Chapter 1: Two Level Systems

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Table of Contents

Background: Pure vs. Mixed Ensembles

- A **pure** ensemble is a collection of physical systems such that every member is characterized by the same ket $|\alpha\rangle$
  - e.g. $|\alpha\rangle$ describes a state with spin pointing in the positive x-direction
- A **mixed** ensemble has a fraction of the members with relative population ω_1 are characterized by $|\alpha_1\rangle$ and some other fraction with relative population ω_2 characterized by $|\alpha_2\rangle$, and so on.
  - mixture of pure states

Sakurai, J., & Napolitano, J. (2017). *Modern Quantum Mechanics* (2nd ed.).

Background: Density Matrices

- A density operator, or matrix, (ρ) contains all the physically significant information about the ensemble of interest
  - Density matrices are Hermitian.
  - A mixed state density matrix can be defined as

$$\rho = \sum_i \omega_i |\alpha_i\rangle\langle\alpha_i|$$

where they must satisfy the condition $\mathrm{tr}(\rho) = 1$ and can contain any eigenvalues

e.g., after diagonalization, the matrix may look like:

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & .3 & 0 & 0 \\ 0 & 0 & .7 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Sakurai, J., & Napolitano, J. (2017). *Modern Quantum Mechanics* (2nd ed.).

Background: Density Matrices

– A pure state density matrix can be defined as

$$\rho = |\alpha_n\rangle\langle\alpha_n|$$

where ω_i equals 1 for $|\alpha_i\rangle$, and equals zero for all other state kets (n = i).

– Satisfies conditions:

$$\rho^2 = \rho \text{ (projection operator) ; } \mathrm{tr}(\rho) = 1$$

– The eigenvalues are either 0 or 1

i.e., after diagonalization, the matrix may look like:

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Example 1: Density matrices (from Final Exam Fall 1998)

Consider a spin 1/2 system. The projection operator P_z projects the component of the wave function that has positive spin along the z-axis.

$$\langle \eta | P_z | \eta \rangle = | \langle z, \uparrow | \eta \rangle |^2$$

a) Express P_z as a matrix in the basis where $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ denotes a state with positive spin along the z-axis.

b) Write down the density matrix for a state that is an incoherent mixture of 50% positive spin along the y-axis and 50% negative spin along the y-axis.

c) If the Hamiltonian is defined as:

$$\mathcal{H} = \alpha + \beta \sigma_x$$

Calculate the expectation of $\mathcal{H}$ for the state described in b.

Solution to Part a

a) Express P_z as a matrix in the basis where $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ denotes a state with positive spin along the z-axis.

To do this, we can find the density matrix for the projection operator starting with the initial state given

Initial state or basis: $|z, \uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\langle z, \uparrow| = \begin{pmatrix} 1 & 0 \end{pmatrix}$

Density matrix: $\rho_z = |z, \uparrow\rangle\langle z, \uparrow| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

Here, we recognize a projection operator is a density matrix of a pure state.

Solution to part b

b) Write down the density matrix for a state that is an incoherent mixture of 50% positive spin along the y-axis and 50% negative spin along the y-axis.

First, find the states: $|y, \uparrow\rangle$ and $|y, \downarrow\rangle$. Recognize these states are the eigenvectors of σ_y.

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Therefore,

$$|y, \uparrow\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$|y, \downarrow\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Solution to part b continued

b) From here, there is a 50% chance of being in either $|y,\uparrow\rangle$ or $|y,\downarrow\rangle$. You superimpose density matrix of $|y,\uparrow\rangle$ and the density matrix $|y,\downarrow\rangle$ to get the density matrix for this mixed state.

$$\rho = \frac{1}{2}\,|y,\uparrow\rangle\,\langle y,\uparrow| + \frac{1}{2}\,|y,\downarrow\rangle\,\langle y,\downarrow|$$

$$\rho = \frac{1}{2}*\frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}\begin{pmatrix}1 & i\end{pmatrix} + \frac{1}{2}*\frac{1}{2}\begin{pmatrix}1\\ -i\end{pmatrix}\begin{pmatrix}1 & -i\end{pmatrix}$$

$$\rho = \frac{1}{4}\begin{pmatrix}1 & i\\ i & -1\end{pmatrix} + \frac{1}{4}\begin{pmatrix}1 & -i\\ -i & -1\end{pmatrix}$$

$$\rho = \frac{1}{4}\begin{pmatrix}2 & 0\\ 0 & -2\end{pmatrix} = \begin{pmatrix}\frac{1}{2} & 0\\ 0 & -\frac{1}{2}\end{pmatrix}$$

Is there a mistake?

Solution to part b continued

b) Yes, we know there is a mistake because trace must equal 1. Previous solution was wrong because the complex conjugate was NOT done when calculating the bras.

$$\rho = \frac{1}{2}\ |y,\uparrow\rangle\ \langle y,\uparrow| + \frac{1}{2}\ |y,\downarrow\rangle\ \langle y,\downarrow|$$

$$\rho = \frac{1}{2}*\frac{1}{2}\begin{pmatrix} 1 \\ -i \end{pmatrix}\ \begin{pmatrix} 1 & i \end{pmatrix} + \frac{1}{2}*\frac{1}{2}\ \begin{pmatrix} 1 \\ i \end{pmatrix}\ \begin{pmatrix} 1 & -i \end{pmatrix}$$

$$\rho = \frac{1}{4}\ \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} + \frac{1}{4}\ \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$$

$$\rho = \frac{1}{4}\ \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

Solution to part c

c) If the Hamiltonian is defined as:

$$\mathcal{H} = \alpha + \beta\sigma_x$$

Calculate the expectation of $\mathcal{H}$ for the state described in *b*.

$$\mathcal{H} = \alpha \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \beta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}$$

$$\langle \mathcal{H} \rangle = \tfrac{1}{2} \langle y, \uparrow | \mathcal{H} | y, \uparrow \rangle + \tfrac{1}{2} \langle y, \downarrow | \mathcal{H} | y, \downarrow \rangle$$

$$\langle \mathcal{H} \rangle = \tfrac{1}{2}\,\tfrac{1}{2} \begin{pmatrix} 1 & -i \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix} + \tfrac{1}{2}\,\tfrac{1}{2} \begin{pmatrix} 1 & i \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\langle \mathcal{H} \rangle = \tfrac{1}{4} \begin{pmatrix} 1 & -i \end{pmatrix} \begin{pmatrix} \alpha + \beta i \\ \beta + \alpha i \end{pmatrix} + \tfrac{1}{4} \begin{pmatrix} 1 & i \end{pmatrix} \begin{pmatrix} \alpha - i\beta \\ \beta - i\alpha \end{pmatrix}$$

$$\langle \mathcal{H} \rangle = \tfrac{1}{4}\, 2\alpha + \tfrac{1}{4}\, 2\alpha$$

$$\langle \mathcal{H} \rangle = \alpha$$

Solution to part c - Second Method

c) This problem can also be done a second way

$$\langle \mathcal{H} \rangle = \text{tr}(\rho \mathcal{H})$$

$$\langle \mathcal{H} \rangle = \text{tr}(\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix})$$

$$\langle \mathcal{H} \rangle = \text{tr}(\begin{pmatrix} \frac{\alpha}{2} & \frac{\beta}{2} \\ \frac{\beta}{2} & \frac{\alpha}{2} \end{pmatrix})$$

$$\langle \mathcal{H} \rangle = \alpha$$

Thank you!