30-01-17

LECTURE #8 (PSO201A)

Linear Algebra

Background needed: (i) R. Shankar, chapter 1
(ii) Griffiths Appendix

- Definition of a linear vector space
- Matrixes and matrix operations (multiplication, transposition, etc..)
- Diagonalizing a matrix
- Eigen values and eigen vectors of a matrix
- Changing the basis of a matrix or vector

- Why need linear algebra?
  - Matrix representation of everything. States are column vectors, Operators are square matrices and operations are matrix operation.
- Why do it this way
  - Convenience for calculations, numerical modeling.

$f(x) \to$ can be represented as a vector.

1. Vectors (states), definition

- The 2D, 3D vectors are written as $\vec{A}$, $\vec{B}$, with an arrowhead.
- A more general vector is written as $|V\rangle$.

discrete: $|V\rangle = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{bmatrix} = v_1 \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} + v_2 \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix} + v_3 \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix} + \cdots = \sum_{i=1}^{n} v_i |i\rangle$; where $|i\rangle = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \end{bmatrix} \to i^{th}$ place

(for a discrete vector you pass on a discrete set of numbers in a basis)

- $|i\rangle$ are the basis vectors

Continuous: $|\psi\rangle = \begin{bmatrix} \psi(x_1) \\ \psi(x_2) \\ \psi(x_3) \\ \vdots \end{bmatrix} = \psi(x_1) \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ \vdots \end{bmatrix} + \psi(x_2) \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \\ \vdots \end{bmatrix} + \psi(x_3) \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix} + \cdots = \int \psi(x) |x\rangle \, dx$

where $|x\rangle = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \end{bmatrix} \to$ at location x

(for continuous vectors, you pass on a continuous set of numbers in a basis, called the function in that basis)

- $|x\rangle$ is the basis vector.

2. Linear Independence

A set of vectors $|1\rangle, |2\rangle, \ldots |n\rangle$ is said to be linearly independent if $\sum_{i=1}^{n} \alpha_i |i\rangle = 0$ has only the trivial solution

$\boxed{\alpha_i = 0 \text{ for all } i}$

or

$\boxed{\det D = 0}$, where D is the matrix consisting of the n vectors as its n columns

- Dimension: A vector space has dimension n if it can accomodate n linearly independent vectors.
- Basis: A set of n linearly independent vectors is called a basis. There can be more than one vector in a vector space and a basis need not be orthogonal.

Examples of basis vectors:

1. $\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix} \to$ linearly dependent

2. $\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \to$ linearly independent

3. $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \to$ linearly independent

Dimension:

A vector space has dimension n if it can accomodate n linearly independent vectors.

Basis: A set of n linearly independent vectors is called a basis. There can be more than one basis in a vector space and a basis need not be orthogonal.

~~Matrix representation of vectors~~

~~discrete:~~ $\cancel{|v\rangle = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{bmatrix} = v_1 \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} + v_2 \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix} + v_3 \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix} + \cdots = \sum_{i=0}^{n} v_i |i\rangle \; ; \; |i\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \rightarrow i^{th} \text{ place}}$

~~continuous:~~ $\cancel{|\psi\rangle = \begin{bmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_3) \\ \vdots \end{bmatrix} = \psi(x_1) \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ \vdots \end{bmatrix} + \psi(x_2) \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \\ \vdots \end{bmatrix} + \cdots = \int \psi(x)|x\rangle\, dx \; ; \; |x\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \rightarrow x^{th} \text{ location}}$

3. Inner Product & Dual space

scaler product: $\vec{A} \cdot \vec{B} = [A_1 \; A_2 \; A_3 \ldots A_n] \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_n \end{bmatrix} = A_1B_1 + A_2B_2 \cdots A_nB_n$

$= [\text{Transpose of } A] \text{ times } B$

inner product: of $|v\rangle$ & $|w\rangle$

$$= [v_1^* \; v_2^* \cdots \; v_n^*] \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = v_1^* w_1 + v_2^* w_2 \cdots v_n^* w_n$$

