product vanishes
Δ We will refer to $\sqrt{\langle v|v\rangle} \equiv |v|$ as the norm or the length of the vector.
Δ A normalized vector has unit norm
Δ A set of basis vectors all of unit norms, which are pairwise orthogonal will be called an orthonormal basis.

We will obtain a formula for the scalar product —

$$|v\rangle = \sum_i v_i |i\rangle$$
$$|w\rangle = \sum_i w_i |j\rangle$$

following the axioms,

$$\langle v|w\rangle = \sum_i \sum_j v_i^* w_j \langle i|j\rangle$$

Now, if we have an orthonormal basis, only the diagonal elements will survive

$\rightarrow$ $\langle i|i\rangle = 1$, $\langle i|j\rangle = 0$, $i \neq j$

$$\Rightarrow \langle i|j\rangle = \begin{cases} 1, & i=j \\ 0, & i\neq j \end{cases} = \delta_{ij}$$

☐ (Gram - Schmidt) — Given a linearly independent basis we can form linear combinations of the basis vectors to obtain an orthonormal basis. (postponing discussion of the process for a while)

Assuming the orthonormal basis,

$$\boxed{\langle v|w\rangle = \sum_i v_i^* w_i}$$

Now, we can see,

$$\langle v|v\rangle = \sum_i |v_i|^2 \geq 0$$ (vanishes only for null vector)

Every vector is associated (can be represented by a column vector —

$$|v\rangle = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

and

$$|w\rangle = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

Therefore, the scalar product may be obtained by,

$$\langle v|w\rangle = \underbrace{[v_1^* \; v_2^* \ldots v_n^*]}_{\text{'Bra v'}} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

Same as Ket, Bra v is just the transpose conjugate (adjoint) of the Ket v column vector.

o If we have a vector,

$$|V\rangle = \sum_i \vartheta_i |i\rangle$$

If we have to select the jth coordinate of the vector, we simply take the dot product with $\langle j|$

$$\langle j|V\rangle = \sum_i \vartheta_i \langle j|i\rangle \quad \rightarrow \cancel{\vartheta}\,\delta_{ij}$$

$$= \vartheta_j$$

Thus, we can represent the vector as,

$$|V\rangle = \sum_i \langle i|V\rangle |i\rangle$$

o Adjoint Operator →

$$\langle aV| = \langle V|a^* \qquad \text{(Yeah, ofc)}$$

Now, if there is a relation among kets,

$$a|V\rangle = b|W\rangle + c|Z\rangle + \cdots$$

We have one among corresponding bras,

$$\langle V|a^* = \langle W|b^* + \langle Z|c^* + \cdots$$

These are called adjoints of each other.

From this, it follows that if we have,

$$|V\rangle = \sum_i |i\rangle\langle i|V\rangle$$

Then,

$$\langle V| = \sum_i \langle V|i\rangle \langle i|$$

→ using skew-symmetric feature of bra-ket.

□ Gram - Schmidt Theorem →

① Rescale the first by its own length, so that it becomes a unit vector. This is the first basis vector

② Subtract from second vector its projection along the first, leaving behind part ⊥ to the first.

③ Rescale this left over vector by its length to make it unit.

Let $|I\rangle, |II\rangle, \ldots$ be lin indep basis.

first vec of orthonormal basis is,

$$|1\rangle = \frac{|I\rangle}{|I|}, \text{ where } |I| = \sqrt{\langle I|I\rangle}$$

Clearly,

$$\langle 1|I\rangle = \frac{\langle I|I\rangle}{|I|^2} = 1$$

for the second vector,

$$|2'\rangle = |II\rangle - |1\rangle\langle 1|II\rangle$$

and,

$$|2\rangle = \frac{|2'\rangle}{|2'|}$$

and

$$|3'\rangle = |III\rangle - |1\rangle\langle 1|III\rangle - |2\rangle\langle 2|III\rangle$$

and so on,

(*) If we had chosen a basis that was lindep, it would vanish at some point due to formation of non-trivial linear combination of vectors.

□ The dimensionality of a space equals $n_\perp$, the max number of mutually orthogonal vectors in it.

(*) Important Inequalities →

I Schwarz Inequality →

$$|\langle V|W\rangle| \leq |V||W|$$

II Triangle Inequality →

$$|V+W| \leq |V|+|W|$$

(?) Proofs omitted here.

Δ Subspaces — Given a vector space $\mathbb{V}$, a subset of its ~~elem~~ elements that form a vector space among themselves is called a subspace. A subspace i of dimensionality n_i will be denoted by $\mathbb{V}_i^{n_i}$

(*) Note that all subspaces must contain the null vector and the inverses of all vectors in it to fulfill axioms for a vector space.

Δ Given two subspaces $\mathbb{V}_i^{n_i}$ and $\mathbb{V}_j^{m_j}$, we define their sum

$\mathbb{V}_i^{n_i} \oplus \mathbb{V}_j^{m_j} = \mathbb{V}_k^{m_k}$ as the set containing -

1. All elements of $\mathbb{V}_i^{n_i}$
2. " " " $\mathbb{V}_j^{m_j}$
3. All possible linear combinations of them.

Ex → $\mathbb{V}_x^1 \oplus \mathbb{V}_y^1 = \mathbb{V}_{xy}^2$ → xy plane

□ Linear Operators →

~~A line~~ An operator Ω is an ~~ins~~ instruction for transforming any given vector $|V\rangle$ into another, $|V'\rangle$. This is represented as,

$$\Omega|V\rangle = |V'\rangle$$

(?) We restrict ourselves to operators that do not take us out of the vector space $\mathbb{V}$, i.e, $|V'\rangle \in \mathbb{V}$

Rules for linear operators →

1. $\Omega \alpha |V_i\rangle = \alpha \Omega |V_i\rangle$
2. $\Omega \{\alpha |V_i\rangle + \beta |V_j\rangle\} = \alpha \Omega |V_i\rangle + \beta \Omega |V_j\rangle$
3. $\langle V_i | \alpha \Omega = \langle V_i | \Omega \alpha$
4. $\{\langle V_i | \alpha + \langle V_j | \beta\} \Omega = \alpha \langle V_i | \Omega + \beta \langle V_j | \Omega$

They can also act on bras –

$$\langle V | \Omega = \langle V' |$$

Ex → The simplest operator is the identity operator, I

$I \longrightarrow$ Leave the vector alone.

Thus,

$$I |V\rangle = |V\rangle \qquad \forall \text{ Kets } |V\rangle$$

and,

$$\langle V | I = \langle V | \qquad \forall \text{ bras } \langle V |$$

Ex: More interesting operator on $\mathbb{V}^3(R)$

$R(\frac{1}{2}\pi \hat{i}) \rightarrow$ Rotate a vector by $\frac{\pi}{2}$ about unit vector $\hat{i}$

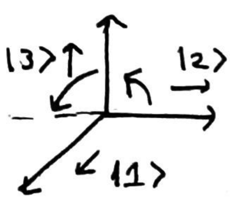
(*) More generally, $R(\vec{\theta})$ represents a rotation of angle $\theta = |\vec{\theta}|$ about the unit vector $\hat{\theta} = \frac{\vec{\theta}}{|\vec{\theta}|}$

Denote $\hat{i} \rightarrow |1\rangle$, $\hat{j} \rightarrow |2\rangle$, $\hat{k} \rightarrow |3\rangle$

$$R(\tfrac{\pi}{2}\hat{i})|1\rangle = |1\rangle$$

$$R(\tfrac{\pi}{2}\hat{i})|2\rangle = |3\rangle$$

$$R(\tfrac{\pi}{2}\hat{i})|3\rangle = -|2\rangle$$



$R(\vec{\theta})$ is clearly linear.

It is nice to know that once the action of an operator (linear) is known on the basis vectors, their action on any vector in that vec space is determined.

If,

$$\Omega|i\rangle = |i'\rangle$$

for a basis, $|1\rangle, \dots, |n\rangle$ in $\mathbb{V}^n$, the for any $V = \sum_i v_i |i\rangle$

$$\Omega|V\rangle = \sum_i \Omega v_i |i\rangle = \sum v_i |i'\rangle$$

Ex → In the ~~case~~ case of $\Omega = R(\frac{\pi}{2}\hat{i})$ if,

$$V = v_1|1\rangle + v_2|2\rangle + v_3|3\rangle$$

Then,

$$R|V\rangle = v_1 R|1\rangle + v_2 R|2\rangle + v_3 R|3\rangle$$

$$\Rightarrow R|V\rangle = v_1|1\rangle + v_2|3\rangle - v_3|2\rangle$$

(!) Essentially changes basis, but not coordinates.

(*) The product of two operators stands for the instruction that the instructions corresponding to the two operators be carried out in sequence,

$$\Lambda\Omega|V\rangle = \Lambda(\Omega|V\rangle) = \Lambda|\Omega V\rangle$$

ket obtained after Ω acts on $|V\rangle$

(!) The order of operations is important.

$$\Lambda \quad \Omega\Lambda - \Lambda\Omega \equiv [\Omega, \Lambda]$$

is called the commutator of Ω and Λ.

