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Density Matrix and Decoherence

Incomplete knowledge about a quantum system adds a new layer of randomness to the state of the system, which can no longer be described by a vector in the state space, a pure state. The description requires ensembles that represent mixed states. The essence of ensembles is encoded in the density matrix, a Hermitian, positive semidefinite operator of unit trace. For quantum systems with two interacting subsystems, also called bipartite systems, the state of any subsystem is generally a mixed state which requires a density matrix for its description, even when the total system is in a pure state. The structure of pure, entangled states of a bipartite system is captured by the Schmidt decomposition, which relates it to the density matrices of the subsystems. We look at decoherence, the process in which the pure state of a subsystem becomes mixed, and consider a phenomenological description of the process via the Lindblad equation. We conclude with a look at measurements in quantum mechanics, contrasting the postulates of the Copenhagen interpretation with insights from decoherence and other interpretations.

22.1 Ensembles and Mixed States

We have seen that probabilities play a central and inescapable role in quantum mechanics. This is quite striking, given that in classical physics probabilities arise *only* due to lack of knowledge about the system. If we toss dice and are unable or unwilling to investigate the myriad factors that in principle determine the outcome, we have to consider probabilities for the possible results. In quantum mechanics, however, perfect knowledge still does not do away with probabilities. Consider a state $|\psi\rangle \in V$, with V an N-dimensional complex vector space. Even if the state is known exactly, its properties, as defined by the observables in the theory, are only determined probabilistically. This is not for lack of information, we believe. We have seen that, at least in the simplest setups, local hidden variables carrying information whose absence leads to probabilities are not consistent with experiment. Given the probabilistic interpretation of quantum mechanics, experiments are understood in the framework provided by an *ensemble*: multiple copies of the quantum system, all in the same state $|\psi\rangle$. Measurements performed on each of the elements of the ensemble can be used to confirm the expected probabilities. This is the *intrinsic* randomness of quantum mechanics.

Interestingly, the randomness that arises in classical mechanics due to lack of knowledge, which requires probabilities, has a counterpart in quantum mechanics and adds a *new layer of randomness* to the theory. We will first consider how this new layer also arises in quantum mechanics due to incomplete knowledge. As we will see, in this situation it is useful to consider more general kinds of ensembles. At a more fundamental level, however, we will note that this new randomness arises naturally in quantum mechanics *even* with complete knowledge. This happens in the description of a *subsystem* that happens to be entangled with the rest of the system. This is a good reason to view this new layer of randomness as a general feature of quantum mechanics. As we discuss the issues and complications associated with general ensembles, we will be led to the concept of a density matrix, an *operator* on the state space of the theory that encodes the quantum state of the system and includes this added layer of randomness. A **pure state** is a familiar state $|\psi\rangle \in V$, a vector in the Hilbert space of the theory, a wave function. On the other hand, if we have extra randomness and the state of the quantum system cannot be described by a vector in V, we have a **mixed state**.

To show how lack of knowledge introduces randomness in quantum mechanics, let us reconsider the Stern-Gerlach experiment. In this experiment the beam of silver atoms that emerges from the hot oven is unpolarized: the spin one-half state of the atoms is random. If we denote the spin state of an atom as $|\mathbf{n}\rangle$ with $\mathbf{n}$ a unit vector, the different atoms have vectors **n** pointing in random directions. Can we find a quantum state $|\psi\rangle$ whose intrinsic randomness affords a description of the atoms in the beam as an ensemble of $|\psi\rangle$? The answer is clearly no. The general state is

$$|\psi\rangle = a_+|+\rangle + a_-|-\rangle, \quad a_+, a_- \in \mathbb{C}, \tag{22.1.1}$$

with $|\pm\rangle$ the familiar $\hat{S}_z$ eigenstates. The state $|\psi\rangle$, a pure state, is fixed when the coefficients a_+ and a_- are fixed, but this also fixes the direction **n** of the spin state. Thus, a state $|\psi\rangle$ as above does not describe states $|\mathbf{n}\rangle$ with random **n**.

While we will deal with the case of random **n** later, let us consider a simpler situation. Assume you have an oven in which 50% of the atoms come out polarized as $|+\rangle$ and the other 50% come out polarized as $|-\rangle$. We can describe the beam by writing the pairs $(p_i, |\psi_i\rangle)$ in which we give the probability p_i of a given atom to be in the quantum state $|\psi_i\rangle$. For the situation we just described, we would write

$$E_z = \left\{ \left(\tfrac{1}{2}, |+\rangle\right), \ \left(\tfrac{1}{2}, |-\rangle\right) \right\}. \tag{22.1.2}$$

We used the label E_z for the *ensemble* of z-polarized states. We say that this ensemble has two *entries*, each entry consisting of a state and its probability. The ensemble here is providing a representation of the mixed state of our system. We can visualize the collection of atoms as a very large ensemble built by joining two equal-size ensembles, one built solely from states that are all $|+\rangle$, and the other built solely from states that are all $|-\rangle$. This is a more general ensemble than one in which all copies of the system are in the same quantum state.

