

5.1: Introduction to the Density Matrix

The **density matrix** or **density operator** is an alternate representation of the state of a quantum system for which we have previously used the wavefunction. Although describing a quantum system with the density matrix is equivalent to using the wavefunction, one gains significant practical advantages using the density matrix for certain time-dependent problems—particularly relaxation and nonlinear spectroscopy in the condensed phase.

The density matrix is defined as the outer product of the wavefunction with its conjugate.

$$\rho(t) \equiv |\psi(t)\rangle\langle\psi(t)| \quad (5.1.1)$$

This implies that if you specify a state $|x\rangle$, then $\langle x|\rho|x\rangle$ gives the probability of finding a particle in the state $|x\rangle$. Its name derives from the observation that it plays the quantum role of a probability density. If you think of the statistical description of a classical observable obtained from moments of a probability distribution P , then ρ plays the role of P in the quantum case:

$$\langle A \rangle = \int A P(A) dA \quad (5.1.2)$$

$$= \langle \psi | A | \psi \rangle = \text{Tr}[A\rho] \quad (5.1.3)$$

where $\text{Tr}[\dots]$ refers to tracing over the diagonal elements of the matrix,

$$\text{Tr}[\dots] = \sum_a \langle a | \dots | a \rangle. \quad (5.1.4)$$

The last expression is obtained as follows. If the wavefunction for the system is expanded as

$$|\psi(t)\rangle = \sum_n c_n(t) |n\rangle \quad (5.1.5)$$

the expectation value of an operator is

$$\langle \hat{A}(t) \rangle = \sum_{n,m} c_n(t) c_m^*(t) \langle m | \hat{A} | n \rangle \quad (5.1.6)$$

Also, from Equation 5.1.1 we obtain the elements of the density matrix as

$$\begin{aligned} \rho(t) &= \sum_{n,m} c_n(t) c_m^*(t) |n\rangle\langle m| \\ &\equiv \sum_{n,m} \rho_{nm}(t) |n\rangle\langle m| \end{aligned}$$

We see that ρ_{nm} , the density matrix elements, are made up of the time-evolving expansion coefficients. Substituting into Equation 5.1.6 we see that

$$\begin{aligned} \langle \hat{A}(t) \rangle &= \sum_{n,m} A_{mn} \rho_{nm}(t) \\ &= \text{Tr}[\hat{A}\rho(t)] \end{aligned}$$

In practice this makes evaluating expectation values as simple as tracing over a product of matrices.

What information is in the density matrix elements, ρ_{nm} ? The diagonal elements ($n = m$) give the probability of occupying a quantum state:

$$\rho_{nn} = c_n c_n^* = p_n \geq 0 \quad (5.1.7)$$

For this reason, diagonal elements are referred to as **populations**. The off-diagonal elements ($n \neq m$) are complex and have a time-dependent phase factor

$$\rho_{nm} = c_n(t) c_m^*(t) = c_n c_m^* e^{-i\omega_{nm}t} \quad (5.1.8)$$

Since these describe the coherent oscillatory behavior of coherent superpositions in the system, these are referred to as **coherences**.

So why would we need the density matrix? It becomes a particularly important tool when dealing with mixed states, which we take up later. Mixed states refer to statistical mixtures in which we have imperfect information about the system, for which we must perform statistical averages in order to describe quantum observables. For mixed states, calculations with the density matrix are greatly simplified. Given that you have a statistical mixture, and can describe p_k , the probability of occupying quantum state $|\psi_k\rangle$, evaluation of expectation values is simplified with a density matrix:

$$\langle \hat{A}(t) \rangle = \sum_k p_k \langle \psi_k(t) | \hat{A} | \psi_k(t) \rangle \quad (5.1.9)$$

$$\rho(t) \equiv \sum_k p_k |\psi_k(t)\rangle \langle \psi_k(t)| \quad (5.1.10)$$

$$\langle \hat{A}(t) \rangle = \text{Tr}[\hat{A}\rho(t)] \quad (5.1.11)$$

Evaluating expectation value is the same for pure or mixed states.

Properties of the Density Matrix

We can now summarize some properties of the density matrix, which follow from the definitions above:

1. ρ is Hermitian since $\rho_{nm}^* = \rho_{mn}$
2. Since probability must be normalized, $\text{Tr}(\rho) = 1$
3. We can ascertain the degree of “pure-ness” of a quantum state from

$$\text{Tr}(\rho^2) \begin{cases} = 1 & \text{for pure state} \\ < 1 & \text{for mixed state} \end{cases} \quad (5.1.12)$$

In addition, when working with the density matrix it is convenient to make note of these trace properties:

1. The trace over a product of matrices is invariant to cyclic permutation of the matrices:

$$\text{Tr}(ABC) = \text{Tr}(CAB) = \text{Tr}(BCA) \quad (5.1.13)$$

2. From this result we see that the trace is invariant to unitary transformation:

$$\text{Tr}(S^\dagger AS) = \text{Tr}(S^{-1}AS) = \text{Tr}(A) \quad (5.1.14)$$

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