We shall discuss the following:

→ Density operators

→ Composite systems

→ Reduced Density operators.

References:

(1) Nielsen & Chuang, Quantum Computation and Information

(2) Breuer & Petruccione, The theory of Open Quantum Systems

Basic Structure of Quantum Mechanics:

* System $\xrightarrow{\text{Associated}}$ Hilbert Space (H)

  State $\xrightarrow[\text{Specification}]{\text{Complete}}$ $|\psi\rangle \in H$ $\quad \because \quad \langle\psi|\psi\rangle = 1.$

* Observables $\longrightarrow$ Hermitian operators on H

  Expectation $\longrightarrow$ $\langle\hat{O}\rangle \equiv \langle\psi|\hat{O}|\psi\rangle$

* Dynamics $\longrightarrow$ $i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$

  $\hat{H} \longrightarrow$ Hamiltonian $\qquad |\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle.$

→ The ~~above~~ Density Matrices! structure is not enough to handle situations with incomplete information, i.e., if we cannot specify the state of the system completely.

→ In the context of OPEN QUANTUM SYSTEMS, we typically encounter the following:

* System can exist in a number of states $\{|\psi_i\rangle\}$ with respective probabilities $\{P_i\}$.

i.e., An ensemble $\{(|\psi_i\rangle, P_i)\}$.

$\sum_i P_i = 1.$

$\downarrow$ Need not be orthogonal

$\langle\psi_i|\psi_i\rangle = 1.$

Example (1):

Consider the hilbert space of a Spin $-\frac{1}{2}$ system spanned by $\{ |\downarrow\rangle, |\uparrow\rangle \}$.

Let us say the system can exist in states $\{ \frac{1}{\sqrt{2}}(|\downarrow\rangle + |\uparrow\rangle), \frac{1}{\sqrt{2}}(|\downarrow\rangle - |\uparrow\rangle), |\downarrow\rangle, |\uparrow\rangle \}$ with respective probabilities $\{ \frac{1}{3}, \frac{1}{3}, \frac{1}{6}, \frac{1}{6} \}$.

Esemble: $\{ (\frac{1}{\sqrt{2}}[|\downarrow\rangle + |\uparrow\rangle], \frac{1}{3}), (\frac{1}{\sqrt{2}}[|\downarrow\rangle - |\uparrow\rangle], \frac{1}{3}),$
$(|\downarrow\rangle, \frac{1}{6}), (|\uparrow\rangle, \frac{1}{6}) \}$.

→ How to compute the averages / expectation values of an observable $\hat{O}$ if the system's state is specified by an ensemble $\{(|\psi_i\rangle, P_i)\}$?

* We proceed by sampling the ensemble:

- Pick a state $|\psi_i\rangle$ with probability P_i.

- Expectation value of $\hat{O}$ in this state → $\langle\psi_i|\hat{O}|\psi_i\rangle$.

- Generate enough samples and sum over the samples to get ⟶ $\langle\hat{O}\rangle = \sum_i \langle\psi_i|\hat{O}|\psi_i\rangle P_i$.

* The result for $\langle \hat{O} \rangle$ alone has two averages:

$$\langle \hat{O} \rangle = \sum_i \underbrace{\langle \psi_i | \hat{O} | \psi_i \rangle}_{\text{QM average}} P_i$$

Statistical average

Consider a complete orthonormal set $\{ |x_i\rangle \}$ on $\mathcal{H}$.

$$\sum_j |x_j\rangle\langle x_j| = \mathbb{1}.$$

→ Rewrite:

$$\langle \hat{O} \rangle = \sum_i \langle \psi_i | \mathbb{1} \, \hat{O} | \psi_i \rangle P_i = \sum_j \sum_i \langle \psi_i | x_j \rangle \underbrace{\langle x_j | \hat{O} | \psi_i \rangle P_i}$$

$$= \sum_j \langle x_j | \hat{O} \left[\sum_i |\psi_i\rangle P_i \langle \psi_i| \right] |x_j\rangle.$$

* Define an object called as DENSITY OPERATOR

or

DENSITY MATRIX,

as

$$\hat{\rho} = \sum_i |\psi_i\rangle P_i \langle \psi_i| \quad \longleftarrow$$

Note: Trace is Basis independent

$\rightarrow$ Using this, $\langle \hat{O} \rangle = \sum_j \langle x_j| \hat{O}\hat{\rho}|x_j\rangle = Tr[\hat{O}\hat{\rho}]$.

$\downarrow$
Trace

* Ensemble: $\{(|\psi_i\rangle, P_i)\} \rightarrow$ Density matrix

$$\hat{\rho} = \sum_i |\psi_i\rangle P_i \langle \psi_i|.$$

Hence we can describe the state of a system without complete information using a density matrix.