For a general ensemble E associated to a quantum system with state space V, we have a list of states and probabilities:

$$E = \left\{ (p_1, |\psi_1\rangle), \ \ldots, (p_n, |\psi_n\rangle) \right\}, \quad p_1, \ldots, p_n > 0, \quad p_1 + \cdots + p_n = 1. \tag{22.1.3}$$

Here $n \geq 1$ is an integer denoting the number of entries in the ensemble. The ensemble provides a description of a general mixed state. The states $|\psi_a\rangle \in V$ above are all normalized:

$$\langle \psi_a | \psi_a \rangle = 1 \quad \text{for all} \quad a = 1, \ldots, n. \tag{22.1.4}$$

However, they are *not* required to be orthogonal to each other. We can imagine the ensemble E containing a large number M of copies of the system, with $p_a \cdot M$ copies in the state $|\psi_a\rangle$, for each $a = 1, \ldots, n$. The number n need not be related to the dimensionality $\dim V$ of the state space. We can have $n = 1$, in which case $p_1 = 1$, and the ensemble represents a pure state $|\psi_1\rangle$; all elements of the ensemble are in this state. For $n \geq 2$, we have a mixed state. We can also have $n > \dim V$ since the states $|\psi_a\rangle$ are not required to be linearly independent. In fact, nothing goes wrong if $n = \infty$, and the ensemble contains an infinite set of entries.

If $\hat{Q}$ denotes a Hermitian operator we are to measure, its expectation value $\langle \hat{Q} \rangle_E$ in the ensemble E is given by

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle = p_1 \langle \psi_1 | \hat{Q} | \psi_1 \rangle + \cdots + p_n \langle \psi_n | \hat{Q} | \psi_n \rangle. \tag{22.1.5}$$

This is clear if we imagine measuring $\hat{Q}$ on the full ensemble E. The expectation value $\langle \psi_a | \hat{Q} | \psi_a \rangle$ of $\hat{Q}$ in the ath subensemble of states $|\psi_a\rangle$ must be weighted by the probability p_a that gives the fraction of all states in E that are in the subensemble. Then we must add the contributions from all values of a. In our example above, where silver atoms emerge as described by the ensemble E_z in (22.1.2), we would see that

$$\langle \hat{Q} \rangle_{E_z} = \tfrac{1}{2} \langle + | \hat{Q} | + \rangle + \tfrac{1}{2} \langle - | \hat{Q} | - \rangle. \tag{22.1.6}$$

Suppose, however, that you are now in possession of an oven that produces 50% of atoms in the state $|x; +\rangle$ and the other 50% in the state $|x; -\rangle$. The ensemble E_x here would be

$$E_x = \Big\{ \big(\tfrac{1}{2}, |x; +\rangle \big), \ \big(\tfrac{1}{2}, |x; -\rangle \big) \Big\}. \tag{22.1.7}$$

The expectation value of $\hat{Q}$ in this ensemble is

$$\langle \hat{Q} \rangle_{E_x} = \tfrac{1}{2} \langle x; + | \hat{Q} | x; + \rangle + \tfrac{1}{2} \langle x; - | \hat{Q} | x; - \rangle. \tag{22.1.8}$$

A curious result emerges if we use $|x; \pm\rangle = \frac{1}{\sqrt{2}} (|+\rangle \pm |-\rangle)$ to rewrite $\langle \hat{Q} \rangle_{E_x}$:

$$\langle \hat{Q} \rangle_{E_x} = \tfrac{1}{4} (\langle + | + \langle - |) \hat{Q} (|+\rangle + |-\rangle) + \tfrac{1}{4} (\langle + | - \langle - |) \hat{Q} (|+\rangle - |-\rangle). \tag{22.1.9}$$

The off-diagonal matrix elements of $\hat{Q}$ cancel out, and we are left with

$$\langle \hat{Q} \rangle_{E_x} = \tfrac{1}{2}\langle + | \hat{Q} | + \rangle + \tfrac{1}{2}\langle - | \hat{Q} | - \rangle = \langle \hat{Q} \rangle_{E_z}. \tag{22.1.10}$$

The expectation values are identical in the two ensembles E_z and E_x. Since this is true for arbitrary observables, we must conclude that no matter how different the ensembles are they are indistinguishable and thus physically equivalent. Both ensembles in fact represent the same beam coming out of the oven; they represent the same mixed state. With rather different ensembles turning out to be equivalent, we are led to find a better way to represent the mixed quantum state of a particle in the beam. This will be done with density matrices.

