Pure versus Mixed States in Quantum Mechanics

Podcast Learn & Fun *

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In quantum mechanics, the state of a system is a fundamental concept. It describes everything that can be known about the system at a given moment in time. The state of a quantum system can be expressed in several ways, but for simplicity, we will focus on two key representations: (1) *Pure States*: A pure state represents complete knowledge of the system. The system is in a definite quantum state, and there is no ambiguity or uncertainty about its state. (2) *Mixed States*: A mixed state, on the other hand, represents incomplete knowledge of the system. The system may not be in a single, well-defined quantum state, but rather in a statistical mixture of several possible pure states.

While these two states are conceptually different, they are also connected in the broader framework of quantum mechanics. Understanding them both is key to navigating the complexities of quantum systems.

Pure States

A *pure state* is the simplest and most fundamental description of a quantum system. It represents a system with complete and precise knowledge of its quantum state. Mathematically, a pure state can be described by a *state vector* or a *wavefunction*. The state vector is typically denoted as $|\psi\rangle$, and it contains all the information about the system. A pure state is always *deterministic*: if we know the pure state of a system, we can predict its future evolution, given the system is not influenced by external randomness.

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Example: Consider a simple quantum system, such as a qubit. A qubit can exist in a superposition of the computational basis states $|0\rangle$ and $|1\rangle$. A pure state of this qubit might look like:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where α and β are complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$. This state represents a superposition of $|0\rangle$ and $|1\rangle$, with α and β determining the probability of measuring the qubit in one of these states. If we measure the qubit in the standard computational basis, there are specific probabilities associated with each outcome. The probability of measuring $|0\rangle$ is $|\alpha|^2$, and the probability of measuring $|1\rangle$ is $|\beta|^2$. These probabilities are *deterministic*, based on the coefficients α and β of the state vector.

There are several key features of pure states: (1) **Coherence**: A pure state represents a situation where all parts of the quantum system are coherent, meaning they work together in a predictable, wave-like manner. For example, interference effects, such as those observed in the famous double-slit experiment, are only observed when the system is in a pure state. (2) **Uncertainty**: While pure states allow for complete knowledge of a system's quantum state, there may still be uncertainty in certain measurements, depending on the basis chosen. For instance, the exact value of an observable like position or momentum may still be uncertain due to the Heisenberg uncertainty principle. However, the state itself is fully determined. (3) **Reversibility**: The evolution of a pure state is reversible, meaning that if we know the state at one point in time, we can calculate the state at any future or past time, given the dynamics of the system.

In a pure state, the quantum system is completely isolated from any outside influences that would cause it to lose its coherence. We can think of a pure state as being in a "well-defined" or "ideal" condition. For example, a photon traveling in a vacuum with a definite energy, frequency, and direction of travel might be described by a pure state.

Mixed States

A *mixed state* represents a situation where the quantum system is not in a single, definite state. Instead, the system is in a probabilistic mixture of multiple possible pure states. This means that, from our perspective, we do not have complete knowledge of the system's state. Instead, we only know the probabilities with which the system could be in each of these possible states.

A mixed state arises when a system is subject to external influences or when we cannot observe all the components of the system. It could also occur due to *decoherence*, which is the loss of quantum coherence caused by interaction with the environment.

Example: Imagine a qubit, but this time, we don't know if it's in the pure state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. Instead, it could be in either $|0\rangle$ with probability p_0, or in $|1\rangle$ with probability p_1, where $p_0 + p_1 = 1$. The state of the qubit is not described by a single state vector, but by the fact that the qubit is in either of the pure states $|0\rangle$ or $|1\rangle$ with some probability. In this case, measuring the state of the qubit would yield either $|0\rangle$ or $|1\rangle$, with the respective probabilities. However, we no longer have any information about the relative phases between the states, and the coherence between $|0\rangle$ and $|1\rangle$ is lost.

There are several key features of pure states: (1) **Incoherence**: Mixed states often describe systems that lack coherence. This means that the system behaves more randomly, and the evolution of the system is not as predictable as for pure states. In fact, measurements on a mixed state will give results that are less deterministic and more probabilistic. (2) **Probabilistic Nature**: A mixed state represents a system that is in a probabilistic combination of pure states. It is not in any one specific pure state, but rather in a "blend" of them. For example, a coin toss could be seen as a mixed state, where the system is in either the heads or tails state, but we don't know which one. (3) **Irreversibility**: Mixed states can arise in open systems that interact with their environment. This interaction often leads to the irreversible loss of coherence, making it impossible to exactly reverse the system's evolution. Unlike pure states, where we can trace the system's evolution backward, the state of a system in a mixed state may be fundamentally unpredictable.

Mixed states often arise in real-world quantum systems where complete isolation from the environment is impossible. For example, a system at thermal equilibrium in a heat bath is typically in a mixed state, where the system's particles are in a range of energy states with varying probabilities, rather than in one well-defined quantum state.

Another example is a qubit in a noisy quantum computer. Even though the qubit may start in a pure state, interactions with the environment (such as electromagnetic noise or imperfections in the hardware) lead the qubit to lose its coherence, and it becomes a mixed state.

Comparing Pure and Mixed States

Knowledge vs. Uncertainty

The most fundamental difference between pure and mixed states is the degree of knowledge about the system. A pure state reflects complete knowledge about the system, whereas a mixed state reflects incomplete knowledge. In other words, when we know the exact pure state, we can predict all future behavior of the system. When we deal with a mixed state, we only know the probabilities of different outcomes, and there is inherent uncertainty in the system's state.

Coherence

Pure states exhibit quantum coherence, which allows for interference effects, superposition, and entanglement. In contrast, mixed states result from a loss of coherence, and as such, they cannot exhibit the same interference effects that pure states can.

Reversibility

The evolution of a pure state is reversible, as we can trace its time evolution in both directions. However, mixed states often result from interactions with an environment, and this process is typically irreversible. The loss of coherence in a mixed state generally leads to the system becoming entangled with its environment, making its evolution much harder to reverse.

Applications

- **Quantum Computing**: In ideal quantum computing scenarios, qubits are initially in pure states. However, in real quantum computers, qubits often end up in mixed states due to noise and decoherence. Quantum error correction methods are used to mitigate the effects of mixed states.

- **Thermal Systems**: Systems at finite temperature are described by mixed states, as the system's particles are in a range of energy states with varying probabilities, rather than in one well-defined quantum state.

- **Quantum Entanglement**: While pure states are ideal for discussing entanglement, mixed states can also exhibit entanglement, though the entanglement is generally weaker and harder to characterize.

Conclusion

To conclude, pure states describe systems with complete knowledge, coherence, and determinism. They allow for predictable behavior and interference effects. In contrast, mixed states represent systems with incomplete knowledge, incoherence, and probabilistic behavior. Understanding the difference between pure and mixed states is key to understanding how quantum systems behave, especially in complex, noisy environments like real-world quantum computers or thermal systems.