It is not generally zero.

Ex, $[R(\frac{\pi}{2}\hat{i}), R(\frac{\pi}{2}\hat{j})] \neq 0$

* Useful identities involving commutators are —

① $$[\Omega, \Lambda\theta] = \Lambda[\Omega, \theta] + [\Omega, \Lambda]\theta$$

② $$[\Lambda\Omega, \theta] = \Lambda[\Omega, \theta] + [\Lambda, \theta]\Omega$$

→ Resemble the chain rule in calculus, for the derivative of a product.

* Not every operator has an inverse.

* $$(\Omega\Lambda)^{-1} = \Lambda^{-1}\Omega^{-1}$$

for only then,

$$(\Omega\Lambda)(\Omega\Lambda)^{-1} = I$$

○ <u>Matrix elements of linear operators</u> →

In the manner a bra or ket may be represented as a row or column vector, an operation on V^n may be represented by an $n\times n$ matrix for a particular basis. — called the matrix elements of the operator for that basis.

We recount the fact that if we know how an operator changes a basis vectors, we know how it changes any vector in that vector space.

$$\Omega|i\rangle = |i'\rangle$$

So,

$$\Omega|V\rangle = \Omega\sum_i v_i|i\rangle = \sum v_i|i'\rangle$$

When we say that $|i'\rangle$ is known, we mean its components in the original basis,

$$\langle j|i'\rangle = \langle j|\Omega|i\rangle \equiv \Omega_{ji}$$

jth component of $|i'\rangle$

These are known.

The n^2 numbers, Ω_{ji}, are the matrix elements of Ω in this basis.

$$\therefore \quad \Omega|V\rangle = |V'\rangle$$

The transformed components of $|V'\rangle$ are expressible in terms of Ω_{ij} and the components of $|V\rangle$.

$$\begin{aligned} v_i' &= \langle i|V'\rangle = \langle i|\Omega|V\rangle \\ &= \langle i|\Omega\Big(\sum_j v_j|j\rangle\Big) \\ &= \sum_j v_j \langle i|\Omega|j\rangle \\ &= \sum_j v_j \Omega_{ij} \end{aligned}$$

This may be cast as,

$$\begin{bmatrix} v_1' \\ v_2' \\ \vdots \\ v_n' \end{bmatrix} = \begin{bmatrix} \langle 1|\Omega|1\rangle & \langle 1|\Omega|2\rangle & \cdots & \langle 1|\Omega|n\rangle \\ \langle 2|\Omega|1\rangle & & \ddots & \vdots \\ \vdots & & & \vdots \\ \langle n|\Omega|1\rangle & \cdots & & \langle n|\Omega|n\rangle \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

<u>Mnemonic</u> $\rightarrow$ The j^{th} column is the image of the j^{th} basis vector after Ω acts on it.

<u>Ex</u> $\rightarrow$ for $R(\frac{\pi}{2}\hat{i})$

$$R\left(\frac{\pi}{2}\hat{i}\right) \leftrightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

Now, a few specific operators and how they look in matrix form —

(I) Identity operator I

$$I_{ij} = \langle i | I | j \rangle = \langle i | j \rangle = \delta_{ij}$$

$$\Rightarrow I_{\cdot} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

(II) Projection operators →

Consider the expansion of an arbitrary ket $|v\rangle$ in a basis.

$$|v\rangle = \sum_{i=1}^{n} |i\rangle\langle i|v\rangle$$

We may write this as,

$$|v\rangle = \left(\sum_{i=1}^{n} |i\rangle\langle i|\right)|v\rangle$$

for this to hold for all basis vectors,

$$I = \sum_{i=1}^{n} |i\rangle\langle i| = \sum_{i=1}^{n} \mathbb{P}_i \longrightarrow \underline{\text{Completeness relation}}.$$

$\mathbb{P}_i$ = projection operator for $|i\rangle$

Consider,

$$\mathbb{P}_i |v\rangle = |i\rangle\langle i|v\rangle = |i\rangle v_i$$

So it takes the projection of a vector along $|i\rangle$.

It can also act on bras,

$$\langle v|\mathbb{P}_i = \langle v|i\rangle\langle i| = v_i^*\langle i|$$

* The completeness relation tells us that that the sum of projections along basis vectors gives us back the original vector.

$P_i P_j = |i\rangle\langle i|j\rangle\langle j| = \delta_{ij} P_j$

Obvious reasons for orthonormal basis

Now, the matrix elements of $\mathbb{P}_i$.

$$|i\rangle = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i^{th} \text{ element}$$

$$\langle i| = \begin{bmatrix} 0 & 0 & \cdots & 1 & \cdots & 0 \end{bmatrix}$$

$$\therefore |i\rangle\langle i| = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & \cdots & 1 & \cdots & 0 \end{bmatrix} = \begin{bmatrix} 0 & \cdots & & 0 \\ \vdots & \ddots & & \vdots \\ & & 1 & \\ 0 & \cdots & & 0 \end{bmatrix}$$

$|v\rangle\langle v| \rightarrow$ Outer product.

Or in a direct approach,

$$(\mathbb{P}_i)_{kl} = \langle k|i\rangle\langle i|l\rangle = \delta_{ki}\delta_{il} = \delta_{kl}\delta_{li}$$

Matrices corresponding to products of operators $\rightarrow$

$$(\Omega\Lambda)_{ij} = \langle i|\Omega\Lambda|j\rangle = \langle i|\Omega I \Lambda|j\rangle$$

$$= \sum_k \langle i|\Omega|k\rangle\langle k|\Lambda|j\rangle$$

$$\Rightarrow \boxed{(\Omega\Lambda)_{ij} = \sum_k \Omega_{ik}\Lambda_{kj}} \rightarrow \text{Typical matrix multiplication.}$$

○ <u>The Adjoint of an operator</u> →

for a given ket, $\alpha|V\rangle \equiv |\alpha V\rangle$, the corresponding bra is, $\langle \alpha V| \equiv \alpha^* \langle V|$

Similarly for a given ket, $|\Omega V\rangle = \Omega|V\rangle$

we have a bra,

$$\langle \Omega V| = \langle V|\Omega^\dagger$$

* → If Ω turns $|V\rangle \to |V'\rangle$, then $\Omega^\dagger$ turns $\langle V| \to \langle V'|$

$$(\Omega^\dagger)_{ij} = \langle i|\Omega^\dagger|j\rangle = \langle \Omega i|j\rangle$$
$$= \langle j|\Omega i\rangle^* = \langle j|\Omega|i\rangle^*$$

$\therefore (\Omega^\dagger)_{ij} = \Omega^*_{ji}$ → <u>Transpose, conjugate</u>

In a given basis, the adjoint operation is the same as taking the transpose conjugate.

$\circledast$ $(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger$

Consider that we have an equation consisting of kets, scalars, and operations —

$$\alpha_1|V_1\rangle = \alpha_2|V_2\rangle + \alpha_3|V_3\rangle\langle V_4|V_5\rangle + \alpha_4\Omega\Lambda|V_6\rangle$$

What is the adjoint?

$$\langle V_1|\alpha_1^* = \langle V_2|\alpha_2^* + \alpha_3^* \cancel{\langle V_3|} \langle V_5|V_4\rangle\langle V_3| + \alpha_4^*\langle V_6|(\Omega\Lambda)^\dagger$$

So, ① Reverse order of all factors,

② $\Omega \leftrightarrow \Omega^\dagger$, $|\rangle \leftrightarrow \langle|$, $\alpha \leftrightarrow \alpha^*$

○ Hermitian, Anti-Hermitian, Unitary

Δ An operator Ω is Hermitian if $\Omega^{\dagger} = \Omega$

Δ An operator Ω is anti-Hermitian if $\Omega^{\dagger} = -\Omega$

An adjoint is to an operator what a complex conjugate is to a number

⇒ Hermitian operators are like real numbers

⇒ Anti-Hermitian operators are like imaginary numbers.

$$\alpha = \frac{\alpha + \alpha^*}{2} + \frac{\alpha - \alpha^*}{2}$$ → Every number may be decomposed into pure real and imaginary parts.

Similarly, we may decompose any operator into Hermitian and anti-Hermitian parts.

$$\Omega = \frac{\Omega + \Omega^{\dagger}}{2} + \frac{\Omega - \Omega^{\dagger}}{2}$$

Δ An operator U is unitary if $UU^{\dagger} = I$

Consequently,

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

⊛ Unitary operators are like complex numbers of unit modulus.

⊛ Imp $U = e^{i\theta}$, $u \cdot u^* = \cancel{e^{2i\theta}}\, e^{i\theta} \cdot e^{-i\theta} = 1$

Unitary operators preserve the inner product between the vectors they act on.

How so?

Let, $|V_1'\rangle = U|V_1\rangle$

$|V_2'\rangle = U|V_2\rangle$

$$\therefore \langle V_2'|V_1'\rangle = \langle V_2 U | U V_1\rangle = \langle V_2|U^{\dagger}U|V_1\rangle$$
$$= \langle V_2|V_1\rangle$$

These are like generalisations of rotation operators from $\mathbb{V}^3(\mathbb{R})$ to $\mathbb{V}^n(\mathbb{C})$ → These operations preserve the length of vectors and their dot products.

