2.4 The density operator

The density operator : The alternate mathematical formulation which is equivalent to the state vector formalism and provides a much more convenient language in quantum mechanics.

2.4.1 Ensembles of quantum states

The density operator formalism provides a convenient means for describing quantum systems whose state is not completely known.

Suppose a quantum system is in one of a number of states $|\psi_i\rangle$, where i is an index, with respective probabilities p_i.

$\{p_i, |\psi_i\rangle\}$: an *ensemble of pure states*

The density operator(density matrix) for the system is defined by

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

All postulates of quantum mechanics can be reformulated in terms of the density operator language.

The state vector formalism and the density operator language give the same results; however it is sometimes much easier to approach problems from one point of view rather than the other.

An unitary evolution for sys. initiated by $|\psi_i\rangle$ with p_i can be described

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \to \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger$$

For a measurement operator M_m, when the initial state was $|\psi_i\rangle$, the probability of getting result m is

$$p(m|i) = \langle\psi_i|M_m^\dagger M_m|\psi_i\rangle = \mathrm{tr}(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|)$$

The probability of obtaining result m is

$$\begin{aligned} p(m) &= \sum_i p(m|i)p_i & (2.1) \\ &= \sum_i p_i \mathrm{tr}(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|) & (2.2) \\ &= tr(M_m^\dagger M_m \rho). & (2.3) \end{aligned}$$

If the initial state was $|\psi_i\rangle$ then the state after obtainging the result m is

$$|\psi_i^m\rangle = \frac{M_m|\psi_i\rangle}{\sqrt{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}}$$

Thus, after a measurement which yields the result m we have an ensemble of states $|\psi_i^m\rangle$ with respective probabilities $p(i|m)$. The coresponding density operator ρ_m is

$$\rho = \sum_i p(i|m)|\psi_i^m\rangle\langle\psi_i^m| = \sum_i p(i|m)\frac{M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}$$

By Bayes's theorem, $p(i|m) = p(m,i)/p(m) = p(m|i)p_i/p(m)$

$$\begin{aligned}\rho_m &= \sum_i p_i \frac{M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m \rho)} \\ &= \frac{M_m \rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m \rho)}\end{aligned}$$

We will complete rephrasing of quantum postulates in next section.

A pure state : if a quantum system whose stat $|\psi\rangle$ is known exactly then we said the system is in a pure state. In this case the density operator is simply $\rho = |\psi\rangle\langle\psi|$.
Otherwise, ρ is in a *mixed state*; it is said to be a *mixture* of the different pure states in the ensemble for ρ.

A pure state stisfies $\mathrm{tr}(\rho^2) = 1$ ($\rho^2 = \rho$), while a mixed state satisfiles $\mathrm{tr}(\rho^2) < 1$ ($\rho^2 \neq \rho$).

1. Sometime people use the term 'mixed state' as a catch-all to include both pure and mixed quantum states. (The origin for this usage seems to be that it implies that the writer is not necessarily *assuming* that a state is pure)
2. The term 'pure state' is often used in reference to a state vector $|\psi\rangle$, to distinguish it from a density operator ρ.

Imagine a quantum system is prepared in the state ρ_i with probability p_i. For pure states, suppose ρ_i from some ensemble $\{p_{ij}, |\psi_{ij}\rangle\}$, so the density matrix of a subsystem i is $\rho_i = \sum_j p_{ij}|\psi_{ij}\langle\psi_{ij}|\rangle$ and the probability for being in the state $|\psi_{ij}\rangle$ is $p_i p_{ij}$. The density matrix for the system is thus

$$\begin{aligned}\rho &= \sum_{ij} p_i p_{ij}|\psi_{ij}\rangle\langle\psi_{ij}| \\ &= \sum_i p_i \rho_i\end{aligned}$$

We say that ρ is a *mixture* of the states ρ_i with probabilities p_i. This concept of a mixture comes up repeatedly in the analysis of problems like quantum noise, there the effect of the noise is to introduce ignorance into our knowledge of the quantum state.

eg) Imagine that our record of the result m of the measuremnt was lost. We would have a quantum system in the state ρ_m with probability $p(m)$, bout would no longer know the actual value of m. The state of such a quantum system would therefore be described by the density operator

$$\rho = \sum_m p(m)\rho_m$$

$$
\begin{aligned}
&= \sum_m \mathrm{tr}(M_m^\dagger M_m\rho)\frac{M_m\rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m\rho)} \\
&= \sum_m M_m\rho M_m^\dagger,
\end{aligned}
$$

a nice compact formula which may be used as the staring point for analysis of further operations on the system.