$= (\text{Transpose-conjugate of } |v\rangle) \text{ times } |w\rangle$

$= (\text{Adjoint of } |v\rangle) \text{ times } |w\rangle$

$= \langle v | w \rangle$ — bra v, ket w

$\langle \; | \; \rangle \equiv$ bracket

} due to Dirac

- $\langle v|$ or bra v is the dual space of ket v, or $|v\rangle$
- representation of vectors in the dual space

  discrete: If $|v\rangle = \sum_{i=0}^{n} v_i |i\rangle$ then $\langle v| = \sum_{i=0}^{n} v_i^* \langle i|$

  continuous: If $|\psi\rangle = \int \psi(x)|x\rangle dx$ then $\langle \psi| = \int \psi^*(x) \langle x| dx$
- $\langle v|w\rangle = \langle w|v\rangle^*$ [This is the main difference between the scalar and inner product]
- $\langle v|v\rangle \equiv$ norm or magnitude of the vector. If $\langle v|v\rangle = 1$ means a normalised vector.
- $\langle v|w\rangle = 0 \Rightarrow$ vectors $|v\rangle$ and $|w\rangle$ orthogonal

~~writing the inner product~~:

4 Orthonormality

In quantum mechanics, we like to work in an orthonormal basis. This means that the vector (state) should have unit norm (or should be normalized) and the basis vectors should be all orthogonal.

discrete: $|V\rangle = \sum_{i=1}^{n} v_i |i\rangle$

(i) $\langle i|j\rangle = 0$ if i & j are two different basis vectors

(ii) $\langle V|V\rangle = 1$

(ii) $\Rightarrow \quad \langle V|V\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} v_i^* v_j \langle i|j\rangle = 1$

$\Rightarrow \langle i|j\rangle = 1$ if $i=j$

such that $\sum_{i=1}^{n} |v_i|^2 = 1$

So, we get $\langle i|j\rangle = \delta_{ij} = 1$ if $i=j$; $= 0$ if $i\neq j$ } The basis vectors of this type that are normalizable to unity are called proper vectors

Continuous: $|\psi\rangle = \int \psi(x)|x\rangle dx$

(i) $\langle x|x'\rangle = 0$ if $x\neq x'$

(ii) $\langle \psi|\psi\rangle = 1$

(ii) $\Rightarrow \quad \langle\psi|\psi\rangle = \iint \psi^*(x)\psi(x') \langle x|x'\rangle dx\, dx' = 1$

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

such that $\langle\psi|\psi\rangle = \int \psi^*(x)\psi(x)dx = 1$

So, we get $\langle x|x'\rangle = \delta(x-x') = \infty$ if $x = x'$; $= 0$ if $x\neq x'$ } The basis vectors of this type that are normalizable to a dirac-delta function are called improper vectors.

(i) $\delta(x-x') = \lim_{\sigma\to 0} \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-x')^2}{2\sigma^2}\right]$

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

* The vector space of both the proper and improper vectors is called the physical Hilbert space

writing the inner product in an orthonormal basis

discrete: $\langle V|W\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} v_i^* w_j \langle i|j\rangle = \sum_{i=1}^{n} v_i^* w_i$

$\langle V|V\rangle = 1 \Rightarrow \sum_{i=1}^{n} |v_i|^2 = 1 \Rightarrow P_i = |v_i|^2$ is the probability that the vector $|V\rangle$ is along $|i\rangle$

continuous: $\langle\psi_1|\psi_2\rangle = \iint \psi_1^*(x)\, \psi_2(x')\, \langle x|x'\rangle\, dx\, dx'$

$= \int \psi_1^*(x)\psi_2(x)\, dx$

So, $\langle\psi|\psi\rangle = \int \psi^*(x)\psi(x)dx = \int |\psi(x)|^2 dx$

$\because \langle\psi|\psi\rangle = 1 \Rightarrow \int |\psi(x)|^2 dx = 1$

- In Q-mech. $\psi(x)$ is called the coeff^n in the x-basis and $|\psi(x)|^2$ is the probability density at x.
- So the total probability is equal to 1 and $p(x) = |\psi(x)|^2$ is the probability density that the vector is along $|x\rangle$.