Properties of the density matrices:

- Hermiticity: $\hat{\rho}^{\dagger} = \hat{\rho}$.

- Semi-Positive definiteness: $\forall |\psi\rangle \in \mathcal{H}, \langle\psi|\hat{\rho}|\psi\rangle \geq 0$.

- Normalization: $\text{Tr}[\hat{\rho}] = 1$.

$\rightarrow$ We can always express the density matrix in an orthonormal basis $\{|x_i\rangle\}$ of $\mathcal{H}$ as,

$$|\psi_i\rangle = \sum_{j} C_{ji}|x_j\rangle.$$

to get $\hat{\rho} = \sum_{i} |\psi_i\rangle P_i \langle\psi_i| \rightarrow \hat{\rho} = \sum_{j,j'} \left[C_{ji} P_i C_{j'i}^{*} \right] |x_j\rangle\langle x_{j'}|$

Example (2):

Construct the density matrix for the Spin-$\frac{1}{2}$ system described by an ensemble in Example (1).

$$\hat{\rho} = \frac{1}{2}\left[|\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\uparrow| \right].$$

What if the ensemble is $\{ (|\downarrow\rangle, \frac{1}{2}), (|\uparrow\rangle, \frac{1}{2}) \}$.

$$\hat{\rho} = \frac{1}{2}\left[|\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\uparrow| \right].$$

→ Ofcourse if we have the complete information of the state of the system. Then the ensemble is $\{(|\psi_i\rangle, 1)\}$.

$$\Rightarrow \quad \hat{\varrho} = |\psi_i\rangle\langle\psi_i|$$

* This is called as a PURE STATE.

Notice! $\hat{\varrho} = |\psi_i\rangle\langle\psi_i| \Rightarrow \hat{\varrho}^2 = \hat{\varrho}^2 \Rightarrow \text{Tr}[\hat{\varrho}^2] = \text{Tr}[\hat{\varrho}] = 1$

i.e., $\text{Tr}[\hat{\varrho}^2] = 1$.

→ We can show that for any density matrix

$$0 \leq \text{Tr}[\hat{\rho}^2] \leq 1.$$

Equality ⟵ holds only for PURE STATES.

* Else we say that the state is a

MIXED STATE.

> For pure states, density matrix formulation is equivalent to standard QM. But allows more flexibility.

Example (3): Verify if the following ensembles (for Spin-$\frac{1}{2}$). describe a pure state or a mixed state.

(i) $\left\{ \left(\frac{1}{\sqrt{2}}[\left|\downarrow\right\rangle + \left|\uparrow\right\rangle] , \frac{1}{2} \right), \left(\frac{1}{2}[\left|\downarrow\right\rangle - \left|\uparrow\right\rangle], \frac{1}{2} \right) \right\}$ (ii) $\left\{ \left(\frac{1}{\sqrt{2}}\left|\downarrow\right\rangle + \frac{\sqrt{2}}{\sqrt{2}}\left|\uparrow\right\rangle , \frac{1}{3} \right), \left(\frac{\sqrt{5}}{4}\left|\downarrow\right\rangle + \frac{\sqrt{2}}{4}\left|\uparrow\right\rangle , \frac{2}{3} \right) \right\}$

* In a fixed orthonormal basis $\{|x_i\rangle\}$ for $\mathcal{H}$, $\hat{\rho}$ can be represented as a matrix:

Basis dependent definitions. But useful.

$$\begin{pmatrix} \langle x_1| \hat{\rho} |x_1\rangle & \cdots & \langle x_1| \hat{\rho} |x_N\rangle \\ \vdots & \ddots & \vdots \\ \langle x_N| \hat{\rho} |x_1\rangle & \cdots & \langle x_N| \hat{\rho} |x_N\rangle \end{pmatrix}.$$

*
$\rightarrow$ Diagonal elements $\rightarrow$ Populations in states $\{|x_i\rangle\}$.

$\rightarrow$ Offdiagonal elements $\rightarrow$ Coherences between states (pair).

→ * Clearly $\hat{e}$ is an operator on H.

* Set of all operators acting on H also (with certain restrictions)

form a Hilbert space with inner product defined between $\hat{A}$ & $\hat{B}$ → $Tr[\hat{A}^{\dagger}\hat{B}]$. → Hilbert Schmidt Inner product

* This Hilbert space is sometimes referred to as LIOUVILLE SPACE.

Example (4) For spin-$\frac{1}{2}$ system, LIOUVILLE space is Span$\{ \mathbb{I}, \sigma_x, \sigma_y, \sigma_z \}$.

$\rightarrow$ What about dynamics?

* We describe it in a similar way to classical set up:

   Given the ensemble $\{(|\psi_i\rangle, P_i)\}$.

   $\quad \rightarrow \hat{\rho}(0) = \sum_i |\psi_i\rangle P_i \langle\psi_i|.$

   - Sample $|\psi_i\rangle$ with probability P_i.

