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Mathematical Physics (1C)
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Building Quantum Operators Modelling Measurement

(Probably, that is)

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Outline

Axioms of Quantum Mechanics

- In these slides, we will explicitly make use of the following axioms of quantum mechanics (QM):

Axioms used

1. The state $|\Psi\rangle$ of a quantum system $\mathcal{S}$ can be represented by a vector in a separable Hilbert space $\mathbb{H}$.
2. Observables on $\mathcal{S}$ can be represented by self-adjoint linear operators $\mathbb{H} \to \mathbb{H}$ on the Hilbert space of states $\mathbb{H}$ of the system $\mathcal{S}$.

- Notice that we have not mentioned an axiom from the Hilbert space formulation of QM, commonly called the **Born rule**. In one form, it states that the probability that a quantum measurement of an observable $\widehat{A}$ makes a state $|\Psi\rangle$ collapse to an eigenstate[1] $|a_k\rangle$ is,

Born rule

$$\mathrm{pr}\left(|a_k\rangle\right) = \langle\Psi\ |a_k\rangle\ \langle a_k\ |\Psi\rangle$$

We are, in fact, going to *derive* the above principle from a simpler assumption!

[1] a notion central to the Copenhagen interpretation of QM

Motivation

- The motivation for this study begins by asking why the Born rule involves an expectation value. Before making the observation[2], let us define the **expectation value** of a self-adjoint operator $\widehat{A} : \mathbb{H} \to \mathbb{H}$,

$$E\left(\widehat{A}\right) := \sum_k \mathrm{pr}\left(|a_k\rangle\right) a_k$$

where $\{a_k\}$ is a normalized eigenbasis for $\mathbb{H}$, i.e., any state $|\Psi\rangle \in \mathbb{H}$ can be written as a unique linear combination (over $\mathbb{C}$) of $\{a_k\}$ and, for all k,

$$\widehat{A}\,|a_k\rangle = a_k\,|a_k\rangle$$

$$\langle a_k | a_l \rangle = \delta_{kl} := \begin{cases} 1 & k = l \\ 0 & k \neq l \end{cases}$$

[2] For simplicity, we assume $\mathbb{H}$ has a dimension that is either finite or countably infinite.

- As a consequence of the above, $\langle a_k \mid a_k \rangle = 1$ and we have,

$$\begin{aligned} a_k &= a_k \langle a_k \mid a_k \rangle \\ &= \langle a_k | a_k | a_k \rangle \\ &= \left\langle a_k \middle| \widehat{A} \middle| a_k \right\rangle \end{aligned}$$

Plugging this into the definition of the expectation value of $\widehat{A}$,

Expectation values, without Born rule

$$E\left(\widehat{A}\right) = \sum_k \mathsf{pr}\left(|a_k\rangle\right) \left\langle a_k \middle| \widehat{A} \middle| a_k \right\rangle$$

Using the Born rule,

$$\begin{aligned} E\left(\widehat{A}\right) = \sum_k \mathsf{pr}\left(|a_k\rangle\right) \left\langle a_k \middle| \widehat{A} \middle| a_k \right\rangle &= \sum_k \langle \Psi \mid a_k \rangle \langle a_k \mid \Psi \rangle \left\langle a_k \middle| \widehat{A} \middle| a_k \right\rangle \\ &= \sum_k \sum_l \langle \Psi \mid a_k \rangle \left\langle a_k \middle| \widehat{A} \middle| a_l \right\rangle \langle a_l \mid \Psi \rangle \\ &= \left\langle \Psi \middle| \widehat{A} \middle| \Psi \right\rangle \end{aligned}$$

- Therefore, the Born rule simplifies the expression for the expectation value of a quantum operator.