$\boxed{+}$ If one treats the columns of an $n \times n$ unitary matrix as components of n vectors, these vectors are orthonormal. Similarly for rows.

⊛ Proof omitted

○ Active and Passive Transformations →

Suppose that we subject all the vectors $|V\rangle$ in a space to a unitary transformation

$$|V\rangle \rightarrow U|V\rangle$$

Under this transformation, the matrix elements of any operator Ω will be modified as follows,

$$\langle V'|\Omega|V\rangle \Rightarrow \langle UV'|\Omega|UV\rangle$$
$$= \langle V'|U^\dagger \Omega U|V\rangle$$

∴ The same change would be affected if we left all the vectors untouched and simply changed all linear operators as –

$$\Omega \rightarrow U^\dagger \Omega U$$

→ Changing the vectors is an active transformation

→ Changing the operator is a passive transformation

wrt vectors.

⊛ Why? We will later see that these give us two equivalent ways of describing the same physical transformation.

⊛ The Eigenvalue Problem →

Consider some linear operator Ω acting on an arbitrary non-zero ket $|V\rangle$

$$\Omega |V\rangle = |V'\rangle$$

Unless the operator is a trivial one - like identity or its multiple, there is no simple (trivial relation b/w $|V\rangle$ and $|V'\rangle$

Each operator, however, has certain kets of its own called eigenkets on which its action is simply rescaling.

$$\Omega |V\rangle = \omega |V\rangle$$

Eigenvalue equation

$|V\rangle \rightarrow$ Eigenket of Ω with eigenvalue ω.

Ex → I - Identity

If $\Omega = I$, $I|V\rangle = |V\rangle$

1. The only eigenvalue is 1
2. All kets are eigenkets with eigenvalue 1.

Ex → $\Omega = \mathbb{P}_V$, projection ~~vector al~~ operator along a normalized ket $|V\rangle$

1. Any ket parallel to $|V\rangle$ ~~wi~~, $\alpha|V\rangle$

$$\mathbb{P}_V |\alpha V\rangle = |V\rangle\langle V|\alpha V\rangle = \alpha|V\rangle |V|^2 = 1\cdot|\alpha V\rangle$$

is an eigenket with eigen value 1

2. Any ket $\perp$ to $|V\rangle$, $\alpha|V'\rangle$

$$\mathbb{P}_V |\alpha V'\rangle = |V\rangle\langle V|\alpha V'\rangle = \alpha|V\rangle\langle V'|V'\rangle$$
$$= 0\cdot|\alpha V\rangle$$

is an eigenket with eigenvalue 0.

(3) Kets that are neither, are not eigenkets

$$\mathbb{P}_v(\alpha|v\rangle + \beta|v_\perp\rangle) = \alpha|v\rangle \neq r(\alpha|v\rangle + \beta|v_\perp\rangle)$$

Ex → Rotation operator $R(\frac{\pi}{2}\hat{i})$

We know,

$$R(\tfrac{\pi}{2}\hat{i})|1\rangle = |1\rangle$$

so it is an eigenket with eigenvalue 1.

Note that if,

$$\Omega|v\rangle = \omega|v\rangle$$

Then,

$$\Omega\alpha|v\rangle = \alpha\Omega|v\rangle = \alpha\omega|v\rangle = \omega\alpha|v\rangle$$

for any multiple α → we do not consider multiples of eigenkets to be different eigenkets with different eigenvalues.

Our intuition says that $R(\frac{\pi}{2}\hat{i})$ has no other eigenvector, but it does have them in $\mathbb{V}^3(\mathbb{C})$. So we need a systematic way of finding them.

o Characteristic equation and the solution to the Eigenvalue Problem →

We rewrite the eigenvalue equation as,

$$(\Omega - \omega I)|v\rangle = |0\rangle$$

Operating both sides with $(\Omega - \omega I)^{-1}$

$$\Rightarrow |v\rangle = (\Omega - I\omega)^{-1}|0\rangle$$

Any finite op acting on the null vec can only give the null vec, but $|v\rangle$ is a nonzero eigenket.

$\Rightarrow (\Omega - I\omega)^{-1}$ cannot exist

Now, for any operator M, $M^{-1} = \frac{1}{\det M} \cdot \text{cofactor}(M^T)$

cofactor (M^T) is finite if M is finite.
$\Rightarrow$ $\det(M) = 0$ for M^{-1} to not exist.

$\therefore \det(\Omega - \omega I) = 0$

This eqn determines the eigenvalues ω. To find them, we proje onto a basis,

$$\langle i | \Omega - \omega I | v \rangle = 0$$

Basically giving us a characteristic polynomial of the form,

$$P^n(\omega) = \sum_{m=0}^{n} C_m \omega^m$$

Called the characteristic polynomial.

⊛ Though this polynomial is determined for a particular basis, the roots are basis independent, - as the definition for eigenvalues are basis independent.

Now by the fundamental theorem of algebra, every nth deg polynomial has n complex roots - not necessarily distinct. Once the eigenvalues are known, the eigenvectors may be found - atleast for Hermitian and unitary matrices.

(*) Hermitian and unitary operators on $V^n(\mathbb{C})$ will have n eigen vectors.

(*) Typically there are only $n-1$ useful equations extracted from putting the eigenvalue into the eigenvalue equation to determine the eigenvector. This helps give the degree of freedom required to include all multiples of the eigenvector.

(*) <u>Notation</u> → The ket (eigen) corresponding to the eigenvalue $\omega = \omega_i$ is labelled as $|\omega = \omega_i\rangle$ or $|\omega_i\rangle$

Δ Phenomena of a single eigenvalue representing more than one eigenvector is called <u>degeneracy</u>.
→ Corresponds to ~~repea~~ repeated roots of characteristic polynomial

The eigenvalues of a Hermitian operator are real.

To every Hermitian operator Ω, there exists at least a basis consisting of its orthonormal eigenvectors.

These theorems strengthen the relation b/w Hermitian operators and real numbers, since they ~~gen~~ ensure that there exists a basis where the Hermitian operator may be expressed as a diagonal matrix of ~~real~~ real ~~numbers~~ numbers.

○ Degeneracy case → Suppose there is a repeated root of the characteristic equation,

$$\omega_1 = \omega_2 = \omega$$

∴ We have two orthonormal vectors obeying,

$$\Omega|\omega_1\rangle = \omega|\omega_1\rangle$$

$$\Omega|\omega_2\rangle = \omega|\omega_2\rangle$$

$$\therefore \Omega[\alpha|\omega_1\rangle + \beta|\omega_2\rangle] = \omega[\alpha|\omega_1\rangle + \beta|\omega_2\rangle]$$

⇒ The whole 2-dim subspace spanned by $|\omega_1\rangle$ and $|\omega_2\rangle$ forms a subspace which has eigenvecs of Ω with eigenvalue ω.

Δ This space is referred to as ~~an~~ an eigenspace of ~~Ω~~ Ω. with eigenvalue ω.

Besides $|\omega_1\rangle$ and $|\omega_2\rangle$ there are infinitely many more orthonormal eigenvectors of Ω in the eigenspace (obtained by rotation) which may be chosen for eigenbasis.

$\Rightarrow$ In face of degeneracy, we have not one, but an infinity of orthonormal eigenbases.

(*) In ~~genera~~ general, if an eigenvalue occurs m_i times, there will be an eigenspace $\mathbb{V}^{m_i}_{\omega_i}$ from which we may choose any m_i orthonormal vectors to form the basis

In the face of degeneracy, the ket $|\omega_i\rangle$ refers to a generic element of the eigenspace $\mathbb{V}^{m_i}_{\omega_i}$ $\longrightarrow$ for a particular element we use $|\omega_i, \alpha\rangle$ where α is a label for the ket in the eigenspace. (Choice of the label will be discussed shortly).

$\boxed{\neg}$ The eigenvalues of an unitary operator are complex numbers of unit modulus.

$\boxed{\neg}$ The eigenvectors of an unitary operator are mutually orthogonal (assuming no degeneracy).

□ Diagonalization of Hermitian matrices →

Let us have a ~~diag~~ Hermitian operator Ω on $\mathbb{V}^n(\mathbb{C})$ represented ~~by a basis~~ in a matrix in some basis $|1\rangle, \ldots, |i\rangle, \ldots |n\rangle$. If we replace this with the eigenbasis $|\omega_1\rangle, \ldots, |\omega_i\rangle, \ldots |\omega_n\rangle$, the matrix representing Ω would become diagonal.

The operator U inducing this change of basis,

$$|\omega_i\rangle = U|i\rangle$$

must be unitary, as it rotates one orthonormal basis to another.

$\boxed{T}$ Every Hermitian matrix on $\mathbb{V}^n(\mathbb{C})$ may be diagonalized by a unitary change of basis.

⇒ If Ω is a Hermitian matrix, $\exists$ a unitary matrix U (built out of ~~it~~ the eigenvectors of Ω) such that $U^\dagger \Omega U$ is diagonal

⇒ finding a basis that diagonalizes Ω is equivalent to solving its eigenvalue problem.