5 [redacted] Completeness of an orthonormal basis

Completeness means that an arbitrary state (vector) can be can be completely expressed in terms of the basis vectors.

discrete:
$$|V\rangle = \sum_{i=1}^{n} v_i |i\rangle \quad \text{where} \quad v_i = \langle i|V\rangle$$

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

$$\Rightarrow \boxed{\sum_{i=1}^{n} |i\rangle\langle i| = I} \rightarrow \text{Identity matrix}$$

- This is the completeness condition that the discrete basis vectors would have to satisfy.

continuous:
$$|\psi\rangle = [redacted] \int \psi(x)|x\rangle dx \quad \text{where} \quad \psi(x) = \langle x|\psi\rangle$$

$$\therefore \quad |\psi\rangle = \int \langle x|\psi\rangle |x\rangle dx = \int |x\rangle\langle x|\psi\rangle dx = \left(\int |x\rangle\langle x| dx\right)|\psi\rangle$$

$$\Rightarrow \boxed{\int |x\rangle\langle x| dx = I}$$

- I is the identity matrix
- Completeness condition in a continuous basis.
-

6. Change of basis

discrete:
$$|V\rangle = \sum_{i=1}^{n} v_i |i\rangle \; ; \quad \text{where} \quad v_i = \langle i|V\rangle \quad — (1)$$

we want to write the state in a new basis $|i'\rangle$, that is:

$$|V\rangle = \sum_{i=1}^{n} v_i' |i'\rangle \; ; \quad \text{where} \quad v_i' = \langle i'|V\rangle = ?$$

$\langle i'| \times (1)$
$$\Rightarrow \therefore \langle i'|V\rangle = \sum_{i=1}^{n} \langle i'|v_i|i\rangle = \sum_{i=1}^{n} v_i \langle i'|i\rangle$$

$$\Rightarrow \boxed{v_i' = \sum_{i=1}^{n} v_i \langle i'|i\rangle}$$

So, if we know the inner product of the two basis vectors, one can write the state in the new basis

Continuous:
$$|\psi\rangle = \int \psi(x)|x\rangle dx \quad — (1) \rightarrow \text{vector (state) in the position basis}$$

$\rightarrow$ $\psi(x)$ in the ~~pos~~ wavefunction in the position basis.

we want to write this in a new basis, say the momentum basis $|p\rangle$

$$\therefore \quad |\psi\rangle = \int \psi(p)|p\rangle dx$$

$\langle p| \times (1)$
$$\Rightarrow \quad \langle p|\psi\rangle = \int \psi(x)\langle p|x\rangle dx$$

$$\Rightarrow \boxed{\psi(p) = \int \psi(x)\langle p|x\rangle dx}$$

- knowing the inner product $\langle p|x\rangle$, one can write the vector in the momentum basis

* $|x\rangle$ is the eigenket of the position operator $\hat{x}$.

* $|p\rangle$ is the eigenket of the momentum operator $\hat{P}$.

Operators

$$\hat{\Omega}|\psi\rangle = |\psi'\rangle$$

1. Basics

⇒ An operator $\hat{\Omega}$ is an instruction for transforming any vector (state) $|\psi\rangle$ into another vector $|\psi'\rangle$

⇒ Operator are represented by square metrices. The inverse of an operator $\hat{\Omega}$ is $\hat{\Omega}^{-1}$. The adjoint (transpose-conjugate) of an operator is $\hat{\Omega}^{\dagger}$, where † is called the dagger.

Adjoint

$a \longrightarrow a^*$

$|\psi\rangle \longrightarrow \langle\psi|$

$\langle\psi| \longrightarrow |\psi\rangle$

$\hat{\Omega} \longrightarrow \hat{\Omega}^{\dagger}$

$\hat{\Omega}^{\dagger} \longrightarrow \hat{\Omega}$

$\langle\psi|\Omega|\psi'\rangle \longrightarrow \langle\psi'|\hat{\Omega}^{\dagger}|\psi\rangle$

2. Matrix representation of an operator

- Operaters are represented in a basis, discrete or continuous. So for a given basis the matrix element of an operator is written as:

discrete: $\langle i|\hat{\Omega}|j\rangle \equiv \Omega_{ij}$

continuous $\langle x|\hat{\Omega}|x'\rangle \equiv \hat{\Omega}_{xx'}$

⇒ So as long as one knows the how an operator acts on a basis vector $[\hat{\Omega}|j\rangle = ?]$ and also the inner product of the basis vectors $[\langle i|j\rangle = ?]$, one can find the matrix element in that particular basis of a given operator.

