2 Denisty Matrix Refresher Course Lecture

Univ of Hyderabad 2024

- Recall states of a quantum system are specified by a vector in a vector space
- The state vector contains all information about the system
- There are systems where we may not have sufficient information to know the state vector.

For such systems* the quantum state is specified by density matrix

---

Examples

① Gas molecules in a container

$\Psi = \Psi(x_1, x_2 \cdots x_N) \quad N \sim 10^{23}$

At temp T : $p(E) \sim e^{-\beta E}/Z$

canonical ensemble

(2) A beam of electrons with spins oriented randomly

(3) Unpolarized light.

Q. What information is needed to specify state completely?

Landau Lifshitz QM

" We will now formulate the meaning of complete description of a state in quantum mechnaics ......" Sec 1 page 5

State vector → Pure States

Mixed State → Density Matrix

What do we want to compute? $\longrightarrow$ Probabilities and average values

If system is described by ψ,

pure state, then

1. Prob that it will be found in state ϕ is $|\langle\psi|\phi\rangle|^2$

2. Prob of X having a value λ_k is

$$|\langle u_k|\psi\rangle|^2$$

$\phi \rightarrow u_k$ eigenvector of $\hat{X}$ with eigenvalue λ_k

3. Average value of X

$$\langle X\rangle_\psi = \langle\psi|\hat{X}|\psi\rangle$$

We will now jump to the definition of density matrix and then relate it to the above statements for pure states.

What is Density Matrix ? It is an operator $\hat{\rho}$ such that

(1) it is hermitian $\hat{\rho}^{+} = \rho$

(2) $Tr\,\rho = 1$

(3) ρ is positive definite

Remark:

If $\rho^2 = \rho$ then the state represented by ρ is a pure state

$\rho^2 \neq \rho \Rightarrow$ mixed state

We need to understand positive defniteness and trace of an operator and more ....

Positive operator

ρ is a positive if for all $|\psi\rangle$

$$\langle\psi|\hat{\rho}|\psi\rangle \geq 0$$

Trace of an operator

Think of an operator as a matrix

Start with an Orthonormal Basis $\{\psi_n\}$

$$\hat{\rho} \longrightarrow (\rho)_{mn} = \langle\psi_m|\hat{\rho}|\psi_n\rangle$$

$$\text{Trace}\,\rho = \sum_n \langle\psi_n|\hat{\rho}|\psi_n\rangle$$

$$\text{or } \langle n|\hat{\rho}|n\rangle$$

Trace AB

$$= \sum_m (AB)_{mm}$$

$$= \sum_{m,n} A_{mn} B_{nm}$$

Just like matrices

A notation : you will see objects

$|\psi\rangle\langle\psi| \longrightarrow$ what is this object?

Recall

$$\sum_n |n\rangle\langle n| = \hat{I}$$

In general $|\chi\rangle\langle\phi|$ is an operator such that

$$(|\chi\rangle\langle\phi|)\;|\psi\rangle = \underbrace{\langle\phi|\psi\rangle}_{\text{complex number}}\;|\chi\rangle$$

If λ is an eigenvalue of $\hat{\rho}$ and if $\hat{\rho}^2 = \hat{\rho}$ then

$$\lambda^2 = \lambda \Rightarrow \lambda = 0, 1$$

Find eigen vector of ρ with eigen value 1. Solve

$$\rho|?\rangle = |?\rangle$$

then solution gives the state vector $|\psi\rangle$ //

$\hat{\rho}$ represents a pure state if and only if $\hat{\rho}^2 = \rho$

Q. $|\psi\rangle$ is unique, eigen value 1 of ρ is non degenerate, why?

Hint: $\mathrm{Tr}\rho = 1$ = sum of eigenvalues

For a pure state represented by $|\psi\rangle$

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

one can show that

$$\hat{\rho}^{\dagger} = \hat{\rho}$$

$$\mathrm{Tr}\,\hat{\rho}\hat{x} = \langle\psi|\hat{x}|\psi\rangle$$

= average value of $\hat{x}$

$$\rho^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|)$$

$$= |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{=1}\langle\psi|$$

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

For pure state $|\psi\rangle$

$$\rho^2 = \rho$$

converse is also true

Mixed state Examples

1) Consider a beam of polarized light $\longrightarrow$ Photon $\longrightarrow$ Pure state

2) unpolarized light photons $\longrightarrow$ mixed state

Electron beam

all spins along z axis
pure state

$\uparrow$ prob of spin up p_1 $\quad S_z = +1$

$\downarrow$ prob of spin down p_2 $\quad S_z = -1$

$$\hat{\rho} = p_1 |1\rangle\langle 1| + p_2 |-1\rangle\langle -1|$$

In matrix notation

$$\hat{\rho} = p_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \underbrace{1 \quad 0} + p_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \underbrace{0 \quad 1}$$

$$= \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix}$$

check $\langle S_z \rangle = p_1 - p_2$?

$$\langle S_z \rangle = \mathrm{Tr}(\rho\, S_z)$$

$$= \mathrm{Tr}\begin{pmatrix} p_1 & \\ & p_2 \end{pmatrix}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

$$= p_1 - p_2$$

In general

for $\psi_1, \psi_2, \psi_3, \ldots \psi_n, \ldots$

prob $p_1, p_2, p_3 \ldots p_n$

Then

$$\hat{\rho} = p_1 |\psi_1\rangle\langle\psi_1| + p_2 |\psi_2\rangle\langle\psi_2| + \ldots$$

$$= \sum p_n |\psi_n\rangle\langle\psi_n|$$

$$\langle x \rangle = \sum p_n \langle\psi_n| \hat{x} |\psi_n\rangle$$

as expected.

If $|\psi_1\rangle \longrightarrow \rho_1$

$|\psi_2\rangle \longrightarrow \rho_2$

then what is $|\langle\psi_1|\psi_2\rangle|^2$

Ans $|\langle\psi_1|\psi_2\rangle|^2$

$= Tr(\rho_1 \rho_2)$

Time evolution $\rightarrow$ Hamiltonian H

$$i\hbar \frac{\partial}{\partial t} |\psi_n t\rangle = H |\psi_n t\rangle$$

$$-i\hbar \frac{\partial}{\partial t} \langle \psi_n t| = \langle \psi_n t| H$$

$$i\hbar \frac{\partial}{\partial t} \rho = i\hbar \frac{\partial}{\partial t} \sum p_n |\psi_n\rangle\langle\psi_n|$$

$$= \sum H p_n |\psi_n\rangle\langle\psi_n|$$

$$- p_n |\psi_n\rangle\langle\psi_n| H$$

$$= H\rho - \rho H$$

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho]$$

von Neuman Eqn

- Don't confuse with Heisenberg equation $i\hbar \frac{d}{dt} \hat{X} = [X, H]$

$$= -[H, X]$$

Matrix mechanics eqn of motion for operators

Example For a spin 1/2 system

$$\rho = (I + s\,\hat{n}\cdot\vec{\sigma})/2$$

(a) What values of s are allowed?
(b) When is it a pure state?
(c) Find spin direction when s corresponds to a pure state
(d) Find average of
(i) S_z (ii) S_x (iii) $\hat{m}\cdot\vec{S}$

$\hat{n}, \hat{m} \rightarrow$ unit vectors

Show that

$$\mathrm{Tr}\,\rho^2 \begin{cases} =1 & \text{for pure state} \\ <1 & \text{for mix state} \end{cases}$$