Expectation values, with Born rule

$$E\left(\widehat{A}\right) = \left\langle \Psi \middle| \widehat{A} \middle| \Psi \right\rangle$$

- It follows that the Born rule itself hides the expectation value of a projection operators corresponding to eigenstates:

$$\begin{aligned}\mathrm{pr}\left(\left|a_k\right\rangle\right) &= \left\langle \Psi \middle| a_k \right\rangle \left\langle a_k \middle| \Psi \right\rangle \\ &= \left\langle \Psi \right| \left| a_k \right\rangle \left\langle a_k \right| \left| \Psi \right\rangle \\ &= E\left(\left|a_k\right\rangle \left\langle a_k\right|\right)\end{aligned}$$

Born rule, with expectation values

$$\mathrm{pr}\left(\left|a_k\right\rangle\right) = E\left(\left|a_k\right\rangle \left\langle a_k\right|\right)$$

- Equipped with the above ideas, we note,

$$E\left(\widehat{I}\right) = \left\langle \Psi \left| \widehat{I} \right| \Psi \right\rangle = \langle \Psi \mid \Psi \rangle$$

But,

$$\begin{aligned} E\left(\widehat{I}\right) &:= \sum_k \mathsf{pr}\left(|a_k\rangle\right) \left\langle a_k \left| \widehat{I} \right| a_k \right\rangle \\ &= \sum_k \mathsf{pr}\left(|a_k\rangle\right) \langle a_k \mid a_k \rangle \\ &= \sum_k \mathsf{pr}\left(|a_k\rangle\right) \\ &:= 1 \end{aligned}$$

Therefore, we have,

Normalization

$$\langle \Psi \mid \Psi \rangle = 1$$

- However, for the purposes of these slides, the above statement is not necessary. We could have, for instance, modified the Born rule without loss or gain of theory as,

Born rule, with explicit normalization

$$\mathrm{pr}\left(|a_k\rangle\right) = \frac{1}{\langle \Psi \mid \Psi \rangle} \langle \Psi \mid a_k \rangle \langle a_k \mid \Psi \rangle$$

Explicit normalization of states then becomes unnecessary as the above rule is invariant under normalization of the form $|\Psi\rangle \to \frac{1}{\langle \Psi \mid \Psi \rangle} |\Psi\rangle$.

- In general, the idea is that scaling states by *any* complex number should not change physics[3]; this idea will be formalized later on.

[3] In *The Principles of Quantum Mechanics*, Paul Dirac gives great attention to this point and how it is related to the idea that eigenstates matter only up to scale as orthogonality of states is a physical distinction and scaling does not disturb orthogonality.

Pure and Mixed Quantum States

- Recall that a quantum system has a state $|\Psi\rangle$ belonging to a [separable] Hilbert space $\mathcal{H}$. But there is more to a state than this notion, as follows.
- A quantum state $|\Psi\rangle$ is **pure** if it is described by a *single* ket, say $|\Psi_1\rangle \in \mathcal{H}$,

$$|\Psi\rangle = |\Psi_1\rangle$$

- A quantum state $|\Psi\rangle$ is **mixed** if it is possibly described by *multiple* kets, say $|\Psi_1\rangle, |\Psi_2\rangle, \ldots |\Psi_N\rangle \in \mathcal{H}$.
  The probability of $|\Psi\rangle$ being described by a given state $|\Psi_\alpha\rangle$ can be described by a probability map,

$$\begin{aligned} \text{pr} : |\Psi_\alpha\rangle \to \text{pr}\left(|\Psi_\alpha\rangle\right) \in [0,1] \\ \sum_\alpha \text{pr}\left(|\Psi_\alpha\rangle\right) = 1 \end{aligned}$$

Density Operators

- In general, the information contained in the possible state(s) of a quantum system are packed into what is called its **density operator** $\widehat{\rho}$,

Density operators

$$\widehat{\rho} := \sum_{\alpha} \mathsf{pr}\left(|\Psi_\alpha\rangle\right) |\Psi_\alpha\rangle \langle\Psi_\alpha|$$

For a pure state $|\Psi\rangle$, the density operator is simply $|\Psi\rangle \langle\Psi|$.