3. Types of Operators

⇒ In quantum mechanics a system is reprented by a state vector. The evolution of the system (rotation, propagation, time evolution) as well as the determination of a physical observable (position, momentum, etc.) happen through the action of an operator on the state.

Correspondingly, we have two kinds of operators.

(i) Unitary operator (evolution) ⇒ $\hat{U}^{\dagger} = \hat{U}^{-1}$

- The evolution of a quantum system is represented through the action of a unitary operator on the state
- The eigenvalues of a unitary operator are complex numbers with unit modules and the eigen vectors are mutually orthogonal ⟶ Prove !!

(ii) Hermitian operator: $\hat{\Omega}^{\dagger} = \hat{\Omega}$ $\left[\Rightarrow \Omega^{*}_{x'x} = \Omega_{xx'}\right] \rightarrow$ Prove !!
(physical observables)

- Corresponding to every physical observable, there is a Hermitian operator.
- The eigenvalue of a Hermitian operator is real !! —— prove !

  → This is definitely a very desired property because any physical quantity is always real and not complex.
- Schrödinger equation that governs the dynamics of a quantum system is also an operator equation

  $\hat{H}|\psi\rangle = i\hbar \frac{\partial}{\partial t}|\psi\rangle$; $\hat{H}$ is called Hamiltonian and is a hermitian operator.

4. Matrix representation of operators in the position basis.

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

what is $|x\rangle$?

↳ position eigenvector or the position basis vector

This means that there is a position operator $\hat{x}$, which acting on $|x\rangle$ will give out x as the eigenvalue, that is

$$\underbrace{\hat{X}}_{\text{position operation}}|x\rangle = \underbrace{x}_{\text{eigenvalue}}|x\rangle$$

∴ The matrix representation of position operator in the position basis

$X_{xx'} = \langle x|\hat{X}|x'\rangle = \langle x|x'|x'\rangle = x'\langle x|x'\rangle = x'\delta(x-x')$

∴ $\boxed{X_{xx'} = x'\delta(x-x')}$

Is $\hat{X}$ Hermitian ?

$X^{*}_{x'x} = \left(x\delta(x'-x)\right)^{*} = x\delta(x-x') = x'\delta(x-x') = X_{xx'}$ $\left[\delta(x-x') = \delta(x'-x)\right.$ ↳ even f^n $\left.\right]$

$\Rightarrow \hat{X}$ is Hermitian

⇒ ~~Without proving let us look~~
what about other operators?

→ ~~Let us consider the momentum operator $\hat{P}$.~~ Without proving the result, lets state that the momentum operator in the position basis is written as

$$\boxed{P_{xx'} = \langle x|\hat{P}|x'\rangle = -i\hbar\,\delta(x-x')\frac{d}{dx'}}$$

~~$\langle p|p'\rangle = \delta(p-p')$~~

$\hat{P}|p\rangle = p|p\rangle$

↳ eigenvalue (momentum)
↳ moment op.
↳ momentum eigenvector

Is $\hat{P}$ Hermitian ?

$P^{*}_{x'x} = \left[-i\hbar\,\delta(x'-x)\frac{d}{dx}\right]^{*} = i\hbar\,\delta(x'-x)\frac{d}{dx} = -i\hbar\,\delta(x'-x)\frac{d}{dx'} = -i\hbar\,\delta(x-x')\frac{d}{dx'}$

$= P_{xx'}$

$\left[\frac{d}{dx}\delta(x-x') = \frac{d}{dx'}\delta(x-x')\right]$ $\left[\delta(x-x') = \delta(x'-x)\right]$

$\Rightarrow \hat{P}$ is hermitian

Change of Basis

We now have the basic understanding about the states and operator. We also know how to represent a state and an operator in a given basis. Now suppose we know the representation in a given basis, can we find the matrix representation in some other basis?