   - Evolve $|\psi_i\rangle$ in time as if we have complete information, i.e., $|\psi_i(t)\rangle = e^{-i\hat{H}t} |\psi_i\rangle.$

   - Generate the ensemble $\{(|\psi_i(t)\rangle, P_i)\}$.

* Hence $\quad \hat{\rho}(t) = \sum_i |\psi_i(t)\rangle \, p_i \, \langle \psi_i(t)|$

$$= e^{-i\hat{H}t} \, \hat{\rho}(0) \, e^{i\hat{H}t}$$

$\Rightarrow \qquad \dfrac{\partial \hat{\rho}(t)}{\partial t} = -i\left[\hat{H}, \hat{\rho}(t)\right] \rightarrow$ Contrast with
Heisenberg equation

$$\dfrac{\partial \hat{O}_H(t)}{\partial t} = i[\hat{H}, \hat{O}_H(t)].$$

* This evolution equation is called LIOUVILLE - VON-NEUMANN EQUATION.

Let us summarize what we have:

Basic structure of Quantum Mechanics :
(with incomplete information)

* Systems $\longrightarrow$ Hilbert Space (H).

  State $\rightarrow$ Density matrix $\begin{cases} \text{Hermitian} \\ \text{positive semi-definite} \\ \text{Normalized.} \end{cases}$

  operator on H.

* Observables $\rightarrow$ Hermitian operator on H.

  Expectation $\rightarrow$ $\text{Tr}[\hat{O}\,\hat{\rho}]$.

* Dynamics $\rightarrow$ $\frac{\partial\hat{\rho}(t)}{\partial t} = -i[\hat{H}, \hat{\rho}(t)]$

  $\hat{H} \rightarrow$ Hermitian operator. $\qquad \hookrightarrow \quad \hat{\rho}(t) = e^{-i\hat{H}t}\,\hat{\rho}(0)\,e^{i\hat{H}t}$

Different pictures of Quantum Dynamics:

$$\langle \hat{O}(t) \rangle = \text{Tr}\left[\underbrace{\hat{O}}_{\hat{O}_S(t)} \underbrace{e^{-i\hat{H}t} \hat{\rho}(0) e^{i\hat{H}t}}_{\hat{\rho}_S(t)} \right] = \text{Tr}\left[\hat{O}_S(t) \hat{\rho}_S(t) \right]$$

Schrodinger

"Cyclic permutations are valid inside traces"

$$= \text{Tr}\left[\underbrace{e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t}}_{\hat{O}_H(t)} \underbrace{\hat{\rho}(0)}_{\hat{\rho}_H(t)} \right] = \text{Tr}\left[\hat{O}_H(t) \hat{\rho}_H(t) \right]$$

Heisenberg

Standard Heisenberg evolution

Let $H = H_0 + H_I$

$$= \text{Tr}\left[\underbrace{e^{i\hat{H}_0 t} \hat{O} e^{-i\hat{H}_0 t}}_{\hat{O}_D(t)} \underbrace{e^{i\hat{H}_0 t} e^{-i\hat{H}t} \hat{\rho}(0) e^{i\hat{H}t} e^{-i\hat{H}_0 t}}_{\hat{\rho}_D(t)} \right]$$

$$= \text{Tr}\left[\hat{O}_D(t) \hat{\rho}_D(t) \right]$$

Dirac / Interaction

Quantum Mechanics of Composite systems:

→ Typically we encounter a situation where the "system" under consideration consists of more than one "sub-system".

→ For the sake of concreteness let us focus on system (s) with two subsystems $\{S_1, S_2\}$.

$$\begin{array}{|c|c|} \hline S_1 & S_2 \\ \hline \end{array}$$

$$S$$
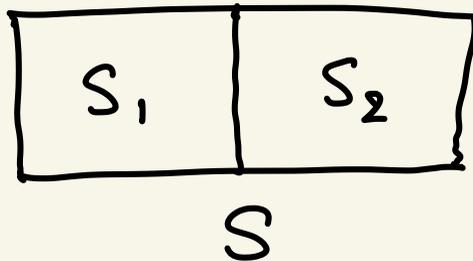
→ Suppose we know how to describe the two sub-systems:

- Individual Hilbert spaces → H_{S_1} & H_{S_2}.

- Observables on each S_1 & S_2 → $\{\hat{O}_{1i}\}$ & $\{\hat{O}_{2i}\}$.

→ How to construct a Hilbert space and observables for the composite system?

$\rightarrow$ The following postulates adresses it:

* The state space of the composite system (S) is the tensor (direct) product of Hilbert spaces of subsystems (S_1, S_2):

$$H_S = H_{S_1} \otimes H_{S_2}$$

If $\dim(H|_{S_1}) = m$ & $\dim(H|_{S_2}) = n$ then $\dim(H_S) = mn$.