2.4.2 General properties of the density operator

The density operator : describing ensembles of quantum states.

Theorem 2.5: (**Characterization of density operators**) An operator ρ is the density operator associated to some ensemble $\{p_i, |\psi_i\rangle\}$ iff it satisfies the conditions:

1. **(Trace dondition)** ρ has trace equal to one
2. **(Positivity condition)** ρ is a positive operator.

Pf.
Suppose $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ is a density operator. Then

$$\mathrm{tr}(\rho) = \sum_i p_i \mathrm{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i p_i = 1,$$

so the trace condition $\mathrm{tr}(\rho) = 1$ is satisfied. Suppose $|\phi\rangle$ is an arbitrary vector in state space. Then

$$
\begin{aligned}
\langle\phi|\rho|\phi\rangle &= \sum_i p_i\langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle \\
&= \sum p_i|\langle\phi|\psi_i\rangle|^2 \\
&\geq 0,
\end{aligned}
$$

so the positivity condition is satisfied.

Conversely, suppose ρ is any operator satisfying the trace and positivity conditions. Since ρ is positive, it must have a spectral decomposition

$$\rho = \sum_j \lambda_j|j\rangle\langle j|,$$

where the vectors $|j\rangle$ are orthogonal, and λ_j are real, non-negative eigenvalues of ρ. From the trace condition we see that $\sum_j \lambda_i = 1$. Therefore, a system in state $|j\rangle$ with probability λ_j will have density operator ρ. That is, the ensemble $\lambda_j, |j\rangle$ is an ensemble of states giving rise to the density operator ρ.

We can define a density operator to be a positive operator ρ which has trace equal to one. Making this definition allows us to reformulate the postulates of quantum mechanics in the density operator picture.

Postulate 1 : Associated to any isolated physical system is a complex vector space with inner product (that is, a Hilbert space) known as *state space* of the system. The system is completely described by its *density operator*, which is a positive operator ρ with trace one, acting on the state space of the system. If a quantum system is in the state ρ_i with probability p_i, then the density operator for the system is $\sum_i p_i \rho_i$.

Postulate 2 : The evolution of a *closed* quantum system is described by *unitary transformation.* That is, the state ρ of the system a time t_1 is related to the state ρ' of the system at time t_2 by a unitary operator U which depends only on the tiems t_1 and t_2,

$$\rho' = U \rho U^\dagger$$

Postulate 3 : Quantum measurements are described by a collection M_m of *measurement operators.* These are operators acting on the state apace of the system being measured. The index m refersto the measurement outcomes that may occur in the experiment. If the state of the quantum system is ρ immediately before the measurement then the probability that result m occurs is given bye

$$p(m) = \mathrm{tr}(M_m^\dagger M_m \rho)$$

and the state of the system after the measurement is

$$\frac{M_m \rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m \rho)}$$

The measurement operators satisfy the completeness relation,

$$\sum_m M_m^\dagger M_m = I.$$

Postulate 4 : The state space of a composite physical system is the tensor product of the state spaces of the component physical systems. Moreover, if we have systems numberd 1 through n, and system number i is prepared in the state ρ_i, then the joint state of the total system is $\rho_i \otimes \rho_2 \otimes \ldots \rho_n$.

Above postulates are mathematically equivalent to the description in terms of the state vector.