discrete:

$$|v\rangle = \sum_{i=1}^{n} v_i |i\rangle \qquad \text{(I)} \qquad \text{where } v_i = \langle i|v\rangle$$

we want to write the state in a new basis $|i'\rangle$, that is

$$|v\rangle = \sum_{i=1}^{n} v_i' |i'\rangle, \quad \text{where } v_i' = \langle i'|v\rangle = ?$$

$$\langle i'| \times \text{(I)} \Rightarrow \quad \langle i'|v\rangle = \sum_{i=1}^{n} \langle i'|v_i|i\rangle = \sum_{i=1}^{n} v_i \langle i'|i\rangle$$

$$\therefore \quad \boxed{v_i' = \sum_{i=1}^{n} v_i \langle i'|i\rangle}$$

→ so if we know the inner product of the two basis vectors, one can write the state in the new basis.

Continuous:

$$|\psi\rangle = \int \psi(x)\, |x\rangle\, dx \quad \text{(II)}; \quad \text{where } \psi(x) = \langle x|\psi\rangle$$

we want to write the state in the momentum basis, that is

$$|\psi\rangle = \int \psi(p)\, |p\rangle\, dp \;;\; \text{where } \psi(p) = \langle p|\psi\rangle \;?$$

$$\langle p| \times \text{(II)} \Rightarrow \quad \langle p|\psi\rangle = \int \psi(x) \langle p|x\rangle\, dx$$

$$\therefore \quad \boxed{\psi(p) = \int \psi(x) \langle p|x\rangle\, dx}$$

So, if we know the inner product $\langle p|x\rangle$, we can write the vector in the momentum basis

⇒ how to find $\langle p|x\rangle$?

⇒ we know that $\hat{p}|p\rangle = p|p\rangle$

or, $\langle x|\hat{p}|p\rangle = p\langle x|p\rangle$

expanding in the $|x'\rangle$ basis, we get

$$\int \langle x|\hat{p}|x'\rangle\langle x'|p\rangle\, dx' = p\langle x|p\rangle$$

or, $$\int -i\hbar\,\delta(x-x')\frac{d}{dx}\langle x'|p\rangle\, dx' = p\langle x|p\rangle$$

or, $$-i\hbar\frac{d}{dx}\langle x|p\rangle = p\langle x|p\rangle \Rightarrow \quad \langle x|p\rangle = A e^{\frac{ipx}{\hbar}} \;\&\; \langle p|x\rangle = A^{*} e^{-ipx/\hbar}$$

what is A?

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

—

$\therefore \int \langle x|p\rangle\langle p|x'\rangle\, dp = \delta(x-x')$

$$\int_{-\infty}^{\infty} e^{-ip(x-x')} = 2\pi\,\delta(x-x')$$

or, $|A|^2 \int e^{i(x-x')p/\hbar}\, dp = \delta(x-x')$

or, $|A|^2\, 2\pi\hbar\, \delta(x-x') = \delta(x-x')$

$\Rightarrow \quad A = \dfrac{1}{\sqrt{2\pi\hbar}}$

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

$\therefore \quad \psi(p) = \langle p|\psi\rangle = \int \psi(x)\langle p|x\rangle\, dx = A\int \psi(x)\, e^{-ipx/\hbar}\, dx$

$$\therefore \boxed{\begin{aligned} \psi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x)\, e^{-ipx/\hbar}\, dx \\ \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int \psi(p)\, e^{ipx/\hbar}\, dp \end{aligned}}$$

$|\psi\rangle \equiv$ state of the system

$\psi(x) \equiv$ ~~position~~ wavefunction in the position basis

$\psi(p) \equiv$ wave-function in the momentum basis.