This means H_S is $\text{Span}\{|x_{1i}\rangle \otimes |x_{2j}\rangle\}$

if $H_1 = \text{Span}\{|x_{1i}\rangle\}$ and $H_2 = \text{Span}\{|x_{2i}\rangle\}$.

* Induced inner product: $\langle \psi_{1i}|\langle \psi_{2j}| |\psi_{1i'}\rangle|\psi_{2j'}\rangle = \langle \psi_{1i}|\psi_{1i'}\rangle\langle \psi_{2j}|\psi_{2j'}\rangle$

Example (5):

Let S_1 & S_2 are Spins $\frac{1}{2}$ systems

Then $\mathbb{H}_{S_1} = $ Span $\{ |\downarrow\rangle_1, |\uparrow\rangle_1 \}$.

$\mathbb{H}_{S_2} = $ Span $\{ |\downarrow\rangle_2, |\uparrow\rangle_2 \}$.

$\mathbb{H}_S = $ Span $\{ |\downarrow\rangle_1 |\downarrow\rangle_2, |\downarrow\rangle_1 |\uparrow\rangle_2, |\uparrow\rangle_1 |\downarrow\rangle_2, |\uparrow\rangle_1 |\uparrow\rangle_2 \}$

$${}_1\langle \sigma_1 | {}_2\langle \sigma_2 | |\sigma_1'\rangle_1 |\sigma_2'\rangle = \langle \sigma_1 | \sigma_1' \rangle_1 {}_2\langle \sigma_2 | \sigma_2' \rangle_2$$

→ Hence every state $|\psi_S\rangle \in H_S$ can be written as

$$|\psi_S\rangle = \sum_{ij} \psi^S_{ij} \ |x_{1i}\rangle \otimes |x_{2j}\rangle$$

$$\downarrow \text{short form}$$

$$|x_{1i}, x_{2j}\rangle.$$
$$\text{or } |x_{1i}\rangle|x_{2j}\rangle$$

→ <u>N</u>ote: It is not always possible to write

any $|\psi_S\rangle \in H_S$ as $\quad |\psi_S\rangle = |\psi_{S_1}\rangle \otimes |\psi_{S_2}\rangle.$

$$\text{Ex: } \frac{1}{\sqrt{2}}\left[|\downarrow\rangle_1 |\downarrow\rangle_2 + |\uparrow\rangle_1 |\uparrow\rangle_2 \right].$$

$$\in H_{S_1} \qquad\qquad H_{S_2}.$$

But if we know for sure that S_1 is in $|\psi_{S_1}\rangle$ and S_2 is in $|\psi_{S_2}\rangle$ then $\quad |\psi_S\rangle = |\psi_{S_1}\rangle \otimes |\psi_{S_2}\rangle.$

* How to compose operators from subsystems:

→ If $\hat{O}_1$ & $\hat{O}_2$ acts on H_{S_1} & H_{S_2} respectively

then $\hat{O} = \hat{O}_1 \otimes \hat{O}_2$ acts on H_S.

$$\downarrow \text{short form}$$
$$\hat{O}_1 \hat{O}_2$$

if $|\psi_S\rangle = \sum_{ij} \psi^S_{ij} |x_{1i}\rangle \otimes |x_{2j}\rangle$

$$\hat{O}|\psi_S\rangle = \hat{O}_1 \otimes \hat{O}_2 |\psi_S\rangle = \sum_{ij} \psi^S_{ij} \hat{O}_1|x_{1i}\rangle \otimes \hat{O}_2|x_{2j}\rangle$$

$\rightarrow$ <u>Note</u>: Not all observables of S are product of observables of S_1 & S_2.

* But if $\hat{O}$ acts on Hs then

$$\hat{O} = \hat{\mathbb{I}} \, \hat{O} \, \hat{\mathbb{I}}$$

Completeness:
$$\hat{\mathbb{I}} = \sum_{ij} |x_{1i}\rangle |x_{2j}\rangle \langle x_{1i}| \langle x_{2j}|$$

$$\hat{O} = \sum_{ij} \sum_{i'j'} |x_{1i}\rangle |x_{2j}\rangle \langle x_{1i}| \langle x_{2j}| \hat{O} |x_{1i'}\rangle |x_{2j'}\rangle \langle x_{1i'}| \langle x_{2j'}|$$

$$O^{ii'}_{jj'}$$

$$\hat{O} = \sum_{i,i'} \sum_{j,j'} O^{ii'}_{jj'} \, |x_{1i}\rangle\langle x_{1i'}| \otimes |x_{2j}\rangle\langle x_{2j'}|$$

Note : $|x_{1i}\rangle|x_{2j}\rangle\langle x_{1i'}|\langle x_{2j'}|$

act on $\#(\Psi_s) \in \mathcal{H}_s$.

i.e.,

* Any operator on $\mathcal{H}_s$ can be written as

  "sum" of "direct product" of operators on $S_1 \, \& \, S_2$.