Simultaneous Diagonalization of Two Hermitian Operators →

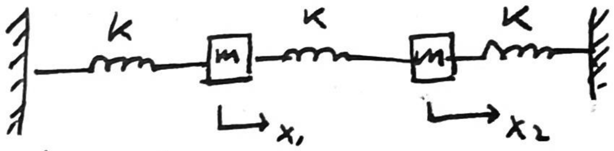
Th. If Ω and Λ are two commuting Hermitian operators, i.e, $[\Omega, \Lambda] = 0$, $\exists$ (atleast) a basis of common eigenvectors that diagonalizes them both.

(*) Proof cut out for brevity.

(*) In general, one can ~~alw~~ always find, for finite n, a set of operators $\{\Omega, \Lambda, \Gamma, \ldots,\}$ the commute with each other and nail down an unique, common, eigenbasis — the elements of which may be labelled unambiguously as $|\omega, \lambda, \gamma, \ldots\rangle$

In study of QMech, it is assumed that such a complete set of commuting operators exist if n is infinite.

(*) IMP Example → Now, there will be a discussion regarding the solution of a simple physical system using the math developed.



We know that the diff eqns of motion are —

$$\left.\begin{aligned} \ddot{x}_1 &= -\frac{2K}{m} x_1 + \frac{K}{m} x_2 \\ \ddot{x}_2 &= -\frac{2K}{m} x_2 + \frac{K}{m} x_1 \end{aligned}\right\} \text{— (I)}$$

The problem is to find $x_1(t)$ and $x_2(t)$ given initial values, i.e, $x_1(0)$, $x_2(0)$, $\dot{x}_1(0)$ and $\dot{x}_2(0)$

We restrict ourselves to case where $\dot{x}_1(0) = 0 = \dot{x}_2(0)$

We rewrite eqn (I) in matrix form,

$$\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix} = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \text{—— (II)}$$

$$\Omega_{11} = \Omega_{22} = -\frac{2k}{m}, \quad \Omega_{12} = \Omega_{21} = \frac{k}{m}$$

Obviously, $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{V}^2(\mathbb{R})$, Ω is an Hermitian operator on $\mathbb{V}^2(\mathbb{R})$

∴ The abstract form of the equation is,

$$|\ddot{x}(t)\rangle = \Omega\,|x(t)\rangle \quad \text{—— (III)}$$

Eqn (I)s can be found from (III) by projecting it onto basis vectors $|1\rangle$ and $|2\rangle$, which have the following significance —

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \leftrightarrow$$ Mass 1 moves unity, Mass 2 remains unchanged

$$|2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \leftrightarrow$$ Mass 1 remains unchanged, Mass 2 moves unity.

In arbitrary scale, when the masses are moved x_1 and x_2 respectively

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} x_1 + \begin{bmatrix} 0 \\ 1 \end{bmatrix} x_2$$

$$\Rightarrow |x\rangle = |1\rangle x_1 + |2\rangle x_2$$

The operator Ω is thus represented in this basis.

This basis has physical significance, but it causes off-diagonal elements to exist in Ω and thus couples the ODEs that we need to solve.

We know that the operator is diagonal in the basis of its normalized eigenvectors. So we switch to that basis, find $|x(t)\rangle$ and then ~~to~~ switch back to normal basis.

Let the eigen vectors be defined as,

$$\Omega |I\rangle = -\omega_1^2 |I\rangle$$
$$\Omega |II\rangle = -\omega_2^2 |II\rangle$$

Solving, we find that,

$$\omega_1 = \left(\frac{k}{m}\right)^{1/2}, \quad |I\rangle \leftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\omega_2 = \left(\frac{3k}{m}\right)^{1/2}, \quad |II\rangle \leftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Now, expanding in new basis,

$$|x(t)\rangle = |I\rangle x_I(t) + |II\rangle x_{II}(t)$$

The matrix eqn now becomes,

$$\begin{bmatrix} \ddot{x}_I \\ \ddot{x}_{II} \end{bmatrix} = \begin{bmatrix} -\omega_I^2 & 0 \\ 0 & -\omega_{II}^2 \end{bmatrix} \begin{bmatrix} x_I \\ x_{II} \end{bmatrix}$$

$$= \begin{bmatrix} -\omega_I^2 x_I \\ -\omega_{II}^2 x_{II} \end{bmatrix}$$

We get the decoupled equations,

$$\ddot{x}_i + \omega_i x_i = 0$$

Which we solve (with $\dot{x}_i(0) = 0$),

$$x_i(t) = x_i(0) \cos(\omega_i t)$$

we get,

$$|x(t)\rangle = |I\rangle x_I(0) \cos \omega_1 t + |II\rangle x_{II}^{(0)} \cos \omega_2 t$$

$$\Rightarrow |x(t)\rangle = |I\rangle \langle I | x_0(0)\rangle \cos(\omega_1 t)$$
$$+ |II\rangle \langle II | x(0)\rangle \cos(\omega_2 t)$$

Now,

$$x_I(0) = \langle I | x(0) \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix}$$

$$= \frac{x_1(0) + x_2(0)}{\sqrt{2}}$$

$$x_{II}(0) = \langle II | x(0) \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix}$$

$$= \frac{x_1(0) - x_2(0)}{\sqrt{2}}$$

$$\therefore |x(t)\rangle = |I\rangle \frac{x_1(0) + x_2(0)}{\sqrt{2}} \cos \omega_I t + |II\rangle \frac{x_1(0) - x_2(0)}{\sqrt{2}} \cos \omega_{II} t$$

Now, we may project onto $|1\rangle$ and $|2\rangle$ to find $x_1(t)$ and $x_2(t)$

$$\therefore x_1(t) = \langle 1 | x(t) \rangle$$

$$= \langle 1 | I \rangle \frac{x_1(0) + x_2(0)}{\sqrt{2}} \cos \omega_1 t + \langle 1 | II \rangle \frac{x_1(0) - x_2(0)}{\sqrt{2}} \cos \omega_{II} t$$

$$= \frac{1}{2}(x_1(0) + x_2(0)) \cos\left(\sqrt{\frac{k}{m}}\, t\right) + \frac{1}{2}(x(0) - x_2(0)) \cos\left(\sqrt{\frac{3k}{m}}\, t\right)$$

Similarly,

$$x_2(t) = \langle 2 | x(t) \rangle$$

$$= \frac{1}{2}(x_1(0) + x_2(0)) \cos\left(\sqrt{\frac{k}{m}}\, t\right) - \frac{1}{2}(x_1(0) - x_2(0)) \cos\left(\sqrt{\frac{3k}{m}}\, t\right)$$

Rewriting in matrix form,

$$\cancel{\frac{x_1(t)}{x_2(t)}}$$

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \dfrac{\cos\omega_1 t + \cos\omega_2 t}{2} & \dfrac{\cos\omega_1 t - \cos\omega_2 t}{2} \\[2ex] \dfrac{\cos\omega_1 t - \cos\omega_2 t}{2} & \dfrac{\cos\omega_1 t + \cos\omega_2 t}{2} \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix}$$

This completes determination of future states dependent on initial states.

The Propagator Matrix

It has the following features —

1. The final state matrix is obtained from the initial state vector upon multiplication by a matrix
2. The matrix is independent of the initial state.

(*) Finding the propagator is tantamount to finding the complete solution to the problem, for any other initial state $x_1(0)$ and $x_2(0)$

This may be expressed as,

$$|x(t)\rangle = u(t)\,|x(0)\rangle$$

Comparing with

$$|x(t)\rangle = |I\rangle\langle I|x(0)\rangle \cos\omega_I t + |II\rangle\langle II|x(0)\rangle \cos\omega_{II} t$$

we find that,

$$u(t) = |I\rangle\langle I| \cos\omega_1 t + |II\rangle\langle II| \cos\omega_2 t$$

$$\Rightarrow u(t) = \sum_{i=I}^{II} |i\rangle\langle i| \cos\omega_i t$$

Taking the matrix elements in $|1\rangle$ and $|2\rangle$ basis, we regain the solution required for our basis.

$$U_{11} = \langle 1|U|1\rangle$$

$$= \langle 1| \{ |I\rangle\langle I| \cos\omega_I t + |II\rangle\langle II| \cos\omega_2 t \} |1\rangle$$

$$= \langle 1|I\rangle\langle I|1\rangle \cos\omega_I t + \langle 1|II\rangle\langle II|1\rangle \cos\omega_{II} t$$

$$= \frac{1}{2}\left(\cos\omega_I t + \cos\omega_{II} t\right)$$

Note that the abstract expression of the propagator matrix is determined entirely by eigenvectors and eigenvalues of Ω

Therefore, we state –

(*) To solve the equation –

$$|\ddot{x}\rangle = \Omega|x\rangle$$

① Solve the eigenvalue problem of Ω

② Construct the propagator in terms of the eigenvalues and eigenvectors

③ $|x(t)\rangle = U(t)|x(0)\rangle$

○ <u>Normal modes</u> –

for the initial value vectors being the eigenkets, the time evolution of the system is particularly simple.

$$|I(t)\rangle = U(t)|I\rangle$$

$$= \left(|I\rangle\langle I|\cos\omega_I t + |II\rangle\langle II|\cos\omega_2 t\right)|I\rangle$$

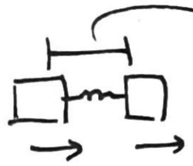
$$= |I\rangle \cos\omega_I t$$

Only modified by overall factor $\cos\omega_I t$

Similar holds for $|II\rangle$

These are the two modes of vibration of the system, clear as,

$$|I\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \rightarrow$$



Both displaced by unity in same dir

$$|II\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} \rightarrow$$

Both disp by unity in opp dir

This can be seen also by representing u in the $|I\rangle, |II\rangle$ basis,

$$u = \begin{bmatrix}\cos\omega_1 t & 0\\ 0 & \cos\omega_2 t\end{bmatrix}$$

The central problem in quantum mechanics is solving the state of a system to described by a ket $|\psi\rangle$ which obeys the Schroedinger equation —

$$\boxed{i\hbar|\dot{\psi}\rangle = H|\psi\rangle}$$

Where $\hbar = \frac{h}{2\pi}$

and H is a hermitian operator called the Hamiltonian.

