Fundamental Concepts-Introduction to Quantum Mechanics- The Density Operator

- A large number or collection of systems are called an *ensemble.*
- Members of the ensemble can be found in one of two or more different quantum states.
- Prepare a large number *N* of systems, where each member of the system can be in one of two state vectors

$$|a\rangle = \alpha|x\rangle + \beta|y\rangle$$
$$|b\rangle = \gamma|x\rangle + \delta|y\rangle$$

- These states are normalized, so $|\alpha|^2 + |\beta|^2 = |\gamma|^2 + |\delta|^2 = 1$
- For a system in state $|a>$, if a measurement is made, then there is a probability $|\alpha|^2$ of finding $|x>$ while there is a probability $|\beta|^2$ of finding $|y>$, and similarly for state $|b>$.

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- Now suppose that we prepare n_a of these systems in state $|a>$ and n_b of the systems in state $|b>$. Since we have N total systems, then

$$n_a + n_b = N$$

- If we divide by N,

$$\frac{n_a}{N} + \frac{n_b}{N} = 1$$

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- The probability that a member of ensemble is found in state $|a>$ is given by $p = n_a/N$
- The probability of finding a member of the ensemble in state $|b>$ is given by $1-n_a/N = 1-p$
- At the level of a single quantum system, where the Born rule gives us the probability of obtaining a given a measurement result.

Max Born (1882–1970)
German physicist and mathematician who was instrumental in the development of quantum mechanics

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- On the ensemble level, where if we draw a member of the ensemble, there is a certain probability that the system was prepared in one state vector or another
- At the ensemble level the use of probability is acting in a *classical* way. That is, it is a simple reflection of incomplete information. So, at the ensemble level, we have a simple statistical mixture.
- We need to weight the calculated quantities by the probabilities of finding different states.
- The proper way to do this is with the ***density operator***.

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- **THE DENSITY OPERATOR FOR A PURE STATE**
- If there exists some orthonormal basis $|u_i\rangle$, then we can expand the state in that basis:

$$|\psi\rangle = c_1|u_1\rangle + c_2|u_2\rangle + \cdots + c_n|u_n\rangle$$

- Then, using the Born rule, we know that the probability of finding the system in state $|u_i\rangle$ upon measurement is given by $|c_i|^2$.

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- When a system is in a definite state like this, we say the system is in a *pure state.*
- The density operator is an average operator that will allow us to describe a statistical mixture.
- we begin by finding the expectation value or *average of some operator A. We write*

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

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- Expanding the state in some orthonormal basis

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \left(c_1^* \langle u_1 | + c_2^* \langle u_2 | + \cdots + c_n^* \langle u_n | \right) A \left(c_1 | u_1 \rangle + c_2 | u_2 \rangle + \cdots + c_n | u_n \rangle \right)$$

$$= \sum_{k,l=1}^{n} c_k^* c_l \langle u_k | A | u_l \rangle$$

$$= \sum_{k,l=1}^{n} c_k^* c_l A_{kl}$$

- Recall how the coefficients in the expansion of a state vector are defined. That is,

$$c_m = \langle u_m | \psi \rangle \quad c_m^* = \langle \psi | u_m \rangle$$

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$$c_k^* c_l = \langle u_l|\psi\rangle\langle\psi|u_k\rangle = \langle u_l|(|\psi\rangle\langle\psi|)|u_k\rangle$$

- We call this the density operator and denote it by *ρ =|ψ><ψ|. So the expectation* or average value of an operator *A with respect to a state* |ψ> *can be written as*

$$\langle A\rangle = \sum_{k,l=1}^{n} c_k^* c_l A_{kl} = \sum_{k,l=1}^{n} \langle u_l|(|\psi\rangle\langle\psi|)|u_k\rangle A_{kl} = \sum_{k,l=1}^{n} \langle u_l|\rho|u_k\rangle A_{kl}$$

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- **Definition: Density Operator for a Pure State**
- The density operator for a state |ψ> *is given by* $\rho = |\psi\rangle\langle\psi|$

$$\langle A\rangle = \sum_{k,l=1}^{n} c_k^* c_l \langle u_k|A|u_l\rangle$$

$$= \sum_{k,l=1}^{n} \langle u_l|\psi\rangle\langle\psi|u_k\rangle\langle u_k|A|u_l\rangle$$

$$= \sum_{k,l=1}^{n} \langle u_l|\rho|u_k\rangle\langle u_k|A|u_l\rangle$$

$$\sum_k |u_k\rangle\langle u_k| = 1$$

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$$
\begin{aligned}
\langle A\rangle &= \sum_{k,l=1}^{n} \langle u_l|\rho|u_k\rangle\langle u_k|A|u_l\rangle \\
&= \sum_{l=1}^{n} \langle u_l|\rho\left(\sum_{k=1}^{n} |u_k\rangle\langle u_k|\right) A|u_l\rangle \\
&= \sum_{l=1}^{n} \langle u_l|\rho A|u_l\rangle \\
&= Tr(\rho A)
\end{aligned}
$$