* We can "lift" operators acting on $\mathcal{H}_1 \, \& \, \mathcal{H}_2$ so that they act on $\mathcal{H}_s = \mathcal{H}_{s_1} \otimes \mathcal{H}_{s_2}$.

  $\hat{O}_1$ acts on $\mathcal{H}_{s_1} \longrightarrow$ $\hat{O}_1 \otimes \hat{\mathbb{I}}_2$ acts on $\mathcal{H}_s$ ← Identity on $\mathcal{H}_{s_2}$

  $\hat{O}_2$ acts on $\mathcal{H}_{s_2} \longrightarrow$ $\underline{\hat{\mathbb{I}}_1 \otimes \hat{O}_2}$ acts on $\mathcal{H}_s$ Identity on $\mathcal{H}_{s_1}$

Example (6):

For the same set up as in Example 6.

If (i) $|\psi_S\rangle = \frac{1}{\sqrt{2}} \left[|\downarrow\rangle_1 |\downarrow\rangle_2 + |\uparrow\rangle_1 |\uparrow\rangle_2 \right]$

(ii) $|\psi_S\rangle = \frac{1}{\sqrt{2}} \left[|\downarrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 |\downarrow\rangle_2 \right]$.

and $\hat{O} = \sigma_1^+ \sigma_2^- + \sigma_2^+ \sigma_1^-$

What is $\langle \psi_S | \hat{O} | \psi_S \rangle$.

here

$\sigma_1^+ |\uparrow\rangle_1 = 0$

$\sigma_1^+ |\downarrow\rangle_1 = |\uparrow\rangle_1$

$\sigma_1^- |\uparrow\rangle_1 = |\downarrow\rangle_1$

$\sigma_1^- |\downarrow\rangle_1 = 0$

Similarly of

σ_2^+, σ_2^- on $\mathcal{H}_{S_2}$.

Partial traces and Reduced Density Matrices:

* Suppose the composite system is prepared in an ensemble $\{ (|\Psi_{Si}\rangle, P_i) \}$

its density matrix is $\quad \in HH_S = HH_{S_1} \otimes HH_{S_2}$

We have knowledge of individual systems.

$$\hat{\rho}_S = \sum_i |\Psi_{Si}\rangle P_i \langle \Psi_{Si}|$$

$\rightarrow$ if $\quad |\Psi_{Si}\rangle = |\Psi_{S_1 p}\rangle \otimes |\Psi_{S_2 q}\rangle$ and $P_i = P_p P_q$

then $\quad \hat{\rho}_S = \hat{\rho}_{S_1} \otimes \hat{\rho}_{S_2}$ with $\quad \hat{Q}_{S_1} = \sum_p |\Psi_{S_1 p}\rangle P_p \langle \Psi_{S_1 p}|$

$\hat{\rho}_{S_2} = \sum_q |\Psi_{S_2 q}\rangle P_q \langle \Psi_{S_2 q}|$

* <u>Note</u>: It is not always possible that $\hat{\rho}_S$ corresponding to every ensemble can be written as $\hat{\rho}_{S_1} \otimes \hat{\rho}_{S_2}$.

Example (7):

Same set up as in Example (6).

if then ensemble is $\left\{ \left(\frac{1}{\sqrt{2}} \left[|\downarrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 |\downarrow\rangle_2 \right], 1 \right) \right\}$

Pure state$^{\downarrow}$ for H_S.

Construct $\hat{\rho}_S$

and argue that $\hat{\rho}_S \neq \hat{\rho}_1 \otimes \hat{\rho}_2$.

* Suppose that the state of the composite system is specified by a density matrix ($\hat{\rho}_S$).

→ If we are only interested in the expectation values of observables of sub system (S), $\{\hat{O}_m\}$

→ Lift the observables to act on H_S → $\{\hat{O}_{1n} \otimes \hat{\mathbb{I}}_2\}$

↓ Identity on H_{S_2}

→ Compute the expectation value.

$$\langle \hat{O}_{1n} \rangle = \text{Tr}\left[\hat{O}_{1n} \otimes \hat{\mathbb{I}}_2 \, \hat{\rho}_S \right].$$