Expectation value of an operator

discrete: $\hat{\Omega}|\omega_i\rangle = \omega_i|\omega_i\rangle$ • Suppose there are n such eigenvalues and eigen vectors

*Suppose the state is not one of the eigen state but
~~For~~ a given state $|V\rangle$:

$$|V\rangle = \sum_{i=1}^{n} c_i|\omega_i\rangle \quad ; \quad c_i = \langle\omega_i|V\rangle$$

$\boxed{\text{* Also, } |V\rangle = \sum v_i|i\rangle \text{ is another decomposition of } |V\rangle \text{ in some other eigen basis}}$

$$P_{\omega_i} = |c_i|^2 = \langle\omega_i|V\rangle\langle\omega_i|V\rangle^* = \langle\omega_i|V\rangle\langle V|\omega_i\rangle$$

→ Summarize adjoint operation

The expectation value is defined as

$$\langle\hat{\Omega}\rangle = \sum_{i=1}^{n}\omega_i P_{\omega_i} = \sum_{i=1}^{n}\omega_i\langle\omega_i|V\rangle\langle V|\omega_i\rangle = \sum_{i=1}^{n}\omega_i\langle V|\omega_i\rangle\langle\omega_i|V\rangle$$

$$= \sum_{i=1}^{n}\langle V|\hat{\Omega}|\omega_i\rangle\langle\omega_i|V\rangle = \langle V|\hat{\Omega}|V\rangle$$

$$\therefore \boxed{\langle\hat{\Omega}\rangle = \langle V|\hat{\Omega}|V\rangle}$$ → expectation value is basis independent

Continuous:

$\Omega|\omega\rangle = \omega|\omega\rangle$ • Continuous set of eigen values and eigen vectors

For a given state $|\psi\rangle$:

$$|\psi\rangle = \int\psi(\omega)|\omega\rangle\, d\omega \quad ; \quad \psi(\omega) = \langle\omega|\psi\rangle$$
$$p(\omega) = \psi(x)\psi^*(x) = \langle\omega|\psi\rangle\langle\psi|\omega\rangle$$

The expectation value is

$$\langle\hat{\Omega}\rangle = \int_{-\infty}^{\infty}\omega\, p(\omega)\,d\omega = \int_{-\infty}^{\infty}\omega\langle\omega|\psi\rangle\langle\psi|\omega\rangle\,d\omega$$

$$= \int_{-\infty}^{\infty}\omega\langle\psi|\omega\rangle\langle\omega|\psi\rangle\,d\omega = \int_{-\infty}^{\infty}\langle\psi|\hat{\Omega}|\omega\rangle\langle\omega|\psi\rangle\,d\omega$$

$$= \langle\psi|\hat{\Omega}|\psi\rangle$$

$$\therefore \boxed{\langle\hat{\Omega}\rangle = \langle\psi|\hat{\Omega}|\psi\rangle}$$ → basis independent definition

Expectation value in the position basis

$$\langle\hat{\Omega}\rangle = \langle\psi|\hat{\Omega}|\psi\rangle = \iint\langle\psi|x\rangle\langle x|\hat{\Omega}|x'\rangle\langle x'|\psi\rangle\,dx\,dx'$$

$$\boxed{\langle\hat{\Omega}\rangle = \iint\psi^*(x)\,\hat{\Omega}_{xx'}\,\psi(x')\,dx\,dx'}$$

⇒ In quantum mechanics any general operator can be written as a function of $\hat{X}$ and $\hat{P}$ operators, that is,

$$\hat{\Omega} = f(\hat{X},\hat{P})$$

$$\therefore \hat{\Omega}_{xx'} = \langle x|\Omega|x'\rangle = \langle x|f(\hat{X},\hat{P})|x'\rangle = \delta(x-x')\left(x', -i\hbar\frac{\partial}{\partial x'}\right)$$

$$\therefore \langle\hat{\Omega}\rangle = \iint\psi^*(x)\delta(x-x')f\left(x', -i\hbar\frac{\partial}{\partial x'}\right)\psi(x')\,dx\,dx'$$

$$\boxed{\langle\hat{\Omega}\rangle = \int\psi^*(x)f\left(x, -i\hbar\frac{\partial}{\partial x}\right)\psi(x)\,dx}$$ — expectation value in the position basis

Also $$\boxed{\langle\hat{\Omega}\rangle = \int\psi^*(p)f\left(i\hbar\frac{\partial}{\partial p}, p\right)\psi(p)\,dp}$$ — expectation value in the momentum basis