Example 22.1. *Unpolarized ensemble.*

The oven in the Stern-Gerlach experiment produces unpolarized silver atoms. We wish to write the expectation value of $\hat{Q}$ in this ensemble and compare it with the result for the E_z ensemble.

In an unpolarized state, the values of $\mathbf{n}$ are uniformly distributed over solid angle. Since the total solid angle is 4π, the probability that the vector $\mathbf{n}$ is within a solid angle $d\Omega$ is $d\Omega/(4\pi)$. The unpolarized ensemble E_{unp} is defined with an infinite number of entries composed by probabilities and states for all possible $d\Omega$:

$$E_{\text{unp}} = \bigcup_{d\Omega} \Big(\tfrac{d\Omega}{4\pi},\ |\mathbf{n}(\theta,\phi)\rangle \Big), \quad |\mathbf{n}(\theta,\phi)\rangle = \cos\tfrac{\theta}{2}|+\rangle + \sin\tfrac{\theta}{2}e^{i\phi}|-\rangle. \tag{22.1.11}$$

The expectation value of any observable $\hat{Q}$ in this ensemble is obtained by integration:

$$\begin{aligned}\langle \hat{Q} \rangle_{E_{\text{unp}}} &= \int \frac{d\Omega}{4\pi} \langle \mathbf{n}(\theta,\phi) | \, \hat{Q} \, | \mathbf{n}(\theta,\phi) \rangle \\ &= \frac{1}{4\pi} \int \sin\theta d\theta d\phi \big(\cos\tfrac{\theta}{2}\langle + | + \sin\tfrac{\theta}{2}e^{-i\phi}\langle - |\big)\hat{Q}\big(\cos\tfrac{\theta}{2}|+\rangle + \sin\tfrac{\theta}{2}e^{i\phi}|-\rangle\big).\end{aligned} \tag{22.1.12}$$

The integral over ϕ kills the off-diagonal matrix elements of $\hat{Q}$, and we find that

$$\langle \hat{Q} \rangle_{E_{\text{unp}}} = \tfrac{1}{2}\int_0^\pi \sin\theta d\theta \big(\cos^2\tfrac{\theta}{2}\langle + | \hat{Q} | + \rangle + \sin^2\tfrac{\theta}{2}\langle - | \hat{Q} | - \rangle\big). \tag{22.1.13}$$

Both integrals evaluate to one, and the result is

$$\langle \hat{Q} \rangle_{E_{\text{unp}}} = \tfrac{1}{2}\langle + | \hat{Q} | + \rangle + \tfrac{1}{2}\langle - | \hat{Q} | - \rangle\big). \tag{22.1.14}$$

This is once more the same expectation value we found in the ensembles E_z and E_x. This shows that the unpolarized ensemble E_{unp} is in fact physically equivalent to the ensembles where half the states are polarized in one direction and the other half in the opposite direction. We checked this for states along z and along x. You should now check it for arbitrary direction.

□

Exercise 22.1. *Prove that the ensemble where 50% of the states are* $|\mathbf{n}; +\rangle$ *and the other 50% are* $|\mathbf{n}; -\rangle$*, for arbitrary but fixed unit vector* $\boldsymbol{n}$*, is physically equivalent to the unpolarized ensemble.*

An even simpler example of quantum states described by ensembles is provided by a pair of entangled states. Let Alice and Bob each have one of two entangled spin one-half states. The entangled state $|\psi_{AB}\rangle$ they share is the singlet state of total spin equal to zero:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\big). \tag{22.1.15}$$

Assume Alice measures the spin of her state along the z-direction. If Alice gets $|+\rangle$, then the state of Bob is $|-\rangle$; if Alice gets $|-\rangle$, the state of Bob is $|+\rangle$. The state of Bob is known if we know the measurement Alice did *and* the result she found. If we do not know the result of her measurement, the situation for Bob is less clear.