$\rightarrow$ Compute the trace using an orthonormal basis of product form

$$\{ \ |x_{1i}\rangle \otimes |x_{2j}\rangle \ \}.$$

as

$$\langle \hat{O}_{1n} \rangle = \sum_{i,j} \underbrace{\langle x_{1i}|\langle x_{2j}| \ \hat{O}_{1n} \otimes \mathbb{I}_2 \ \hat{\varrho}_S |x_{1i}\rangle |x_{2j}\rangle}_{\downarrow}$$

$$= \sum_{i,j} \left[\langle x_{1i}|\hat{O}_{1n} \right] \langle x_{2j}| \ \hat{\varrho}_S |x_{1i}\rangle |x_{2j}\rangle$$

expand $\hat{\varrho}_S$ in some arbitrary orthonormal basis in product form $\{ \ |\xi_{1p}\rangle \otimes |\xi_{2q}\rangle \ \}.$

$$\hat{\varrho}_S = \sum_{\substack{p,q \\ p',q'}} \underbrace{|\xi_{1p}\rangle |\xi_{2q}\rangle \langle \xi_{1p}| \langle \xi_{2q}|}_{\text{II}} \hat{\varrho}_S |\xi_{1p'}\rangle \underbrace{|\xi_{2q'}\rangle \langle \xi_{1p'}| \langle \xi_{2q'}|}_{\text{III}}$$

Substituting in above equation,

$$\langle \hat{O}_{1n} \rangle = \sum_{ij} \sum_{\substack{p,q \\ p',q'}} \left[\langle x_{1i} | \hat{O}_{1n} \right] \langle x_{2j} | x$$

$$|\xi_{1p}\rangle |\xi_{2p}\rangle \langle \xi_{1p}| \langle \xi_{2q}| \hat{\varrho}_S |\xi_{1p'}\rangle |\xi_{2q'}\rangle \langle \xi_{1p'}| \langle \xi_{2q'}|$$
$$|x_{1i}\rangle |x_{2j}\rangle.$$

$$= \sum_{ij} \sum_{\substack{p,q \\ p',q'}} \langle x_{1i} | \hat{O}_{1n} |\xi_{1p}\rangle \langle x_{2j} | \xi_{2p}\rangle$$
$$\langle \xi_{1p}| \langle \xi_{2q}| \hat{\varrho}_S |\xi_{1p'}\rangle |\xi_{2q'}\rangle \langle \xi_{2q'} | x_{2j}\rangle$$
$$\langle \xi_{1p'} | x_{1i}\rangle$$

$$\langle \hat{O}_{1n} \rangle = \sum_{i} \langle x_{1i}| \; \hat{O}_{1n} \; \hat{\varrho}_{S_1} |x_{1i}\rangle$$

where

$$\hat{\varrho}_{S_1} = \sum_{j} \sum_{\substack{p,q \\ p',q'}}$$

$$|\xi_{1p}\rangle \langle x_{2j}|\xi_{2q}\rangle \langle \xi_{1p}|\langle \xi_{2q}| \hat{\varrho}_S |\xi_{1p'}\rangle |\xi_{2q'}\rangle$$

$$\sum_{j} \langle \xi_{2q'}|x_{2j}\rangle \langle x_{2j}|\xi_{2q}\rangle = \delta_{qq'}$$

$$\langle \xi_{2q'}|x_{2j}\rangle$$
$$\langle \xi_{1p'}|$$

$$= \sum_{\substack{p,p' \\ q}} |\xi_{1p}\rangle \Big[\langle \xi_{1p}| \langle \xi_{2q}| \hat{\varrho}_S |\xi_{1p'}\rangle |\xi_{2q}\rangle \Big] \langle \xi_{1p'}|$$

$$\hat{\rho}_{S_1} = \sum_q \left[\hat{\Pi}_1 \otimes \langle \xi_{2q} | \right] \hat{\rho}_S \left[\hat{\Pi}_1 \otimes | \xi_{2q} \rangle \right]$$

$\downarrow$

Nontrivial operation

Acting identity in $\mathbb{H}_{S_1}$
and
Projector in $\mathbb{H}_{S_2}$.

Density matrix in $\mathbb{H}_S = \mathbb{H}_{S_1} \otimes \mathbb{H}_{S_2}$

Operator in $\mathbb{H}_{S_1}$

In short form this operation is denoted as $\mathrm{Tr}_{S_2}[*]$

$$\hat{\rho}_{S_1} = \mathrm{Tr}_{S_2}[\hat{\rho}_S] = \sum_q \left[\hat{\Pi}_1 \otimes \langle \xi_{2q} | \right] \hat{\rho}_S \left[\hat{\Pi}_1 \otimes | \xi_{2q} \rangle \right].$$

The quantity $\hat{\varrho}_{S_1} = \text{Tr}_{S_2}[\hat{\varrho}_S]$ has Trace over only $H|_{S_2}$ of an ~~operator~~ acting on $H|_S = H|_{S_1} \otimes H|_{S_2}$

* This is Called as PARTIAL TRACE.

Note:

$\rightarrow$ Partial trace is a ~~basis~~ independent operation.