Commutator and the Heisenberg Uncertainty relation

The commutator of two operators $\hat{\Omega}$ and $\hat{\Lambda}$ is defined as

$$[\hat{\Omega}, \hat{\Lambda}] \equiv \hat{\Omega}\hat{\Lambda} - \hat{\Lambda}\hat{\Omega} \quad \text{— commutator}$$

$$\{\hat{\Omega}, \hat{\Lambda}\} \equiv \hat{\Omega}\hat{\Lambda} + \hat{\Lambda}\hat{\Omega} \quad \text{— anti-commutator}$$

- $[\hat{\Omega}, \hat{\Lambda}] = 0 \Rightarrow$ $\hat{\Omega}$ and $\hat{\Lambda}$ operators are compatible. This means that the order of operation of $\hat{\Omega}$ and $\hat{\Lambda}$ does not change the measurement outcome

- $[\hat{\Omega}, \hat{\Lambda}] \neq 0 \Rightarrow$ $\hat{\Omega}$ and $\hat{\Lambda}$ are not compatible. The order of operation of $\hat{\Omega}$ and $\hat{\Lambda}$ does change the measurement outcome.

$\Rightarrow$ For every pair of ~~incompatible~~ non-commuting operators, there is an uncertainty relation that needs to be satisfied

Uncertainty:

$$\Delta\Omega \equiv \langle (\hat{\Omega} - \langle \Omega \rangle)^2 \rangle^{\frac{1}{2}}$$
$$= \sqrt{\langle \hat{\Omega}^2 \rangle - \langle \hat{\Omega} \rangle^2}$$

Pair of ~~[illegible]~~ non-commuting operators	Heisenberg uncertainty relation
$\hat{X}$ & $\hat{P}$; $[\hat{X}, \hat{P}] = i\hbar\hat{I}$	$\Delta x \Delta P \geq \frac{\hbar}{2}$
t and E	$\Delta t \Delta E \geq \frac{\hbar}{2}$

$*$ $\langle x | f(\hat{X}, \hat{P}) | x' \rangle = \delta(x - x')\, (x' - i\hbar \frac{\partial}{\partial x'})$

Prove; also given as a homework problem

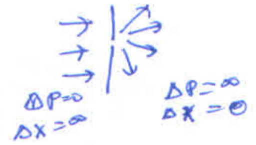
$\Rightarrow$ Prove the commutation relation $[\hat{X}, \hat{P}] = i\hbar\hat{I}$

$\Rightarrow$ Prove the Heisenberg uncertainty relation $\Delta\hat{X}\Delta\hat{P} \geq \frac{\hbar}{2}$

$\Rightarrow$ Position - momentum uncertainty

$$\Delta\hat{X}\Delta\hat{P}_x \geq \frac{\hbar}{2} \quad \text{similarly} \quad \Delta\hat{Y}\Delta\hat{P}_y \geq \frac{\hbar}{2} \;\&\; \Delta\hat{Z}\Delta\hat{P}_z \geq \frac{\hbar}{2}$$

$$\Delta\hat{X} = 0 \Rightarrow \Delta\hat{P}_x = \infty$$



$\rightarrow$ time - energy uncertainty relation

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$

$\rightarrow$ angle - OAM uncertainty relation

$$\Delta\theta \Delta l \geq \frac{\hbar}{2}$$

Ex. $\Delta t = 10^{-8}$ sec (atom excitation time)

$$\Delta E \geq \frac{\hbar}{2\Delta t} = \frac{6.6 \times 10^{-34}}{2\pi \times 2 \cdot 10^{-8}} \sim \frac{3.3}{6} \times 10^{-26}\ \text{J} = 0.5 \times 10^{-26}$$

$$h\frac{c}{\lambda} = \frac{6.6 \times 10^{-34} \times 3 \times 10^{8}}{500 \times 10^{-9}} = \frac{6.6 \times 3}{5} \times 10^{-19} \approx 4 \times 10^{-19}\ \text{J}.$$

Schrödinger Equation

The schrödinger equation in the Dirac notation is written as

$$\hat{H}(t)\,|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle$$

→ H is the Hamiltonian of the system

→ $H = K.E + P.E$

we write this equation in the position basis.