The density operator approach really shines for two applications:

- The description of quantum systems whose state is not known
- The description of subsystems of a composite quantum system

It is tempting fallacy to suppose that the eigenvlues and eigenvectors of a density matrix have some special significance with regard to the ensemble of quantum states represented by that density matrix.

eg) Suppose that a quantum system with density matrix

$$\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|.$$

And suppose we define other vectors

$$\begin{aligned}|a\rangle &\equiv \sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle \\ |b\rangle &\equiv \sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle\end{aligned}$$

and the quantum system is prepared in the state $|a\rangle$ with probability 1/2 and in the state $|b\rangle$ with probability 1/2. Then

$$\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b| = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$$

That is, these two different ensembles of quantum states give rise to the same density matrix. In general, the eigenvectors and eigenvalues of a density matrix just indicate *one* of many possible ensembles that may give rise to a specific density matrix, and there is no reason to suppose it is an especially privileged ensemble.

What classes of ensembles does give rise to a particular density matrix? The solution to this problem has suprisingly many applications in quantum computation and quantum information, notably in the understanding of quantum noise and quantum error-correction. For the solution it is convenient to make use of vectors $|\tilde{\psi}_i\rangle$ which may not be normalized to unit length. We say the set $|\tilde{\psi}_i\rangle$ *generates* the operator $\rho \equiv \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|$, and thus the connection to the usual ensemble pircture of density operators is expressed by the equation $|\tilde{\psi}_i\rangle = \sqrt{p_i}|\psi_i\rangle$. When do two sets of vectors, $|\tilde{\psi}_i\rangle$ and $|\tilde{\phi}_j\rangle$ generate the same operator ρ? The solution to this problem will enable us to answer the question of what ensembles give rise to a given density matrix.

Theorem 2.6: **Unitary freedom in the ensemble for density matrices** The set $|\tilde{\psi}_i\rangle$ and $|\tilde{\phi}_j\rangle$ generate the same density matrix iff

$$|\tilde{\psi}_i\rangle = \sum_j u_{ij}|\tilde{\phi}_j\rangle$$

where u_{ij} is a unitary matrix of complex numbers, with indices i and j, and we 'pad' whichever set of vectors $|\tilde{\psi}_i\rangle$ or $|\tilde{\phi}_j\rangle$ is smaller with additional vectors 0 so that the two sets have the same number of elements.

As a consequence of the theorem, note that $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ for normalized state $|\psi_i\rangle, |\phi_i\rangle$ and probability distributions p_i and q_i iff

$$\sqrt{p_i}|\psi_i\rangle = \sum_j u_{ij}\sqrt{q_i}|\phi_j\rangle,$$

for some unitary matrix u_{ij}, and we may pad the smaller ensemble with entries having probability zero in order to make the two ensembles the same size. Thus, Theorem 2.6 characterizes the freedom in ensembles $\{p_i, |\psi_i\rangle\}$ giving rise to a given density matrix ρ.

Pf.
Suppose $|\tilde{\psi}_i\rangle = \sum_i u_{ij}|\tilde{\phi}_j\rangle$ for some unitary u_{ij}. Then

$$\begin{aligned}\sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| &= \sum_{ijk} u_{ij}u_{ik}^*|\tilde{\phi}_j\rangle\langle\tilde{\phi}_k| \\ &= \sum_{jk}\left(\sum_i u_{ki}^\dagger u_{ij}\right)|\tilde{\phi}_j\rangle\langle\tilde{\phi}_k|\end{aligned}$$

$$
\begin{aligned}
&= \sum_{jk} \delta_{kj} |\tilde{\phi}_j\rangle\langle\tilde{\phi}_k| \\
&= \sum_{j} |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j|
\end{aligned}
$$

which shows that $|\tilde{\psi}_i\rangle$ and $|\tilde{\phi}_j\rangle$ generate the same operator.