The problem is to find $|\psi(t)\rangle$ given $|\psi(0)\rangle$

Since the equation is first order in t, no assumptions need to be made about $|\dot{\psi}(0)\rangle$, which is fixed by the Schroedinger equation to be —

$$|\dot{\psi}(0)\rangle = \frac{-i}{\hbar} H|\psi(0)\rangle$$

⊗ In most cases, H is time-independent

The algorithm used to solve this is analogous to the one just used.

① Solve the eigenvalue problem of H

② Find the propagator $U(t)$ in terms of the eigenvectors and eigenvalues of H.

③ $|\psi(t)\rangle = U(t)|\psi(0)\rangle$

O <u>Functions of Operators</u> →

We have encountered two types of objects that act on vectors –

functions of 'c' numbers

① Scalars → 'c' numbers ($\sin x$, $\log(x)$, etc)

↳ Commute with each other and with operators

② Operators → 'q' numbers

↳ Do not generally commute with each other.

Now, we are not familiar with functions of q numbers like we are familiar with functions of c numbers.

(*) We will restrict ourselves to functions that can be written as a power series.

$$f(x) = \sum_{n=0}^{\infty} a_n x^n$$

is a <u>power series</u>

Now consider x is a q number instead of a c number.

$$\therefore \quad f(\Omega) = \sum_{n=0}^{\infty} a_n \Omega^n$$

(*) → This definition only makes sense if the sum converges to a definite limit.

Ex →

$$e^{\Omega} = \sum_{n=1}^{\infty} \frac{\Omega^n}{n!}$$

Let us restrict ourselves to a Hermitian Ω.

Going to eigenbasis of Hermitian Ω, the power series may be computed easily.

$$\Omega = \begin{bmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_n \end{bmatrix}$$

$$\Rightarrow \quad \Omega^m = \begin{bmatrix} \omega_1^m & & & \\ & \omega_2^m & & \\ & & \ddots & \\ & & & \omega_n^m \end{bmatrix}$$

$$\Rightarrow \quad e^{\Omega} = \begin{bmatrix} \sum_{m=0}^{\infty} \frac{\omega_1^m}{m!} & & \\ & \ddots & \\ & & \sum_{m=0}^{\infty} \frac{\omega_n^m}{m!} \end{bmatrix}$$

○ Derivatives of ~~Power~~ Operators with respect to parameters —

Consider a parameter λ, and an operator $\theta(\lambda)$ with dependence on it.

$$\frac{d(\theta(\lambda))}{d\lambda} = \lim_{\Delta\lambda \to 0} \left[\frac{\theta(\lambda + \Delta\lambda) - \theta(\lambda)}{\Delta\lambda} \right]$$

If $\theta(\lambda)$ is written as a matrix in some basis, then the matrix representing $\frac{d\theta(\lambda)}{d\lambda}$ is obtained by differentiating the matrix elements of $\theta(\lambda)$

A special case of $\theta(\lambda)$ is —

$$\theta(\lambda) = e^{\lambda\Omega}$$

where Ω is Hermitian.

In the eigenbasis of Ω,

$$\frac{d\theta(\lambda)}{d\lambda} = \Omega e^{\lambda\Omega} = e^{\lambda\Omega}\Omega = \theta(\lambda)\Omega$$

The same result may be obtained from the power series as well.

(*) → In the eigenbasis, the q numbers behave like c numbers. if the same q number — or powers of it enter the picture, everything even commutes.

However, if more than one q number exists then things are not as simple.

$$e^{\alpha\Omega} e^{\beta\Omega} = e^{(\alpha+\beta)\Omega} \quad \text{is true}$$

But, $$e^{\alpha\Omega} e^{\beta\theta} = e^{\alpha\Omega+\beta\Omega} \quad \text{is not true.}$$

or even
$$e^{\alpha\Omega} e^{\beta\theta} e^{-\alpha\Omega} = e^{\beta\theta} \quad \text{is not true}$$

unless $[\Omega, \theta] = 0$

likewise, in differentiating the product,

$$\frac{d}{d\lambda} e^{\lambda\Omega} e^{\lambda\theta} = \Omega e^{\lambda\Omega} e^{\lambda\theta} \neq e^{\lambda\Omega} e^{\lambda\theta}\theta$$

Generalization to infinite dimensions —

In previous discussions, the dimension of the space was unspecified but finite. Now we generalize them to infinite dimensions.

Consider a function defined in some interval, say $a \le x \le b$.

A concrete example is provided by displacements of a string $f(x,t)$ clamped at $x=0$ and $x=L$.

Let us denote by $f_n(x)$ the discrete approximation to $f(x)$ that coincides with it at n points and vanishes in between. Let us now interpret the ordered ~~tupple~~ n-tuple — $(f_n(x_1), f_n(x_2), \dots, f_n(x_n))$ as components of a ket $|f_n\rangle$ in a vector space $\mathbb{V}^n(\mathbb{R})$

$$|f_n\rangle \leftrightarrow \begin{bmatrix} f_n(x_1) \\ f_n(x_2) \\ \vdots \\ f_n(x_n) \end{bmatrix}$$

The basis vectors in this space are

$$|x_i\rangle \leftrightarrow \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow \underline{\underline{i^{\text{th}}\text{ place}}}$$

This will correspond to a discrete function which is unity at $x = x_i$ and zero elsewhere.

$\langle x_i | x_j \rangle = \delta_{ij}$ (orthogonality)

$$\sum_{i=1}^{n} |x_i\rangle\langle x_i| = I \quad \text{(completeness)}$$

To every possible discrete approximation, there is a correspon-ding ket.

(*) The set of all kets that represent discrete functions ~~have~~ that vanish at $x=0$ and $x=L$ and are specified at n points in between, form a vector space.

We define the inner product in this space —

$$\langle f_n | g_n \rangle = \sum_{i=1}^{n} f_n(x_i)\, g_n(x_i)$$

~~fn are~~ $f_n(x)$ and $g_n(x)$ are said to be orthogonal if

$$\langle f_n | g_n \rangle = 0$$

Now let us approximate the string at every point.

$f_\infty(x) \equiv f(x)$ is specified by an ordered infinity of numbers. an $f(x)$ for each point.

Each function is now represented by a ket $|f_\infty\rangle$ in an infinite dimensional vector space

(*) Vector addition and scalar multiplication are defined as before.

Now, for the inner product if n goes to infinity, the sum goes to infinity too. — we need a definition where a smooth limit obtains.

A natural choice is,

$$\langle f_n | g_n \rangle = \sum_{i=1}^{n} f_n(x_i)\, g_n(x_i)\, \Delta \,, \quad \Delta = \frac{L}{n+1}$$

Now as $n \to \infty$

$$\langle f|g\rangle = \int_0^L f(x)g(x)\,dx$$

$$\langle f|f\rangle = \int_0^L f^2(x)\,dx$$

If we wish to consider complex functions as well -

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)\,dx$$

What are the basis vectors of this space, and how are they normalized?

The orthogonality of the bases ensure -

$$\langle x|x'\rangle = 0 \quad , \; x \neq x'$$

What if $x = x'$? will $\langle x|x'\rangle = 1$?