- For future use, we define the trace of a linear operator,

Trace of linear operators

$$\mathsf{tr}\left(\widehat{A}\right) := \sum_{k} \left\langle a_k \middle| \widehat{A} \middle| a_k \right\rangle = \sum_{k} a_k$$

We will soon use these constructions to simplify the expression for the expectation value of a linear operator.

Properties of Trace

- Firstly, trace is a **linear** operation as,

$$\begin{aligned}
\operatorname{tr}\left(c\widehat{A}\right) &:= \sum_k \left\langle a_k \left| c\widehat{A} \right| a_k \right\rangle \\
&= c \sum_k \left\langle a_k \left| \widehat{A} \right| a_k \right\rangle \\
&= c \operatorname{tr}\left(\widehat{A}\right) \\
\operatorname{tr}\left(\widehat{A} + \widehat{B}\right) &:= \sum_k \left\langle a_k \left| \left(\widehat{A} + \widehat{B}\right) \right| a_k \right\rangle \\
&= \sum_k \left[\left\langle a_k \left| \widehat{A} \right| a_k \right\rangle + \left\langle a_k \left| \widehat{B} \right| a_k \right\rangle \right] \\
&= \sum_k \left\langle a_k \left| \widehat{A} \right| a_k \right\rangle + \sum_k \left\langle a_k \left| \widehat{B} \right| a_k \right\rangle \\
&= \operatorname{tr}\left(\widehat{A}\right) + \operatorname{tr}\left(\widehat{B}\right)
\end{aligned}$$

- Secondly, trace is a *symmetric* operation,

$$\operatorname{tr}\left(\widehat{A}\widehat{B}\right) := \sum_m \left\langle a_m \left| \widehat{A}\widehat{B} \right| a_m \right\rangle$$

$$= \sum_m \langle a_m| \left(\sum_i \sum_j \left\langle a_i \left| \widehat{A} \right| a_j \right\rangle |a_i\rangle \langle a_j| \right) \left(\sum_k \sum_l \left\langle a_k \left| \widehat{B} \right| a_l \right\rangle |a_k\rangle \langle a_l| \right) |a_m\rangle$$

$$= \sum_m \sum_i \sum_j \sum_k \sum_l \left\langle a_i \left| \widehat{A} \right| a_j \right\rangle \left\langle a_k \left| \widehat{B} \right| a_l \right\rangle \langle a_m|\, a_i\rangle \langle a_j|\, a_k\rangle \langle a_l|\, a_m\rangle$$

$$= \sum_m \cancel{\sum_i} \sum_j \cancel{\sum_k} \cancel{\sum_l} \left\langle a_{\cancel{i}} \left| \widehat{A} \right| a_j \right\rangle \left\langle a_{\cancel{k}} \left| \widehat{B} \right| a_{\cancel{l}} \right\rangle \delta_{m\cancel{i}}\, \delta_{j\cancel{k}}\, \delta_{\cancel{l}m}$$

$$= \sum_m \sum_j \left\langle a_m \left| \widehat{A} \right| a_j \right\rangle \left\langle a_j \left| \widehat{B} \right| a_m \right\rangle$$

$$= \sum_m \sum_j \left\langle a_j \left| \widehat{B} \right| a_m \right\rangle \left\langle a_m \left| \widehat{A} \right| a_j \right\rangle$$

$$= \sum_m \sum_j \left\langle a_m \left| \widehat{B} \right| a_j \right\rangle \left\langle a_j \left| \widehat{A} \right| a_m \right\rangle$$

$$= \operatorname{tr}\left(\widehat{B}\widehat{A}\right)$$

- To summarize,

Properties of trace

1. Linearity

$$\text{tr}\left(c\widehat{A}\right) = c\text{tr}\left(\widehat{A}\right)$$
$$\text{tr}\left(\widehat{A}+\widehat{B}\right) = \text{tr}\left(\widehat{A}\right) + \text{tr}\left(\widehat{B}\right)$$

2. Symmetry

$$\text{tr}\left(\widehat{A}\widehat{B}\right) = \text{tr}\left(\widehat{B}\widehat{A}\right)$$