Conversely, suppose

$$A = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j|.$$

Let $A = \sum_k \lambda_k |k\rangle\langle k|$ be a decomposition for A such that $|k\rangle$ are orthonormal, and the λ_k are strictly positive. Let $|\psi\rangle$ be any vector orthonormal to the space spanned by $|\tilde{k}\rangle$ ($|\tilde{k}\rangle = \sqrt{\lambda_i}|k\rangle$), so $\langle\psi|\tilde{k}\rangle\langle\tilde{k}|\psi\rangle = 0$ for all k, and

$$0 = \langle\psi|A|\psi\rangle = \sum_i \langle\psi|\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|\psi\rangle = \sum_i |\langle\psi|\tilde{\psi}_i\rangle|^2.$$

Thus $\langle\psi|\tilde{\psi}_i\rangle = 0$ for all i and all $|\psi\rangle$ orthonormal to the space spanned by the $|\tilde{k}\rangle$. It follows that each $|\tilde{\psi}_i\rangle$ can be expressed as a linear combination of the $|\tilde{k}\rangle$, $|\tilde{\psi}_i\rangle = \sum_k c_{ik}|\tilde{k}\rangle$. Since $A = \sum_k |\tilde{k}\rangle\langle\tilde{k}| = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|$ we see that

$$\sum_k |\tilde{k}\rangle\langle\tilde{k}| = \sum_{kl} \left(\sum_i c_{ik} c_{il}^* \right) |\tilde{k}\rangle\langle\tilde{l}|.$$

The operators $|\tilde{k}\rangle\langle\tilde{l}|$ are easily seen to be *linearly independent*, and thus it must be that $\sum_i c_{ik}c_{il}^* = \delta_{kl}$. This ensures that we may append extra columns to c to obtain a unitary matrix v such that $|\tilde{\psi}_i\rangle = \sum_k v_{ik}|\tilde{k}\rangle$, where we have appended zero vectors to the list of $|\tilde{k}\rangle$. Similarly, we can find a unitary matrix w such that $|\tilde{\phi}_j\rangle = \sum_k w_{jk}|\tilde{k}\rangle$. Thus $|\tilde{\psi}_i\rangle = \sum_j u_{ij}|\tilde{\phi}_j\rangle$, where $u = vw^\dagger$ is unitary.

2.4.3 The reduced density operator

The deepest application of the density operator may be as a descriptive tool for *subsystems* of a composite quantum system. Such a description is provided by *reduced density operator*.

Suppose we have physical systems A and B, whose state is described by a density operator ρ^{AB}. The reduced density operator for system A is defined by

$$\rho^A \equiv tr_B(\rho^{AB}),$$

where tr_B is a map of operators known as the *partial trace* over system B. The partial trace is defined by

$$
\begin{aligned}
\mathrm{tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) &\equiv |a_1\rangle\langle a_2|\mathrm{tr}(|b_1\rangle\langle b_2|) \\
&= \langle b_2|b_1\rangle|a_1\rangle\langle a_2|
\end{aligned}
$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in the state space A, and $|b_1\rangle$, $|b_2\rangle$ are of B.

The physical justification for making this identification is that the reduced density operator provides the correct measrement statistics for measurements made on system A.

*eg)*Suppose a quantum system is in the product state $\rho^{AB} = \rho \otimes \sigma$, where ρ is a density operator for system A, and σ is a density operator for system B. Then

$$\rho^A = \mathrm{tr}_B(\rho \otimes \sigma) = \rho \mathrm{tr}(\sigma) = \rho,$$

which is the result we intuitively expect. Similarly, $\rho^B = \sigma$ for this state.

eg) For the Bell state, the density operator

$$\begin{aligned}
\rho &= \left(\frac{|00\rangle + |11\rangle}{\sqrt{2}}\right)\left(\frac{\langle 00| + \langle 11|}{\sqrt{2}}\right) \\
&= \frac{|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|}{2}.
\end{aligned}$$

Tracing out the second qubit, we find the reduced density operator of the first qubit,

$$\begin{aligned}
\rho^1 &= \mathrm{tr}_2(\rho) \\
&= \frac{\mathrm{tr}_2(|00\rangle\langle 00|) + \mathrm{tr}_2(|11\rangle\langle 00|) + \mathrm{tr}_2(|00\rangle\langle 11|) + \mathrm{tr}_2(|11\rangle\langle 11|)}{2} \\
&= \frac{|0\rangle\langle 0|\langle 0|0\rangle + |1\rangle\langle 0|\langle 1|0\rangle + |0\rangle\langle 1|\langle 0|1\rangle + |1\rangle\langle 1|\langle 1|1\rangle}{2} \\
&= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} \\
&= \frac{I}{2}
\end{aligned}$$