That will be naive - ~~as~~ we must proceed via completeness.

$$\therefore \quad \int_a^b |x'\rangle\langle x'|\,dx' = I$$

We dot with Ket $|f\rangle$ (arbitrary function) from right, and basis bra $\langle x|$ from left,

$$\int_a^b \langle x|x'\rangle\langle x'|f\rangle\,dx' = \langle x|I|f\rangle$$

$$= \langle x|f\rangle$$

Now, $\langle x'|f\rangle = f(x')$, $\langle x|f\rangle = f(x)$

(Just component of function at that point

$$\Rightarrow \quad \int_a^b \langle x|x'\rangle f(x')\,dx' = f(x)$$

Now, ~~at~~ as $\langle x|x'\rangle$ vanishes at all points $x \neq x'$, we denote it by some function $\delta(x',x)$

We pull out $f(x)$ (approx),

$$f(x) \int_a^b \delta(x, x')\,dx = f(x)$$

$$\Rightarrow \int_a^b \delta(x, x')\,dx = 1$$

as we can restrict it to infinitesimal area $a = x - \epsilon$, $b = x + \epsilon$ (due to local nature of δ)

Since δ depends only on the difference $x - x'$, let us write it as,

$\delta(x - x')$

This function has the properties,

$\circledast$ $\delta(x - x') = 0, \quad x \neq x'$

$\circledast$ $\int_a^b \delta(x - x')\,dx' = 1, \quad a < x < b$

is called the 'Dirac delta function' and it fixes the normalization of the basis vectors.

$$\langle x | x' \rangle = \delta(x - x')$$

$\circledast$ The dirac delta cannot be finite at $x = x'$, otherwise the integral will not be finite

→ Skipping rest of the Dirac material – too difficult atm.

~~o Operators in Infinite Dimensions →~~

Unfortunately (?) the next section cannot be understood without this section on the dirac delta.

→ we may view the delta function as the limit of a Gaussian

$$g_\Delta(x-x') = \frac{1}{\sqrt{x\Delta^2}} \exp\left[-\frac{(x-x')^2}{\Delta^2}\right]$$

The Gaussian is centered at $x = x'$, has width Δ and a maximum height $\frac{1}{\sqrt{\pi\Delta^2}}$ and unit area → Indep of Δ.

As $\Delta \to 0$, g_Δ approximates the delta function.

From the Gaussian model it is clear that the delta function is even., as $g_\Delta(-x) = g_\Delta(x)$

$$\Rightarrow \delta(x-x') = \langle x | x' \rangle = \langle x' | x \rangle^*$$

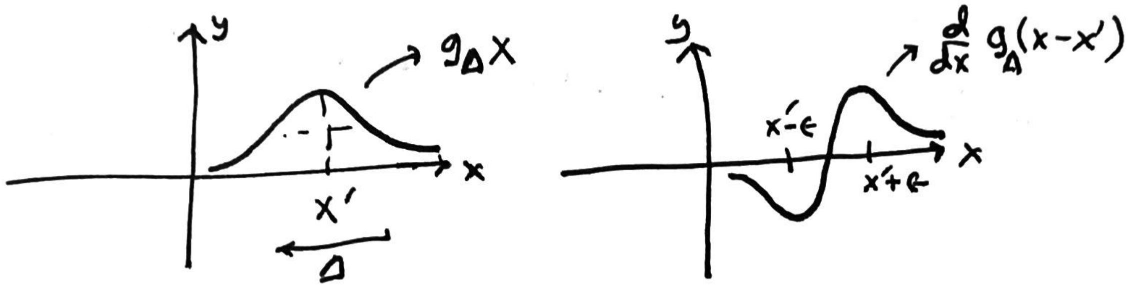
$$= \delta(x'-x)^* = \delta(x'-x)$$

as the delta function is real.

o Derivative of the Delta function →

$$\delta'(x-x') = \frac{d}{dx}\delta(x-x') = -\frac{d}{dx'}\delta(x-x')$$

How does δ' behave under the integral?
Using the integral of gaussian model, we see that



We see that $\frac{dg_\Delta(x-x')}{dx} = -\frac{dg_\Delta(x-x')}{dx'}$

Consider these a function of x'. As $\Delta \to 0$, each of these two bumps becomes δ function to a scale.

The first bump will sample $-f(x-\epsilon)$ and the second one will sample $+f(x+\epsilon)$ (upto a scale)

$$\therefore \int \delta'(x-x') f(x') dx' \propto f(x+\epsilon) - f(x-\epsilon)$$

$$= 2\epsilon \left.\frac{df}{dx'}\right|_{x=x'}$$

The constant of proportionality is $\frac{1}{2\epsilon}$

$$\Rightarrow \int \delta'(x-x') f(x') dx' = \left.\frac{df}{dx'}\right|_{x=x'} = \frac{df(x)}{dx}$$

The result is verified by,

$$\int \delta'(x-x') f(x') dx' = \int \frac{d\delta(x-x')}{dx} f(x') dx'$$

$$= \frac{d}{dx} \int \delta(x-x') f(x') dx'$$

$$= \frac{d}{dx} f(x)$$

(*) Note that $\delta'(x-x')$ is odd.

(*) This may be encapsulated by —

$$\delta'(x-x') = \delta(x-x') \frac{d}{dx}$$

→ The diff operator acts on any function that appears with delta in the integrand.

Also, generalizing,

$$\frac{d^n \delta(x-x')}{dx^n} = \delta(x-x') \frac{d^n}{dx^n}$$

~~Skipping the Fourier Stuff atleast.~~

~~(*) Read Fourier transforms to continue.~~

From Fourier Analysis, we know that, given a function $f(x)$ we may define its transform as,

$$f(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{-ikx} f(x)\,dx \quad \text{— (I)}$$

and its inverse is,

$$f(x') = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{ikx} f(k)\,dk \quad \text{— (II)}$$

feeding eqn (I) into (II),

$$f(x') = \int_{-\infty}^{\infty} \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x'-x)} \right] f(x)\,dx$$

Now, this looks like,

$$f(x') = \int_{-\infty}^{\infty} \delta(x'-x)\, f(x)\,dx$$

$$\Rightarrow \quad \delta(x'-x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x'-x)}$$

□ Operators in Infinite Dimensions →

Now that we are familiar with the elements of this function space — kets $|f\rangle$ and basis vectors $|x\rangle$, let us turn to the linear operators in this space.

Consider the equation,

$$\Omega|f\rangle = |\tilde{f}\rangle$$

→ Ω takes a function $f(x)$ and outputs another function $\tilde{f}(x)$

An example of such an operator is the differential operator, which acts on $f(x)$ to give us $\frac{d}{dx}(f(x)) = \tilde{f}(x)$

We can describe this as,

$$D|f\rangle \equiv |df/dx\rangle$$

What are the matrix elements of D in the $|x\rangle$ basis? To find them, we dot both sides with $|x\rangle$

$$\langle x|D|f\rangle = \left\langle x \middle| \frac{df}{dx} \right\rangle = \frac{df(x)}{dx}$$

and using the identity,

$$\int \langle x|D|x'\rangle\langle x'|f\rangle\, dx' = \frac{df}{dx}$$

Comparing this with

$$\int \delta'(x'-x) f(x')\, dx = \frac{df(x)}{dx}$$

we see that,

$$\langle x|D|x'\rangle = D_{xx'} = \delta'(x-x') = \delta(x-x')\frac{d}{dx'}$$

(4) View $D_{xx'}$ as a matrix acting to the right on the components $f_{x'} \equiv f(x')$ of a vector $|f\rangle$.

Thus, we integrate $D_{xx'} = \delta'(x-x')$ over the second index (x') and this pulls out the derivative of f at the first index (x).

Thus, the differential operator is an infinite dimensional matrix with the given elements.

Normally, when one thinks of an operator acting on a vector, there is a sum over a common index.

In fact,

$$\int \langle x|D|x'\rangle\langle x'|f\rangle\, dx' = \frac{df}{dx}$$

contains such a sum over the index x'

However replacing the $\langle x|D|x'\rangle \equiv D_{xx'}$ as

$$D_{xx'} = \delta(x-x')\frac{d}{dx'},$$

$$\int \delta(x-x')\frac{d}{dx'}f(x')\,dx'$$

$$= \left.\frac{df}{dx'}\right|_{x'=x} = \frac{df}{dx}$$

renders the integration trivial.

Now, we examine whether D is Hermitian and examine its eigenvalue problem.

Now, $D_{xx'} = \delta'(x-x')$

while,

$$D^*_{x'x} = \delta'(x'-x)^* = \delta'(x'-x)$$

$$= -\delta'(x-x') \qquad [D^\dagger \text{ has components } D^*_{x'x}]$$

as $\delta'(x-x')$ is odd.

$\Rightarrow$ D is not hermitian.

But we can invent an operator,

$$K = -iD$$

Such that,

$$K^*_{x'x} = [-i\delta'(x'-x)]^* = i\delta'(x'-x)$$

$$= -i\delta(x-x')$$

$$= K_{xx'}$$

Note that this does not guarantee that K is Hermitian.

O Determination of whether K is Hermitian (dense portion) →

Let $|f\rangle$ and $|g\rangle$ be two kets in the function space whose images in the $|x\rangle$ basis are two functions $f(x)$ and $g(x)$ in the interval a to b.