- As a corollary,

$$\text{tr}\left(\left(\widehat{A}_1 \ldots A_{M-1}\right)\widehat{A}_M\right) = \text{tr}\left(\widehat{A}_M\left(\widehat{A}_1 \ldots \widehat{A}_{M-1}\right)\right) = \ldots$$

Cyclicity

$$\text{tr}\left(\widehat{A}_1 \ldots \widehat{A}_M\right) = \text{tr}\left(\widehat{A}_M\widehat{A}_1 \ldots \widehat{A}_{M-1}\right) = \text{tr}\left(\widehat{A}_{M-1}\widehat{A}_M\widehat{A}_1 \ldots \widehat{A}_{M-2}\right) = \ldots$$

Expectation Values Using Density Operators

- For a pure quantum state $|\Psi\rangle$,

$$
\begin{aligned}
E\left(\widehat{A}\right) = \left\langle \Psi \left| \widehat{A} \right| \Psi \right\rangle &= \left(\sum_k \langle \Psi \, | a_k \rangle \langle a_k | \right) \widehat{A} \left(\sum_l | a_l \rangle \langle a_l | \, \Psi \rangle \right) \\
&= \sum_k \sum_l \langle \Psi \, | a_k \rangle \langle a_l \, | \Psi \rangle \left\langle a_k \left| \widehat{A} \right| a_l \right\rangle \\
&= \sum_k \sum_l \langle \Psi \, | a_k \rangle \langle a_l \, | \Psi \rangle \langle a_k \, | a_k | \, a_k \rangle \\
&= \sum_k \sum_l \langle \Psi \, | a_k \rangle \langle a_l \, | \Psi \rangle \langle a_k | \, a_l \rangle \, a_k \\
&= \mathrm{tr} \left(\sum_k \sum_l \langle \Psi \, | a_k \rangle \langle a_l \, | \Psi \rangle | a_l \rangle \langle a_k | \, a_k \right) \\
&= \mathrm{tr} \left[\left(\sum_k \langle \Psi \, | a_k \rangle \langle a_k | \right) \left(\sum_l | a_l \rangle \langle a_l | \, \Psi \rangle \right) \widehat{A} \right] \\
&= \mathrm{tr} \left(| \Psi \rangle \langle \Psi | \, \widehat{A} \right)
\end{aligned}
$$

- Let us redefine the expectation value of a linear operator $\widehat{A}$ taking into account mixed states,

$$E\left(\widehat{A}\right) := \sum_{\alpha} \mathrm{pr}\left(|\Psi_\alpha\rangle\right) E_\alpha\left(\widehat{A}\right)$$

where $E_\alpha\left(\widehat{A}\right)$ is the previously-defined notion of expectation values, which holds for pure states $|\Psi\rangle = |\Psi_\alpha\rangle$.

$$\begin{aligned}
E\left(\widehat{A}\right) &= \sum_{\alpha} \mathrm{pr}\left(|\Psi_\alpha\rangle\right) \mathrm{tr}\left(|\Psi\rangle\langle\Psi| \widehat{A}\right) \\
&= \sum_{\alpha} \mathrm{tr}\left(\mathrm{pr}\left(|\Psi_\alpha\rangle\right) |\Psi\rangle\langle\Psi| \widehat{A}\right) \\
&= \mathrm{tr}\left(\sum_{\alpha} \mathrm{pr}\left(|\Psi_\alpha\rangle\right) |\Psi\rangle\langle\Psi| \widehat{A}\right) \\
&= \mathrm{tr}\left(\widehat{\rho}\widehat{A}\right)
\end{aligned}$$

Expectation values, with Born rule, using density operators

$$E\left(\widehat{A}\right) = \mathrm{tr}\left(\widehat{\rho}\widehat{A}\right)$$

- This leads to the following corollary,

Born rule, with density operators

$$\mathsf{pr}\left(|a_k\rangle\right) = \mathsf{tr}\left(\widehat{\rho}\,|a_k\rangle\,\langle a_k|\right)$$