$$\langle x|\hat{H}(t)|\psi(t)\rangle = i\hbar \,\langle x|\frac{d}{dt}|\psi(t)\rangle$$

$$\langle x|\hat{H}(t)|\psi(t)\rangle = i\hbar \frac{d}{dt}\langle x|\psi(t)\rangle$$

or, $$\int \langle x|\hat{H}(t)|x'\rangle\langle x'|\psi(t)\rangle\,dx' = i\hbar\frac{d}{dt}\psi(x,t)$$

or, $$\int \langle x|\hat{H}(t)|x'\rangle\,\psi(x',t)\,dx' = i\hbar\frac{d}{dt}\psi(x,t)$$

$$\langle x|\hat{H}(t)|x'\rangle = ? \quad = \delta(x-x')\,H\left(x, -i\hbar\frac{\partial}{\partial x'}, t\right)$$

$[H = K.E. + P.E.]$

or, $$H\left(x, -i\hbar\frac{\partial}{\partial x}, t\right)\psi(x,t) = i\hbar\frac{d}{dt}\psi(x,t)$$

Now $H = K.E + P.E$

$$\therefore H\left(x, -i\hbar\frac{\partial}{\partial x}, t\right) = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + V(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$$

$$\therefore \boxed{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\psi(x,t) = i\hbar\frac{d}{dt}\psi(x,t)}$$

— This is the Schrödinger equation in the $|x\rangle$ basis

~~[illegible]~~ Lecture #3

$$\left[-\frac{\hbar^2}{2m} + V(x,t)\right]\psi(x,t) = i\hbar\frac{d}{dt}\psi(x,t)$$

- ~~Quantity~~ Equation in terms of the wavefunction
- Describes wave-particle dual systems, wavef^n.
- Aim: Given $\psi(x_0, t_0)$ at $t=t_0$, how to find the wave-function $\psi(x_1, t_1)$ at $t = t_2$.

- Newton's equation $m\frac{d^2x}{dt^2} = \frac{dp}{dt}$
  - describes particle
  - equation in terms of x & p
  - Aim: given (x_0, p_0) at $t=t_0$ find out (x_1, p_1) at $t=t_1$
- Wave equation: $\nabla^2 E = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}$; $\nabla^2 B = \frac{1}{c^2}\frac{\partial^2 B}{\partial t^2}$
  - describes waves
  - equation in term of E & B
  - Aim: ~~Find out~~ (E_0, B_0) at $t=t_0$, find out (E_1, B_1) at $t=t_1$

Properties of $\psi(t)$

(i) It must be a single-valued wavefunction

(ii) It must be continuous

(iii) It must be square-integrable $\int|\psi(x)|^2 dx < \infty$

(iv) ~~[illegible]~~ The formulation of the theory must be consistent with de-Broglie-Einstein postulates

(v) ~~The theory must~~ If $\psi_1(x,t)$ and $\psi_2(x,t)$ are two solutions of SE then $\psi(x,t) = c_1\psi_1(x,t) + c_2\psi_2(x,t)$ must also be a solution to SE. This comes from ~~the~~ linearity of SE

(vi) $\psi(x,t)$ is complex-valued f^n.

→ $\psi(x,t) = A\sin(kx-\omega t)$ is not a solution to the SE eq. (although $A\sin(kx-\omega t)$ is a solution of the wave-equation)

→ $\psi(x,t) = e^{i(kx-\omega t)}$ is a solution

→ $\psi^*(x,t) = e^{-i(kx-\omega t)}$ is not a solution to the SE equation but to its conjugate equation $\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right]\psi^*(x,t) = -i\hbar\frac{d}{dt}\psi^*$

$$\frac{\partial^2}{\partial x^2}e^{+i(kx-\omega t)} = (ik)^2 e^{i(kx-\omega t)} = -k^2 e^{i(kx-\omega t)}$$

$$-i\hbar\frac{d}{dt}e^{i(kx-\omega t)} = (-i\hbar)(-i\omega) = \hbar\omega$$

$$\Rightarrow -\frac{\hbar^2}{2m}(-k^2) + V = \hbar\omega$$

~~If V=0~~ or $\frac{\hbar^2k^2}{2m} + V = \hbar\omega$

or $\boxed{\frac{p^2}{2m} + V = \hbar\omega} \Rightarrow \boxed{K.E + V = E}$