If K is Hermitian, it must satisfy,

$$\langle g|K|f\rangle = \langle g|Kf\rangle = \langle Kf|g\rangle^*$$

$$= \langle f|K^\dagger|g\rangle^* = \langle f|K|g\rangle^*$$

Now,

$\langle g|K|f\rangle$ can be represented as,

$$\int_a^b\int_a^b \langle g|x\rangle\langle x|K|x'\rangle\langle x'|f\rangle\,dx\,dx' \quad \text{— (I)}$$

and $\langle f|K|g\rangle^*$ can be represented as,

$$\left[\int_a^b\int_a^b \langle f|x\rangle\langle x|K|x'\rangle\langle x'|g\rangle\,dx\,dx'\right]^* \quad \text{— (II)}$$

(Sums over appropriate indices)

Now, we are concerned whether (I) is equal to (II).

with the LHS,

$$\int_a^b\int_a^b \langle g|x\rangle\langle x|K|x'\rangle\langle x'|f\rangle\,dx\,dx'$$

$$\cancel{\Rightarrow \int_a^b \langle g|x\rangle\left[\int_a^b \delta(x-x')\frac{d}{dx'}f(x')\,dx'\right]dx}$$

$$\Rightarrow \int_a^b \langle g|x\rangle\left[\int_a^b -i\delta(x-x')\frac{d}{dx'}f(x')\,dx'\right]dx$$

$$= \int_a^b \langle g|x\rangle\left[-i\frac{df(x)}{dx}\right]dx$$

$$= \int_a^b \langle g|x\rangle\langle x|-i\frac{df}{dx}\rangle\,dx$$

using the definition of the inner product, this may be written as —

$$= \int_a^b g^*(x)\left[-i\frac{df(x)}{dx}\right]dx \quad \text{— III}$$

Similarly with the RHS (tery) we get –

$$\left[\int_a^b\int_a^b \langle f|x\rangle\langle x|K^\dagger|x'\rangle\langle x'|g\rangle dx\,dx'\right]^*$$

$$= \left[\int_a^b f^*(x)\left\{-i\frac{dg(x)}{dx}\right\}dx\right]^*$$

$$= i\int_a^b \frac{dg^*}{dx}\cdot f(x)\,dx \quad \text{— IV}$$

Now, we must see if III and IV are equal.

Note the $\frac{dg^*}{dx}$ term in IV and the $g^*(x)$ term in III. If we integrate by parts with $g^*(x)$ as the first function, we would get same terms. So we do that with III.

$$\int_a^b g^*(x)\left[-i\frac{df(x)}{dx}\right]dx$$

$$= -ig^*(x)f(x)\Big|_a^b + i\int_a^b\frac{dg^*(x)}{dx}f(x)\,dx$$

Thus, I is equal to II iff

$$-ig^*(x)f(x)\Big|_a^b = 0$$

or the 'surface' terms vanish.

Thus, in infinite dimensional case only the condition $K_{xx'} = K^*_{x'x}$ is not sufficient for an operator to be Hermitian.

We also have to look at the behaviour of the functions at the endpoints a and b.

(*) One set of functions that form a space and obey this condition are the possible configurations $f(x)$ of the string clamped ~~at~~ at $x = 0, L$, as $f(x)$ vanishes at the end points.

(*) Another example of a function that obeys this condition is a function in 3D space parametrized by r, θ and ϕ where ϕ is the angle measured about the z axis. Let us require that these functions be single valued. – if we start at a certain point and go once around the z axis we return to the original point.

$$f(\phi) = f(\phi + 2\pi)$$

In the space of such periodic functions,

$K = -i \dfrac{d}{d\phi}$ is a Hermitian operator.

The surface term vanishes,

$$-ig^*(\phi) f(\phi) \Big|_0^{2\pi} = -i \left[g^*(2\pi) f(2\pi) - g^*(0) f(0) \right]$$

$$= 0$$

In Q Mech, we study function defined over $(-\infty, \infty)$

They fall into two classes –

① Those that vanish as $|x| \to \infty$

② Those that do not, i.e e^{ikx} like

When $K = -i\frac{d}{dx}$ is sandwitched between two functions of type ①-①, ①-② or ②-① satisfies the criteria for being Hermitian (as the surface term vanishes).

But when it is sandwitched between two functions of type ②, it depends on whether,

$$e^{ikx} e^{-ikx} \Big|_{-\infty}^{\infty} = 0$$

<u>or not</u>.

→ If $k = k'$, the contribution from one end cancels the other.

→ If $k \neq k'$, $e^{i(k-k')x}$ oscillates rather than approaching a limit as $|x| \to \infty$

We thus invent a prescription/method of defining a limit for such a function: the limit as $|x| \to \infty$ is defined to be the average over a large interval.

As $x \to \infty$

$$\lim_{x\to\infty} e^{ikx} e^{-ik'x} = \lim_{\substack{L\to\infty \\ \Delta\to\infty}} \frac{1}{\Delta} \int_{0}^{L+\Delta} e^{i(k-k')x}\, dx = 0$$

⇒ <u>K is Hermitian in this space</u>

○ Eigenvalue problem of K →

We have to find roots of an infinite-order characteristic polynomial and get characteristic eigenvectors.

Let,

$$\mathbb{K}|K\rangle = K|K\rangle$$ (Confusing notation, yes)

Standard procedure →

$$\langle x|\mathbb{K}|K\rangle = K\langle x|K\rangle$$

$$= \int \langle x|\mathbb{K}|x'\rangle\langle x'|K\rangle dx = K\psi_K(x)$$

where ψ_K is the function represented by the ket $|K\rangle$

$$= -i\frac{d}{dx}\psi_K(x) = K\psi_K(x)$$

($\psi_K(x) = \langle x|K\rangle$)

⊛ We could also have directly substituted $K = -i\frac{d}{dx}$ in the $|x\rangle$ basis.

The solution to this ODE is simply,

$$\psi_K(x) = Ae^{iKx}$$

A is a free parameter unspecified by eigenvalue problem.

⇒ Any real number K is an eigenvalue, and the corresponding eigenfunction is given by Ae^{iKx}.

We use the freedom in ~~sela~~ scale to normalise,

$A = \left(\frac{1}{2\pi}\right)^{1/2}$ so that,

$$|K\rangle \leftrightarrow \frac{1}{(2\pi)^{1/2}} e^{ikx}$$

why do we select this value? remember that — (from fourier)

~~$\delta(x-x$~~

$$\cancel{\delta(x-x') = \frac{1}{2\pi}\int e^{i(k-k')x}}$$

$$\delta(x-x') = \frac{1}{2\pi}\int e^{ik(x-x')}dk$$

So, when we do,

$$\langle K|K'\rangle = \int_{-\infty}^{\infty}\langle K|x\rangle\langle x|K'\rangle dx$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i(K-K')x} dx$$

$$= \delta(K-K')$$

(*) $\langle K|K\rangle$ is infinite — no choice in A can normalize $|K\rangle$ to unity. The delta function normalization is the natural one when the eigenvalue spectrum is continuous.

(*) Why did we not consider complex eigenvalues like $K = K_1 + iK_2$? note that in that case, there will be a real exponential part that blows up to infinity or -ve infinity as $x \to \infty$, it would not oscillate like in our case with real eigenvalues.

In restricting ourselves to real K, we have restricted ourselves to the physical Hilbert Space, which is of interest in QMech.
This space is defined as the space of functions that can either be normalized to unity or to to the Dirac Delta.

form Dirac Delta.

(*) We assume that the theorem proved for finite dimension, namely that the eigen functions of a Hermitian operator form a complete basis, holds in the ~~this~~ Hilbert Space.

We have to state this separately because in infinite dimensional spaces you need to have infinitely many normal eigenvectors for an orthonormal basis. — you can not be sure that you have them all.

Since K is a Hermitian operator, functions that were expanded in the x basis with components $f(x) = \langle x | f \rangle$ must also have an expansion in the K basis.

$$f(K) = \langle K | f \rangle = \int_{-\infty}^{\infty} \langle K | x \rangle \langle x | f \rangle dx$$

$$= \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{-iKx} f(x) dx$$

Similarly, to get back to x basis,

$$f(x) = \langle x | f \rangle = \int_{-\infty}^{\infty} \langle x | K \rangle \langle K | f \rangle dK$$

$$= \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{iKx} f(K) dK$$

⇒ The fourier transform is just the passage from one complete basis $|x\rangle$ to another $|K\rangle$, and vice-versa.

(*) The matrix elements of K in the K basis are trivial –

$$\langle k|K|k'\rangle = k'\langle k|k'\rangle = k'\delta(k-k')$$

⇒ The K basis was generated by the Hermitian operator K.