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$$Tr(\rho) = \sum_j \langle u_j|\rho|u_j\rangle = \sum_j \langle u_j|\psi\rangle\langle\psi|u_j\rangle = \sum_j c_j c_j^* = \sum_j |c_j|^2 = 1$$

- This expression can be summarized by saying that *due to the conservation of probability,* the trace of the density operator is always 1.
- Example: A system is in the following state, where the $|u_k>$ *constitute an orthonormal* basis. Write down the density operator, and show it has unit trace.
- $$|\psi\rangle = \frac{1}{\sqrt{3}}|u_1\rangle + i\sqrt{\frac{2}{3}}|u_2\rangle$$

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- Solution:

$$\langle\psi| = \frac{1}{\sqrt{3}}\langle u_1| - i\sqrt{\frac{2}{3}}\langle u_2|$$

$$\rho = |\psi\rangle\langle\psi| = \left(\frac{1}{\sqrt{3}}|u_1\rangle + i\sqrt{\frac{2}{3}}|u_2\rangle\right)\left(\frac{1}{\sqrt{3}}\langle u_1| - i\sqrt{\frac{2}{3}}\langle u_2|\right)$$

$$= \frac{1}{3}|u_1\rangle\langle u_1| - i\frac{\sqrt{2}}{3}|u_1\rangle\langle u_2| + i\frac{\sqrt{2}}{3}|u_2\rangle\langle u_1| + \frac{2}{3}|u_2\rangle\langle u_2|$$

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$$Tr(\rho) = \sum_{i=1}^{2} \langle u_i|\rho|u_i\rangle = \langle u_1|\rho|u_1\rangle + \langle u_2|\rho|u_2\rangle$$

$$= \frac{1}{3}\langle u_1|u_1\rangle\langle u_1|u_1\rangle - i\frac{\sqrt{2}}{3}\langle u_1|u_1\rangle\langle u_2|u_1\rangle + i\frac{\sqrt{2}}{3}\langle u_1|u_2\rangle\langle u_1|u_1\rangle + \frac{2}{3}\langle u_1|u_2\rangle\langle u_2|u_1\rangle$$

$$+ \frac{1}{3}\langle u_2|u_1\rangle\langle u_1|u_2\rangle - i\frac{\sqrt{2}}{3}\langle u_2|u_1\rangle\langle u_2|u_2\rangle + i\frac{\sqrt{2}}{3}\langle u_2|u_2\rangle\langle u_1|u_2\rangle + \frac{2}{3}\langle u_2|u_2\rangle\langle u_2|u_2\rangle$$

$$= \frac{1}{3} + \frac{2}{3} = 1$$

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- There are a couple of things to notice:
  - The sum of the diagonal elements of the matrix is one. This shouldn't be surprising, since we showed earlier that *Tr(ρ)=1 because probabilities sum* to one.
  - The values along the diagonal are the probabilities of finding the system in the respective states.
  - The off-diagonal elements of the density matrix are called *coherences.*

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- **Time Evolution of the Density Operator**

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle \qquad\qquad H = H^\dagger$$

- → $$-i\hbar\frac{d}{dt}\langle\psi| = \langle\psi|H$$

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

- → $$\frac{d\rho}{dt} = \frac{d}{dt}(|\psi\rangle\langle\psi|) = \left(\frac{d}{dt}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{d}{dt}\langle\psi|\right)$$

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- →

$$\frac{d\rho}{dt} = \left(\frac{H}{i\hbar}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\langle\psi|\frac{H}{-i\hbar}\right) = \frac{H}{i\hbar}\rho - \rho\frac{H}{i\hbar} = \frac{1}{i\hbar}[H, \rho]$$

$$i\hbar\frac{d\rho}{dt} = [H, \rho]$$

- For a closed system, *If we let ρ(t) represent the density operator at* some later time *t and ρ(t_o) represent the density operator at an initial time t_o, then*
-
$$\rho(t) = U\rho(t_o)U^\dagger$$

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- Finally, looking at the definition $\rho = |\psi\rangle\langle\psi|$, *it is obvious that the density operator* is Hermitian, meaning $\rho = \rho^\dagger$. *In the case of pure states, since*

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

- we have the following definition. If a system is in a pure state $|\psi\rangle$ *with density* operator $\rho = |\psi\rangle\langle\psi|$, *then*

- $$Tr(\rho^2) = 1 \quad \text{(pure state only)}$$

Fundamental Concepts-Introduction to Quantum Mechanics- The Density Operator

- **THE DENSITY OPERATOR FOR A MIXED STATE**
- What we are looking for is a density matrix that describes an ensemble. This can be done by following these three steps:
  - Construct a density operator for each individual state that can be found in the ensemble.
  - Weight it by the probability of finding that state in the ensemble.
  - Sum up the probabilities.