Notice that this state is a *mixed state*, since $\mathrm{tr}((I/2)^2) = 1/2 < 1$. This is quite a remarkable result. The state of the joint system of two qubits is a pure state; however, the first qubit is in a mixed state, a state about which we apparently do not have maximal knowledge. This strange property, that the joint state of a system can be completely known, yet a sybsystem be in mixed states, another hallmark of quantum entanglement.

Quantum teleportatin and the reduced density operator

A useful application of the reduced density operator is to the analysis of quantum teleportation.

Before Alice makes her measurement the quantum state of the three qubits is:

$$|\psi_2\rangle = \frac{1}{2}\left[|00\rangle\left(\alpha|0\rangle + \beta|1\rangle\right) + |01\rangle\left(\alpha|1\rangle + \beta|0\rangle\right) + |10\rangle\left(\alpha|0\rangle - \beta|1\rangle\right) + |11\rangle\left(\alpha|1\rangle - \beta|0\rangle\right)\right].$$

Measuring in Alice's computational basis, the state of the system after the measurement is:

$$|00\rangle\left[\alpha|0\rangle + \beta|1\rangle\right] \text{ with probability } \frac{1}{4}$$
$$|01\rangle\left[\alpha|1\rangle + \beta|0\rangle\right] \text{ with probability } \frac{1}{4}$$

$$|10\rangle\,[\alpha|0\rangle - \beta|1\rangle] \ \text{ with probability } \frac{1}{4}$$
$$|11\rangle\,[\alpha|1\rangle - \beta|0\rangle] \ \text{ with probability } \frac{1}{4}$$

The density operator of the system is thus

$$\begin{aligned}\rho = \frac{1}{4}[\quad & |00\rangle\langle 00|\,(\alpha|0\rangle + \beta|1\rangle)\,(\alpha^*\langle 0| + \beta^*\langle 1|) + |01\rangle\langle 01|\,(\alpha|1\rangle + \beta|0\rangle)\,(\alpha^*\langle 1| + \beta^*\langle 0|) \\ & +|10\rangle\langle 10|\,(\alpha|0\rangle - \beta|1\rangle)\,(\alpha^*\langle 0| - \beta^*\langle 1|) + |11\rangle\langle 11|\,(\alpha|1\rangle - \beta|0\rangle)\,(\alpha^*\langle 1| - \beta^*\langle 0|)].\end{aligned}$$

Tracing out Alice's system, we see that the reduced density operator of Bob's system is

$$\begin{aligned}\rho^B &= \frac{1}{4}[\,(\alpha|0\rangle + \beta|1\rangle)\,(\alpha^*\langle 0| + \beta^*\langle 1|) + (\alpha|1\rangle + \beta|0\rangle)\,(\alpha^*\langle 1| + \beta^*\langle 0|) \\ &\quad + (\alpha|0\rangle - \beta|1\rangle)\,(\alpha^*\langle 0| - \beta^*\langle 1|) + (\alpha|1\rangle - \beta|0\rangle)\,(\alpha^*\langle 1| - \beta^*\langle 0|)\,] \\ &= \frac{2\left(|\alpha|^2 + |\beta|^2\right)|0\rangle\langle 0| + 2\left(|\alpha|^2 + |\beta|^2\right)|1\rangle\langle 1|}{4} \\ &= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} \\ &= \frac{I}{2},\end{aligned}$$

Thus, the state of Bob's system after Alice has performed the measurement but before Bob has learned the measurement result is $I/2$. This state has no dependence upon the state $|\psi\rangle$ being teleported, and thus any measurements performed by Bob will contain no informatin about $|\psi\rangle$, thus preventing Alice from using teleportation to transmit information to Bob faster than light.