Now, we attempt to find the operator that is responsible for the orthonormal x basis. Let us call it the X operator. The kets $|x\rangle$ are its eigenvectors with the eigenvalue x.

$$X|x\rangle = x|x\rangle$$

The matrix elements of X in the x basis are,

$$\langle x'|X|x\rangle = x\delta(x'-x)$$

Let us find its action on functions,

$$X|f\rangle = |\tilde{f}\rangle$$

Now,

$$\langle x|X|f\rangle = \int \langle x|X|x'\rangle\langle x'|f\rangle dx'$$

$$= x f(x)$$

$$= \langle x|\tilde{f}\rangle$$

$$= \tilde{f}(x)$$

$$\Rightarrow \tilde{f}(x) = x f(x)$$

→ The effect of X is to multiply $f(x)$ by x

Summarised as,

$$X|f(x)\rangle = |x f(x)\rangle$$

There is a nice reciprocity between X and K operators which manifests itself if we compute the matrix elements of X in the K basis.

$$\langle K | X | K' \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iKx} \, x \, e^{iK'x} \, dx$$

$$= i \frac{d}{dK} \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(K'-K)x} \, dx \right]$$

$$= i \delta'(K - K')$$

Thus if $|g(K)\rangle$ is a ket whose image in the K basis is $g(K)$, then,

$$X |g(K)\rangle = \left| \frac{i \, dg(K)}{dK} \right\rangle$$

$\Rightarrow$ In X basis, X acts as x and K as $-i\frac{d}{dx}$ (on $f(x)$), while in K basis K acts as K and X as $i\frac{d}{dK}$ (on $f(K)$)

Operators that have such a relationship are called <u>conjugates</u> of one another.

$\circledast$ Conjugate operators X and K do not commute. We may compute their commutator, (in X basis)

$$X|f\rangle \rightarrow x \, f(x)$$

$$K|f\rangle \rightarrow -i \frac{df(x)}{dx}$$

$$XK|f\rangle \rightarrow -ix \frac{df(x)}{dx}$$

$$KX|f\rangle \rightarrow -i \frac{d}{dx}(x f(x))$$

$$\Rightarrow [X, K]|f\rangle \Rightarrow -ix\frac{df}{dx} + ix\frac{df}{dx} + if$$

$$= iI|f\rangle$$

$$\Rightarrow [X, K] = iI \quad (\text{as } |f\rangle \text{ is arbitrary})$$

This is ~~the~~ the end on the conversation about Hilbert Space.

(*) Imp Example → (Normal Mode Problem in Hilbert Space)

Consider a string of length L clamped at its two ends $x = 0$ and L.
The displacement $\psi(x, t)$ obeys the differential equation,

$$\frac{\partial^2 \psi}{\partial t^2} = \frac{\partial^2 \psi}{\partial x^2} \quad (\text{velocity unity wave eqn})$$

Given $\psi(x, 0)$ ~~and~~ and $\dot{\psi}(x, 0) = 0$, we wish to determine the time evolution of the string.

(*) This is identical to the two coupled masses problem, except the fact that this is done on an infinite dimensional space.

We identify $\psi(x, t)$ as components of a vector $|\psi(t)\rangle$ in Hilbert Space. — the elements of which are in correspondence with all the possible displacements of the string, i.e. functions that are continuous on $0 \leq x \leq L$ interval and vanish at the end points. (These form a vector space)

The operator here is $\frac{\partial^2}{\partial x^2}$, which we recognise to be $-K^2$ where $K \leftrightarrow -i\frac{\partial}{\partial x}$

Since K acts in a space where the functions vanish at the endpoints, i.e, $\psi(0) = \psi(L) = 0$, it is Hermitian ⇒ so is K^2. Thus we get the abstract counterpart,

$$|\ddot{\Psi}(t)\rangle = -K^2 |\Psi(t)\rangle$$

We use the same algorithm —

(i) Solve eigenvalue problem of $-K^2$

(ii) Construct propagator $U(t)$ in terms of eigenvectors and eigenvalues

(iii)
$$|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$$

Step i → The equation to solve is,

$$K^2|\Psi\rangle = k^2|\Psi\rangle$$

In X basis,

$$-\frac{d^2}{dx^2}\psi_k(x) = k^2 \psi_k(x)$$

Which has the general solution —

$$\psi_k(x) = A\cos kx + B\sin kx$$

where A and B are arbitrary.

Not all of these solutions lie in the Hilbert Space.

So we try,

$$\psi_k(0) = 0 = A \Rightarrow A = 0$$

while at $x = L$,

$$\psi_k(L) = 0 = B\sin kL$$

We do not want the trivial solution of $A = B = 0$

$$\Rightarrow \sin kL = 0 \Rightarrow kL = m\pi, \quad m \in \mathbb{N}$$

(We do not consider m -ve as there are no new solutions that are generated, as $\sin(-mx) = -\sin(mx)$)

Now we need to fix B.

Remember the condition that in the Hilbert Space,

$$\int_0^L \psi_m(x)\,\psi_{m'}(x)\,dx = \delta_{mm'}$$

(Normalisation condition)

Set $m = m'$ (As for $m \neq m'$ the integral evaluates to zero)

$$B^2 \int_0^L \sin^2\left(\frac{m\pi x}{L}\right) dx = \delta_{mm} = 1$$

$$\Rightarrow B^2 \cdot \frac{1}{2}\left[\int_0^L \left\{1 - \cos\left(\frac{2m\pi x}{L}\right) dx\right\}\right] = 1$$

$$\Rightarrow \frac{B^2}{2}\left\{\left[x\right]_0^L - \left[\frac{\sin\left(\frac{2m\pi x}{L}\right)}{\frac{2m\pi}{L}}\right]_0^L\right\} = 1$$

$$\Rightarrow B^2 \cdot \frac{L}{2} = 1$$

$$\Rightarrow B = \left(\frac{2}{L}\right)^{1/2}$$

The allowed eigenvectors then form a discrete set labelled by m,

$$\psi_m(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{m\pi x}{L}\right)$$

So let us associate each solution ~~to~~ labelled by the integer m with an abstract Ket $|m\rangle$

$$|m\rangle \xrightarrow[x\text{ basis}]{} \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{m\pi x}{L}\right)$$

Note that in $|m\rangle$ basis, K is diagonal with the eigenvalues being

$$K^2 = \frac{m^2\pi^2}{L^2}$$

So we project $|\psi(t)\rangle$ on the $|m\rangle$ basis.

$$\frac{d^2}{dt^2}\langle m|\psi(t)\rangle = -\left(\frac{m^2\pi^2}{L^2}\right)\langle m|\psi(t)\rangle$$

This may be solved via ansatz to be,

$$\langle m|\psi(t)\rangle = \langle m|\psi(0)\rangle \cos\left(\frac{m\pi t}{L}\right)$$

(subject to $\dot{\psi}(x,0)=0$)

Now,

$$|\psi(t)\rangle = \sum_{m=1}^{\infty}|m\rangle\langle m|\psi(t)\rangle \quad \text{(completeness)}$$

$$= \sum_{m=1}^{\infty}|m\rangle\langle m|\psi(0)\rangle \cos\left(\frac{m\pi t}{L}\right)$$

$$= \left(\sum_{m=1}^{\infty}|m\rangle\langle m| \cos\left(\frac{m\pi t}{L}\right)\right)|\psi(0)\rangle$$

$$= U(t)|\psi(0)\rangle$$

where,

$$U(t) = \sum_{m=1}^{\infty}|m\rangle\langle m|\cos\left(\frac{m\pi t}{L}\right)$$

Now in the x basis,

$$\langle x|\psi(t)\rangle = \psi(x,t)$$

$$= \langle x|U(t)|\psi(0)\rangle$$

$$= \int_0^L \langle x|U(t)|x'\rangle\langle x'|\psi(0)\rangle dx'$$

Now we must find $\langle x|U(t)|x'\rangle$ i.e the matrix elements of the propagator in the x basis.

It follows from

$$U(t) = \sum_{m=1}^{\infty} |m\rangle\langle m| \cos\left(\frac{m\pi t}{L}\right)$$

$$\cancel{\sum_{m=}}$$

$$\Rightarrow \langle x|U(t)|x'\rangle = \sum_{m=1}^{\infty} \langle x|m\rangle\langle m|x'\rangle \cos\left(\frac{m\pi t}{L}\right)$$

$$\Rightarrow \langle x|U(t)|x'\rangle = \sum_{m=1}^{\infty} \left(\frac{2}{L}\right) \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{m\pi x'}{L}\right) \cos\left(\frac{m\pi t}{L}\right)$$

Since we ~~kn~~ know this,
we just need to know some $\langle x'|\psi(0)\rangle = \psi(x',0)$
to perform the integral,

$$\langle x|\psi(t)\rangle = \int_0^L \langle x|U(t)|x'\rangle\langle x'|\psi(0)\rangle\, dx'$$

to get $\langle x|\psi(t)\rangle = \psi(x,t)$

Alternatively, we could start with,

$$|\psi(t)\rangle = \sum_{m=1}^{\infty} |m\rangle\langle m|\psi(0)\rangle \cos\left(\frac{m\pi t}{L}\right)$$

$$\Rightarrow \langle x|\psi(t)\rangle = \sum_{m=1}^{\infty} \langle x|m\rangle\langle m|\psi(0)\rangle \cos\left(\frac{m\pi t}{L}\right)$$

$$= \sum_{m=1}^{\infty} \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{m\pi x}{L}\right) \cos\left(\frac{m\pi t}{L}\right) \langle m|\psi(0)\rangle$$

Given $|\psi(0)\rangle$ we compute,

$$\langle m|\psi(0)\rangle = \left(\frac{2}{L}\right)^{1/2} \int_0^L \sin\left(\frac{m\pi x}{L}\right) \psi(x,0)\, dx$$

We approximate using a few m only to get solution.