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$$|a\rangle = \alpha|x\rangle + \beta|y\rangle$$

$$|b\rangle = \gamma|x\rangle + \delta|y\rangle$$

- The density operators for each of these states are

$$\rho_a = |a\rangle\langle a|$$

$$\rho_b = |b\rangle\langle b|$$

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$$\rho_a = |a\rangle\langle a| = (\alpha|x\rangle + \beta|y\rangle)(\alpha^*\langle x| + \beta^*\langle y|)$$
$$= |\alpha|^2|x\rangle\langle x| + \alpha\beta^*|x\rangle\langle y| + \alpha^*\beta|y\rangle\langle x| + |\beta|^2|y\rangle\langle y|$$
$$\rho_b = |b\rangle\langle b| = (\gamma|x\rangle + \delta|y\rangle)(\gamma^*\langle x| + \delta^*\langle y|)$$
$$= |\gamma|^2|x\rangle\langle x| + \gamma\delta^*|x\rangle\langle y| + \gamma^*\delta|y\rangle\langle x| + |\delta|^2|y\rangle\langle y|$$

- $\rightarrow$

$$\rho = p\rho_a + (1-p)\rho_b = p|a\rangle\langle a| + (1-p)|b\rangle\langle b|$$

$$\rho = \sum_{i=1}^{n} p_i \rho_i = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|$$

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- **KEY PROPERTIES OF A DENSITY OPERATOR**
  - The density operator is Hermitian, meaning $\rho = \rho^{\dagger}$.
  - $Tr(\rho)=1$.
  - *ρ is a positive operator, meaning* $\langle u|\rho|u\rangle \geq 0$ *for any state vector* $|u\rangle$.

- Recall that an operator is positive if and only if it is Hermitian and has nonnegative eigenvalues.

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- **Expectation Values**

- The result that we found in the pure state case for calculating the expectation value of a given operator holds true in the general case of a statistical mixture. That is, the expectation value of an operator with respect to a statistical mixture of states can be calculated using

$$\langle A \rangle = Tr(\rho A)$$

-

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- **Probability of Obtaining a Given Measurement Result**
- Given a projection operator $P_n = |u_n\rangle\langle u_n|$ *corresponding to measurement result a_n, the probability of obtaining a_n can be calculated using the density operator as* follows:

$$p(a_n) = \langle u_n|\rho|u_n\rangle = Tr(|u_n\rangle\langle u_n|\rho) = Tr(P_n\rho)$$

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- The probability of obtaining measurement result *m associated with measurement operator* M_m *is*

$$P(m) = Tr(M_m^\dagger M_m \rho)$$

- After a measurement, the system is in the state described by

$$\rho \rightarrow \frac{P_n \rho P_n}{Tr(P_n \rho)}$$

- The state of the system after measurement is

- $$\frac{M_m \rho M_m^\dagger}{Tr(M_m^\dagger M_m \rho)}$$

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- **CHARACTERIZING MIXED STATES**
  - A mixed state is a classical statistical mixture of two or more states. The state has no coherences. Therefore the off-diagonal terms of the density operator are zero, that is, $\rho_{mn} = 0$ *when* $m = n$.
  - A pure state will have nonzero off-diagonal terms.
- In summary:
  - $Tr(\rho^2) < 1$ *for a mixed state.*
  - $Tr(\rho^2) = 1$ *for a pure state.*

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- **Completely Mixed States**
- In a completely mixed state the probability for the system to be in each given state is identical. the state space has *n dimensions, then*

$$\rho = \frac{1}{n} I$$

$$Tr(\rho^2) = Tr\left(\frac{1}{n^2} I\right) = \frac{1}{n^2} Tr(I) = \frac{1}{n}$$

- In most if not all cases of interest to us, *n =2.*

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- **THE PARTIAL TRACE AND THE REDUCED DENSITY OPERATOR**
- A very important application of the density operator is in the characterization of composite systems.
- The density operator is a very useful tool for characterizing and working with states of subsystems.