$\rightarrow$ The ~~object~~ obtained by partial trace, $\text{Tr}_{S_2}[\hat{\varrho}_S]$ is still an operator on $H|_{S_1}$.

Useful for calculations: (prove using def.)

→ Partial trace is a linear operation.

i.e., $\text{Tr}_{S_2}[\alpha \hat{X} + \alpha' \hat{X}'] = \alpha \text{Tr}_{S_2}[\hat{X}] + \alpha' \text{Tr}_{S_2}[\hat{X}']$

$\hat{X}, \hat{X}'$ are operators on H_5 & $\alpha, \alpha' \in \mathbb{C}$.

→ $\text{Tr}_{S_2}\left[|\Psi_1\rangle |\Psi_2\rangle \langle \Psi_1'| \langle \Psi_2'| \right]$ ← Reducing of products.

$$= \langle \Psi_2' | \Psi_2 \rangle \ |\Psi_1\rangle \langle \Psi_1'|.$$

Example (8):

Example demonstrating partial trace operation:

Consider the composite system with two Spin-$\frac{1}{2}$'s

let us say $\quad \hat{\rho}_S = |\Psi_S\rangle\langle\Psi_S| \quad |\Psi_S\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2\right]$

Construct $\quad \hat{\rho}_{S_1} = Tr_{S_2}\left[\hat{\rho}_S\right]$

Ans: $\quad \hat{\rho}_S = \frac{1}{2}\left[|\uparrow\rangle_1 |\downarrow\rangle_2 \,_1\langle\uparrow| \,_2\langle\downarrow| + |\uparrow\rangle_1 |\downarrow\rangle_2 \,_1\langle\downarrow| \,_2\langle\uparrow| \right.$

$$\left. + |\downarrow\rangle_1 |\uparrow\rangle_2 \,_1\langle\uparrow| \,_2\langle\downarrow| + |\downarrow\rangle_1 |\uparrow\rangle_2 \,_1\langle\downarrow| \,_2\langle\uparrow| \right].$$

Now $\hat{\rho}_{S_1} = \text{Tr}_{S_2}\left[\hat{\rho}_S\right]$

$\hat{\rho}_{S_1} =$

$\frac{1}{2}\left\{\text{Tr}_{S_2}\left[|\uparrow\rangle_1 |\downarrow\rangle_2 {}_1\langle\uparrow| {}_2\langle\downarrow|\right] + \text{Tr}_{S_2}\left[|\uparrow\rangle_1 |\downarrow\rangle_2 {}_1\langle\downarrow| {}_2\langle\uparrow|\right]\right.$

$+ \left.\text{Tr}_{S_2}\left[|\downarrow\rangle_1 |\uparrow\rangle_2 {}_1\langle\uparrow| {}_2\langle\downarrow|\right] + \text{Tr}_{S_2}\left[|\downarrow\rangle_1 |\uparrow\rangle_2 {}_1\langle\downarrow| {}_2\langle\uparrow|\right]\right\}.$

$\hat{\rho}_{S_1} = \frac{1}{2}\left\{ \overbrace{{}_2\langle\downarrow|\downarrow\rangle_2}^{1} |\uparrow\rangle_1 {}_1\langle\uparrow| + \overbrace{{}_2\langle\uparrow|\downarrow\rangle_2}^{0} |\uparrow_1\rangle \langle\downarrow|_2 \right.$

$\left. + \underbrace{{}_2\langle\downarrow|\uparrow\rangle_2}_{0} |\downarrow\rangle_1 {}_1\langle\uparrow| + \underbrace{{}_2\langle\uparrow|\uparrow\rangle_2}_{1} |\downarrow\rangle_1 {}_1\langle\downarrow|\right\}$

$\hat{\rho}_{S_1} = \frac{1}{2}\left\{ |\uparrow\rangle_1 {}_1\langle\uparrow| + |\downarrow\rangle_1 {}_1\langle\downarrow|\right\}.$

Now going back,

$$\langle \hat{O}_{1n} \rangle = \sum_i \langle x_{1i} | \hat{O}_{1n} \, \hat{\rho}_{S_1} | x_{1i} \rangle$$

$$\langle \hat{O}_{1n} \rangle = \text{Tr}_{S_1} [\, \hat{O}_{1n} \, \hat{\rho}_{S_1} \,].$$

* So expectation values of all operators acting
on H_{S_1}, with respect to $\hat{\rho}_{S_1}$ are same as
the expectation value of lifted operators
with respect to $\hat{\rho}_S$.

* Furthermore, $Tr_{S_2}[\hat{\rho}_S] = \hat{\rho}_{S_1}$ satisfies

the properties of density matrices:
hermiticity, positive semi-definiteness and
normalization.

* Hence $\hat{\rho}_{S_1}$ completely specifies the
state of subsystem S_1. It is a density matrix
for S_1 and called as REDUCED DENSITY MATRIX.

