

Quantum Mechanics II Lecture 2

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Density Matrix

Assume we have an ensemble of N_{tot} particles, each of which can be in one of n states. Then the density matrix of that system can be expressed in one of two ways:

$$\rho = \frac{1}{N_{tot}} \sum_{i=1}^{N_{tot}} |\psi_i\rangle \langle \psi_i| \quad (1)$$

$$\rho = \sum_{i=1}^n p_i |\psi_i\rangle \langle \psi_i| \quad (2)$$

where p_i is the probability of being in state i . Equation 1 assumes that each particle is in a well defined state and sums over all particles in the ensemble, while equation 2 sums over all possible *states* of the particles and multiplies by the probability of that state.

Claim:

The density matrix contains all possible knowable information about a system. This can be proven by showing that the expectation value of any arbitrary operator can be found with no other knowledge of the system.

Proof:

First we need to slightly redefine the expectation value of an operator: It is now an average over the expectation values for all possible states (indicated by the $\langle \rangle$ brackets), weighted by probability (indicated by an overbar):

$$\langle \overline{\mathcal{O}} \rangle = \sum_i p_i \langle \psi_i | \mathcal{O} | \psi_i \rangle \quad (3)$$

We start by taking the trace of the matrix $\mathcal{O}\rho$.¹

$$\begin{aligned} \text{Tr}(\mathcal{O}\rho) &= \sum_j \langle j | \mathcal{O}\rho | j \rangle \\ &= \sum_{i,j} \langle j | \mathcal{O} p_i | \psi_i \rangle \langle \psi_i | j \rangle \\ &= \sum_{i,j} p_i \langle \psi_i | j \rangle \langle j | \mathcal{O} | \psi_i \rangle \\ &= \sum_i p_i \langle \psi_i | \mathcal{O} | \psi_i \rangle = \langle \overline{\mathcal{O}} \rangle \end{aligned} \quad (4)$$

So, all knowable information about the system is contained within the density matrix.

Vector space of operators

Given some vector space \mathbb{V} with basis $|j\rangle$. We can now define a corresponding vector space $\mathbb{V} \otimes \mathbb{V}$ of all *operators* on \mathbb{V} . Clearly, operators can be added, multiplied with scalars etc. in a linear fashion. But we can also define an inner (scalar) product between operators,

$$\mathcal{O}_1 \cdot \mathcal{O}_2 = \text{Tr}(\mathcal{O}_1^\dagger \mathcal{O}_2). \quad (5)$$

This can be proven to fulfill all of the requirements for an inner product; it also makes sense if you think of an operator as a $n \times n$ matrix which can be “stretched” into a single column by arranging the second column below the first one and so on. In that case, the trace is just the usual scalar product between the two resulting “vectors”. We can now find orthonormal bases for this vector space; one “obvious” example is

$$\mathcal{O}_{ij} = \frac{1}{\sqrt{n}} |i\rangle \langle j|. \quad (6)$$

¹The trace of a square matrix is the sum of its diagonal components.

As a consequence, we can expand any operator in this basis, with coefficients given by the inner product:

$$\mathcal{P} = \sum_{i,j} Tr(\mathcal{O}_{ij}^\dagger \mathcal{P}) \mathcal{O}_{ij}. \quad (7)$$

Polarization

Let's consider the vector space for operators on spin- $\frac{1}{2}$ particles, \mathbb{V}^4 . In this space there are a multitude of bases that will span the entire space, but only two that we normally focus on:

The "special basis": $\frac{1}{\sqrt{2}}|\uparrow\rangle\langle\uparrow|$, $\frac{1}{\sqrt{2}}|\uparrow\rangle\langle\downarrow|$, $\frac{1}{\sqrt{2}}|\downarrow\rangle\langle\uparrow|$, $\frac{1}{\sqrt{2}}|\downarrow\rangle\langle\downarrow|$

The Pauli spin matrix basis: $\frac{1}{\sqrt{2}}\sigma_0$, $\frac{1}{\sqrt{2}}\sigma_x$, $\frac{1}{\sqrt{2}}\sigma_y$, $\frac{1}{\sqrt{2}}\sigma_z$

We can write any operator in that vector space as a sum of the basis vectors:

$$\mathcal{O} = \frac{1}{\sqrt{2}} \sum_{j=0}^3 o_j \sigma_j \quad (8)$$

or

$$\begin{aligned} \mathcal{O} &= \frac{1}{\sqrt{2}} \sum_j Tr(\mathcal{O} \frac{1}{\sqrt{2}} \sigma_j) \sigma_j \\ &= \frac{1}{2} \sum_j Tr(\mathcal{O} \sigma_j) \sigma_j \end{aligned} \quad (9)$$

Now let's look again at the expectation value of an operator

$$\begin{aligned} \langle \overline{\mathcal{O}} \rangle &= \sum_i p_i \langle \psi_i | \mathcal{O} | \psi_i \rangle \\ &= \sum_i p_i \left\langle \psi_i \left| \frac{1}{2} \sum_j Tr(\mathcal{O} \sigma_j) \sigma_j \right| \psi_i \right\rangle \\ &= \sum_j \frac{1}{2} \underbrace{Tr(\mathcal{O} \sigma_j)}_{a_j} \underbrace{\sum_i p_i \langle \psi_i | \sigma_j | \psi_i \rangle}_{P_j} \\ &= \sum_j a_j P_j \end{aligned} \quad (10)$$

where a_j is the analyzing power² and P_j is the polarization.³ Note that, because of the definition, $P_0 = 1$ always.

Extreme Cases for Polarization

1: All particles are in the same state $|\psi_i\rangle$

In this case, the total polarization, $|\vec{P}|$ will be 1, which indicates the ensemble of particles is "pure". The polarization vector will point in the same direction that is given by the state vector for all particles.

2: All particles are in totally random states

In this case, \vec{P} will be 0, meaning there is no preferred state vector for the ensemble as a whole. One interesting point to be made about this case is that an ensemble of totally randomly oriented state vectors is indistinguishable from an ensemble of exactly half spin-up and half spin-down particles: both have $\vec{P} = 0$, but as stated before, the result of *any* measurement is completely determined by \vec{P} .

To make a connection between the polarization and the density matrix, recall that we can express any operator as a sum of the Pauli matrix vectors (including the density matrix). So,

$$\rho = \frac{1}{2} \sum_j Tr(\rho\sigma_j)\sigma_j \quad (11)$$

But what is $Tr(\rho\sigma_j)$? Well, let's express the trace as a sum:

$$\begin{aligned} Tr(\rho\sigma_j) &= \sum_k \left\langle k \left| \sum_i p_i |\psi_i\rangle \right. \right\rangle \langle \psi_i | \sigma_j | k \rangle \\ &= \sum_i p_i \langle \psi_i | \sigma_j | \psi_i \rangle \\ &= P_j \end{aligned} \quad (12)$$

So it turns out that $Tr(\rho\sigma_j)$ is simply the j^{th} component off the polarization, which leads to

$$\rho = \frac{1}{2} \sum_j P_j \sigma_j \quad (13)$$

²The analyzing power only contains information about the operator, not the system.

³The polarization contains information about the distribution of particle states in the system.

The density matrix is the only thing you need to know to have all knowledge of a system **IF** all the particles have no knowledge of each other. This is a much deeper statement than simply saying the particles don't interact, as we will see.