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- A typical example is imagining that Alice and Bob each share one member of an entangled EPR pair. Let's suppose that the system is in one of the Bell states

$$|\beta_{10}\rangle = \frac{|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle}{\sqrt{2}}$$

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- We construct the density operator for a composite system the same way we have been doing for individual systems. The density operator for this particular state is

$$
\begin{aligned}
\rho &= |\beta_{10}\rangle\langle\beta_{10}| \\
&= \left(\frac{|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle}{\sqrt{2}}\right)\left(\frac{\langle 0_A|\langle 0_B| - \langle 1_A|\langle 1_B|}{\sqrt{2}}\right) \\
&= \frac{|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B| - |1_A\rangle|1_B\rangle\langle 0_A|\langle 0_B| + |1_A\rangle|1_B\rangle\langle 1_A|\langle 1_B|}{2}
\end{aligned}
$$

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- Now, if Alice and Bob fly off in opposite directions, neither one of them alone has access to the complete system. We need a tool that will tell us what Alice alone sees and what Bob alone sees.
- To implement the partial trace, we compute the trace by summing over the basis states of one party alone. Let's say for the sake of example that we're in Bob's shoes. Then we need to trace over Alice's basis states. We have

$$\rho_B = Tr_A(\rho) = Tr_A(|\beta_{10}\rangle\langle\beta_{10}|) = \langle 0_A|(|\beta_{10}\rangle\langle\beta_{10}|)|0_A\rangle + \langle 1_A|(|\beta_{10}\rangle\langle\beta_{10}|)|1_A\rangle$$

-

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- Using our expression for *ρ, we have*

$$
\begin{aligned}
&\langle 0_A|(|\beta_{10}\rangle\langle\beta_{10}|)|0_A\rangle \\
&= \langle 0_A|\left(\frac{|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B|-|0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|-|1_A\rangle|1_B\rangle\langle 0_A|\langle 0_B|+|1_A\rangle|1_B\rangle\langle 1_A|\langle 1_B|}{2}\right)|0_A\rangle \\
&= \frac{1}{2}\left(\frac{\begin{array}{c}\langle 0_A|0_A\rangle|0_B\rangle\langle 0_B|\langle 0_A|0_A\rangle - \langle 0_A|0_A\rangle|0_B\rangle\langle 1_B|\langle 0_A|1_A\rangle - \langle 0_A|1_A\rangle|1_B\rangle\langle 0_B|\langle 0_A|0_A\rangle \\ + \langle 0_A|1_A\rangle|1_B\rangle\langle 1_B|\langle 1_A|0_A\rangle\end{array}}{2}\right) \\
&= \frac{|0_B\rangle\langle 0_B|}{2}
\end{aligned}
$$

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$$
\begin{aligned}
&\langle 1_A|(|\beta_{10}\rangle\langle\beta_{10}|)|1_A\rangle \\
&\quad = \langle 1_A|\left(\frac{|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B|-|0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|-|1_A\rangle|1_B\rangle\langle 0_A|\langle 0_B|+|1_A\rangle|1_B\rangle\langle 1_A|\langle 1_B|}{2}\right)|1_A\rangle \\
&\quad = \frac{1}{2}\left(\frac{\begin{array}{c}\langle 1_A|0_A\rangle|0_B\rangle\langle 0_B|\langle 0_A|1_A\rangle - \langle 1_A|0_A\rangle|0_B\rangle\langle 1_B|\langle 0_A|1_A\rangle - \langle 1_A|1_A\rangle|1_B\rangle\langle 0_B|\langle 0_A|1_A\rangle \\ +\langle 1_A|1_A\rangle|1_B\rangle\langle 1_B|\langle 1_A|1_A\rangle\end{array}}{2}\right) \\
&\quad = \frac{|1_B\rangle\langle 1_B|}{2}
\end{aligned}
$$

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- So the density operator for Bob is

$$\rho_B = Tr_A(\rho) = Tr_A(|\beta_{10}\rangle\langle\beta_{10}|) = \langle 0_A|(|\beta_{10}\rangle\langle\beta_{10}|)|0_A\rangle + \langle 1_A|(|\beta_{10}\rangle\langle\beta_{10}|)|1_A\rangle$$
$$= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2}$$

- We dropped the subscripts because this is Bob's state alone. The matrix representation with respect to Bob's {|0>,|1>} basis is

$$\rho_B = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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- Notice that *$Tr(\rho_B)$=1/2+1/2=1 (remember, the trace of a density matrix is always 1).*
- Now let's square it. This is easy because we just have the identity matrix:

$$\rho_B = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{I}{2}, \Rightarrow \rho_B^2 = \frac{I^2}{4} = \frac{1}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

- Then we have $Tr(\rho_B^2) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2} < 1$
- That is, Bob has a *completely mixed state.*