→ Similarly reduced density matrix $\hat{\rho}_{S_2}$ can be constructed
for S_2.

* Few important observations:

→ If $\hat{\rho}_S = \hat{\rho}_{S_1} \otimes \hat{\rho}_{S_2}$ → Uncorrelated

  then $Tr_{S_2}[\hat{\rho}_S] = \hat{\rho}_{S_1}$ & $Tr_{S_1}[\hat{\rho}_S] = \hat{\rho}_{S_2}$.

→ But for arbitrary $\hat{\rho}_S$,

  $\hat{\rho}_{S_1} = Tr_{S_2}[\hat{\rho}_S]$ & $\hat{\rho}_{S_2} = Tr_{S_1}[\hat{\rho}_S] \not\Rightarrow \hat{\rho}_S = \hat{\rho}_{S_1} \otimes \hat{\rho}_{S_2}$

→ If $\hat{\rho}_S$ is a pure state, i.e., $\hat{\rho}_S = |\psi_S\rangle\langle\psi_S|$,

  this doesnot imply $Tr_{S_2}[\hat{\rho}_S] = \hat{\rho}_{S_1}$ & $Tr_{S_2}[\hat{\rho}_S] = \hat{\rho}_{S_2}$

  are pure states.   This happens only if

  uncorrelated → $|\psi_S\rangle = |\psi_{S_1}\rangle \otimes |\psi_{S_2}\rangle$

Example (9)

Consider the same state as in Example (8)

for composite system of two spins-$\frac{1}{2}$ systems.

$$\hat{\rho}_S = |\Psi_S\rangle\langle\Psi_S| \text{ with } |\Psi_S\rangle = \frac{1}{\sqrt{2}}\left[|+\rangle_1|\uparrow\rangle_2 + |\uparrow\rangle_1|+\rangle_2\right]$$

↳ pure state

then Compute

$$\hat{\rho}_{S_1} = \text{Tr}_{S_2}\left[\hat{\rho}_S\right] \quad \& \quad \hat{\rho}_{S_2} = \text{Tr}_{S_1}\left[\hat{\rho}_S\right].$$

Show that $\hat{\rho}_{S_1}$ & $\hat{\rho}_{S_2}$ are mixed states.

→ Suppose the initial state of the composite system is $\hat{\rho}_S(0)$. Let us say it is "isolated" and subjected to evolution with respect to $\hat{H}_S$. Typical structure of $\hat{H}_S$ is

$$\hat{H}_S = \hat{H}_{S_1} \otimes \hat{\mathbb{1}}_2 + \hat{\mathbb{1}}_1 \otimes \hat{H}_{S_2} + \sum_{i,j} \lambda_{ij} \underset{\underset{\text{acts on } H_{S_1}}{\uparrow}}{\hat{O}_{1i}} \otimes \underset{\underset{\text{acts on } H_{S_2}}{\downarrow}}{\hat{O}_{2j}}$$

Then
$$\hat{\rho}_S(t) = e^{-i\hat{H}_S t} \hat{\rho}_S(0) e^{i\hat{H}_S t}.$$

Now the reduced density matrices for $S_1 \& S_2$

at time t are

$$\hat{\rho}_{S_1}(t) = \text{Tr}_{S_2}[\hat{\rho}_S(t)] \overset{\text{Typically}}{\neq} e^{-i\hat{H}_{S_1}t}\,\text{Tr}_{S_2}[\hat{\rho}_S(0)]\,e^{i\hat{H}_{S_1}t}$$

$$\hat{\rho}_{S_2}(t) = \text{Tr}_{S_1}[\hat{\rho}_S(t)] \neq e^{-i\hat{H}_{S_2}t}\,\text{Tr}_{S_1}[\hat{\rho}_S(0)]\,e^{i\hat{H}_{S_2}t}$$

Also

$$\frac{\partial\hat{\rho}_1(t)}{\partial t} = -i\,\text{Tr}_{S_2}\left[[\hat{H}_S,\hat{\rho}_S(t)]\right] \neq -i\left[\hat{H}_{S_1},\text{Tr}_{S_2}[\hat{\rho}_S^{(t)}]\right]$$

$$\frac{\partial\hat{\rho}_2(t)}{\partial t} = -i\,\text{Tr}_{S_1}\left[[\hat{H}_S,\hat{\rho}_S(t)]\right] \neq -i\left[\hat{H}_{S_2},\text{Tr}_{S_1}[\hat{\rho}_S(t)]\right]$$

* In general the closed equations satisfied by subsystems reduced density matrices are very complex and sometimes even extremely challenging to obtain (if not impossible).

* To obtain closed equations describing the evolution of reduced density matrices for subsystems and studying their dynamics constitutes OPEN QUANTUM SYSTEMS THEORY.

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