Suppose all we know is that Alice measured along the z-direction. What then is the state of Bob's particle? To answer this we can again think in terms of an ensemble in which each element contains the entangled pair $|\psi_{AB}\rangle$. If Alice measures along z, about half of the time she will get $|+\rangle$, and the other half of the time she will get $|-\rangle$. As a consequence, in half of the elements of the ensemble the state of Bob will be $|-\rangle$, and in the other half, the state of Bob will be $|+\rangle$. The state of Bob can be described by the ensemble E_{Bob} that reads

$$E_{\text{Bob}} = \Big\{\big(\tfrac{1}{2}, |+\rangle\big), \big(\tfrac{1}{2}, |-\rangle\big)\Big\}. \tag{22.1.16}$$

Suppose, instead, that Alice decides to measure in an arbitrary direction **n**. To analyze this, it is convenient to use the rotational invariance of the singlet state to rewrite it as follows:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\big(|\mathbf{n};+\rangle_A|\mathbf{n};-\rangle_B - |\mathbf{n};-\rangle_A|\mathbf{n};+\rangle_B\big). \tag{22.1.17}$$

If Alice measures and the result is not known, the state of Bob is again an ensemble. Since the probabilities that she finds $|\mathbf{n};-\rangle$ and $|\mathbf{n};+\rangle$ are the same, the correlations in the entangled state imply that this time the ensemble for Bob's state is

$$E_{\text{Bob}} = \Big\{\big(\tfrac{1}{2}, |\mathbf{n};+\rangle\big), \big(\tfrac{1}{2}, |\mathbf{n};-\rangle\big)\Big\}. \tag{22.1.18}$$

The two ensembles that we get, from Alice measuring along z and along **n**, are equivalent, as we demonstrated before by considering expectation values. Again, we wish to have a better understanding of why the state of Bob's particle did not depend on the direction Alice used to make her measurement.

Example 22.2. *Absence of a pure-state description of an entangled particle.*

Let us now consider again the same entangled state of two particles, one held by Alice and the other by Bob:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\big). \tag{22.1.19}$$

Is there a state $|\psi_A\rangle$ of Alice's particle that summarizes all we know about this particle?

If such a state existed, we would require the expectation value of any observable $\hat{Q}$ in $|\psi_A\rangle$ to be equal to the expectation value of $\hat{Q} \otimes \mathbb{1}$ in $|\psi_{AB}\rangle$:

$$\langle\psi_A|\hat{Q}|\psi_A\rangle = \langle\psi_{AB}|\hat{Q}\otimes\mathbb{1}|\psi_{AB}\rangle? \tag{22.1.20}$$

We will see that there is *no* such state $|\psi_A\rangle$. No pure state can represent Alice's state if it is entangled with another state. To see this we examine the cases when $\hat{Q}$ is σ_x, σ_y, and σ_z. Note that

$$\begin{aligned}
\sigma_x \otimes \mathbb{1}|\psi_{AB}\rangle &= \tfrac{1}{\sqrt{2}}\big(|-\rangle_A|-\rangle_B - |+\rangle_A|+\rangle_B\big),\\
\sigma_y \otimes \mathbb{1}|\psi_{AB}\rangle &= i\tfrac{1}{\sqrt{2}}\big(|-\rangle_A|-\rangle_B + |+\rangle_A|+\rangle_B\big),\\
\sigma_z \otimes \mathbb{1}|\psi_{AB}\rangle &= \tfrac{1}{\sqrt{2}}\big(|+\rangle_A|-\rangle_B + |-\rangle_A|+\rangle_B\big).
\end{aligned} \tag{22.1.21}$$

It follows quickly that all three expectation values vanish:

$$\langle\psi_{AB}|\sigma_x \otimes \mathbb{1}|\psi_{AB}\rangle = \langle\psi_{AB}|\sigma_y \otimes \mathbb{1}|\psi_{AB}\rangle = \langle\psi_{AB}|\sigma_z \otimes \mathbb{1}|\psi_{AB}\rangle = 0. \tag{22.1.22}$$

If a pure-state representative $|\psi_A\rangle$ of Alice's particle exists, then it must then satisfy

$$\langle\psi_A|\sigma_x|\psi_A\rangle = \langle\psi_A|\sigma_y|\psi_A\rangle = \langle\psi_A|\sigma_z|\psi_A\rangle = 0. \tag{22.1.23}$$

There is in fact a simple proof that the state $|\psi_A\rangle$ with vanishing expectation values for σ_x, σ_y, and σ_z does not exist. Any spin state points somewhere, and therefore $|\psi_A\rangle = \gamma|\mathbf{n}\rangle$, for some constant $\gamma \neq 0$ and some direction $\mathbf{n}$. But we also have $\langle\mathbf{n}|\mathbf{n}\cdot\boldsymbol{\sigma}|\mathbf{n}\rangle = 1$. This means $\mathbf{n}\cdot\boldsymbol{\sigma}$ has a nonzero expectation value in $|\psi_A\rangle$, but this is impossible if all three Pauli matrices have zero expectation value in $|\psi_A\rangle$.

□

We have thus shown that there is no pure state representing the quantum state of Alice's particle when entangled. How do we describe such a quantum state? By using a density matrix. The description of the state of an entangled particle is given in all generality in section 22.4.