### Introduction to Quantum Mechanics

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### **Density Operators**

- What if the system in consideration interacts with the environment?
- Can describe their combined behaviour by a  $|\psi\rangle$ .
- May not be able to describe the behaviour of the system with a pure state.
- Density operators.
- Encoding some classical uncertainity within the already present quantum uncertainity.

## **Density Operators**

• If a system exists in the states  $|\psi_i\rangle$  with probabilities  $p_i$ , then its density operator  $\rho$  is defined as

$$\rho = \sum_{i} p_{i} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right|$$

- The density operator is positive and has unit trace. The converse holds.
- Unitary evolution

$$\rho = \sum_{i} p_{i} |\psi_{i}\rangle \langle \psi_{i}| \rightarrow \sum_{i} p_{i} U |\psi_{i}\rangle \langle \psi_{i}| U^{*} = U \rho U^{*}$$

Measurements

$$p(m) = Tr(M_m^* M_m \rho)$$

$$\rho_m = \frac{M_m \rho M_m^*}{Tr(M_m^* M_m \rho)}$$

# Some more points

- We can even have a mixture of density operators  $\{\rho_i, p_i\}$ , such that  $\rho = \sum_i p_i \rho_i$  describes the state of the system. Can be viewed as  $\sum_{ij} q_{ij} |\psi_{ij}\rangle \langle \psi_{ij}|$ . A simple example is the action of  $\mathcal{M} = \{M_m\}$  on  $\rho$  without knowing the outcome.
- The postulates can be reformed in the density operator language.
- A  $\rho$  is pure iff  $tr(\rho^2) = 1$ .
- Set of density ops is convex, and the pure states occupy the boundary of this set. Intuitive example: two qubits.

### Formation of density operators

Freedom in generation of the density operator.

#### Theorem 2.6 of QCQI

The vectors  $\left| ilde{\phi}_i 
ight>$  and  $\left| ilde{\psi}_j 
ight>$  generate the same density matrix (i.e.,

$$\sum_{i} \left| \tilde{\phi}_{i} \right\rangle \left\langle \tilde{\phi}_{i} \right| = \sum_{j} \left| \tilde{\psi}_{j} \right\rangle \left\langle \tilde{\psi}_{j} \right| ) \text{ iff}$$

$$\left|\tilde{\phi}_{i}\right\rangle = \sum_{j} u_{ij} \left|\tilde{\psi}_{j}\right\rangle$$

where  $U = [u_{ij}]$  is a unitary matrices.

Note In the above theorem, we absorbed the probabilities into the vectors as  $\left|\tilde{\psi}\right.\rangle\equiv\sqrt{p}\left|\psi\right.\rangle$ .

### Analyzing subsystems

If we have systems A and B, described by the density operator  $\rho_{AB}$ , we define the density operator for the subsystem A as

$$\rho_A \equiv Tr_B(\rho_{AB})$$

with the partial trace operation Tr<sub>B</sub> being defined as

$$\mathit{Tr}_{\mathcal{B}}(\ket{a_1}\bra{a_2}\otimes\ket{b_1}\bra{b_2})\equiv\ket{a_1}\bra{a_2}\mathit{tr}(\ket{b_1}\bra{b_2}))$$

and for general states  $\rho_{AB}$  the definition extends by superposition. Or,

$$Tr_B(\rho_{AB}) := \sum_j (I_A \otimes \langle j|_B) \rho_{AB} (I_A \otimes |j\rangle_B)$$

### A nice example

Consider

$$|\psi\rangle_{AB} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

Thus,  $\rho_{AB} = |\psi\rangle_{AB} \langle \psi|_{AB}$ . Now, we can compute  $\rho_A = Tr_B(\rho_{AB})$ . (compute)

(comment on  $S(\cdot)$ )

# Why the partial trace?

- The unique operation that preserves observable statistics.
- Let  $M = \sum_m m P_m$  be an observable on the system A
- Let M' be the corresponding observable on the system AB. Thus, any state  $|m\rangle_A |\psi\rangle_B$  of AB should have p(m)=1.
- Thus, the corresponding projector for measuring m on AB is  $P_m \otimes I_B$  and thus

$$M' = \sum_{m} m P_m \otimes I_B = M \otimes I_B$$

## Why the partial trace?

- Now, we want a map  $f(\cdot)$  such that  $f(\rho_{AB})$  gives us the density operator describing the state of A.
- We need

$$tr(Mf(\rho_{AB})) = tr((M \otimes I_B)\rho_{AB}) - (\#)$$

• Let  $M_i$  be an orthonormal basis of the space of hermitian operators w.r.t. the inner product  $(A, B) \equiv Tr(AB)$ . Expand  $f(\rho_{AB})$  as

$$f(\rho_{AB}) = \sum_{i} M_{i} tr(M_{i} f(\rho_{AB})) = \sum_{i} M_{i} tr((M \otimes I_{B}) \rho_{AB})$$

- Thus such an f is unique.
- Now see that  $f = tr_B$  satisfies (#).

### Schmidt Decomposition

This is a very useful theorem in quantum information.

#### Theorem 2.7 of QCQI

Let  $|\psi\rangle \in \mathcal{H}_{AB}$ . Then there exist orthonormal states  $|i_A\rangle \in \mathcal{H}_A$  and orthonormal states  $|i_B\rangle \in \mathcal{H}_B$  such that

$$|\psi\rangle = \sum_{i} \lambda_{i} |i_{A}\rangle \otimes |i_{B}\rangle$$

where  $\lambda_i \geq 0$  and  $\sum_i \lambda_i^2 = 1$ .

#### Purification

- Suppose we are given the state  $\rho_A$  for the system A.
- With the help of the previous theorem, we come up with an auxilliary system R, such that the combined state of these two systems is a pure state.
- Purification.
- Suppose

$$\rho_A = \sum_i p_i \ket{i_A} \bra{i_A}$$

- Introduce R with  $\mathcal{H}_R = \mathcal{H}_A$  and a orthonormal basis  $|i_R\rangle$ .
- Define

$$|\psi_{AR}\rangle \equiv \sum_{i} \sqrt{p_i} |i_A\rangle |i_R\rangle$$

See that

$$\rho_{A} = Tr_{R}(|\psi_{AR}\rangle \langle \psi_{AR}|)$$