Measurements, Observables and the Uncertainty Relations

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1 Summary

Some basic principles of quantum mechanics.

1. Measurement changes the state. A measurement modeled by an observable (operator) $\hat{A}$ on a state $|\alpha\rangle$ changes the state to one of the eigenstates of $\hat{A}$:
$$\hat{A}\,|\alpha\rangle \propto |a\rangle$$
where $\hat{A}\,|a\rangle = a\,|a\rangle$.

2. The probability of measuring an eigenvalue a is given by
$$P(a) = |\langle a\,|\alpha\,\rangle|^2$$
Notice that this is consistent in two respects. If the state $|\alpha\rangle$ is already the eigenstate $|a\rangle$, then we measure a with certainty,
$$P(a) = |\langle a\,|a\,\rangle|^2 = 1$$
and for an arbitrary state, the probability of measuring one of the eigenvalues of $\hat{A}$ is 1, that is, we always get one of the eigenvalues:
$$\begin{aligned} P(some\,a_i) &= \sum_i |\langle a_i\,|\alpha\,\rangle|^2 \\ &= \sum_i \langle \alpha\,|a_i\,\rangle \langle a_i\,|\alpha\,\rangle \\ &= \langle\alpha|\left(\sum_i |a_i\rangle\langle a_i|\right)|\alpha\rangle \\ &= \langle\alpha|\,1\,|\alpha\rangle \\ &= \langle\alpha\,|\alpha\,\rangle \\ &= 1 \end{aligned}$$
where we use the completeness of the set of eigenvectors.

3. The expectation value of an operator is
$$\begin{aligned} \langle\alpha|\hat{A}\,|\alpha\rangle &= \langle\alpha|\left(\sum_i |a_i\rangle\langle a_i|\right)\hat{A}\left(\sum_j |a_j\rangle\langle a_j|\right)|\alpha\rangle \\ &= \sum_{i,j} \langle\alpha\,|a_i\,\rangle \langle a_i|\,a_j\,|a_j\rangle \langle a_j\,|\alpha\,\rangle \\ &= \sum_{i,j} a_j \delta_{ij} \langle\alpha\,|a_i\,\rangle \langle a_j\,|\alpha\,\rangle \\ &= \sum_i a_i \langle\alpha\,|a_i\,\rangle \langle a_i\,|\alpha\,\rangle \\ &= \sum_i a_i\,|\langle a_i\,|\alpha\,\rangle|^2 \\ &= \sum_i a_i P(a_i) \end{aligned}$$

2 Examples: Spin operators

We can construct any operator from its eigenstates and eigenvalues as

$$\hat{A} = \sum_i a_i |a_i\rangle \langle a_i|$$

For $\hat{S}_x$, we know that acting on S_z eigenkets $|\pm\rangle$, we have equal probability of finding $|S_x, \pm\rangle$. Therefore, we must have

$$|S_x, +\rangle = \frac{1}{\sqrt{2}} e^{i\delta_1} |+\rangle + \frac{1}{\sqrt{2}} e^{i\delta_2} |-\rangle$$

for arbitrary phases δ_1, δ_2. Since the overall phase is arbitrary and nonphysical we can eliminate one of these and write

$$|S_x, +\rangle = \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} e^{i\delta} |-\rangle$$

Since $|S_x, +\rangle$ and $|S_x, -\rangle$ must be orthogonal (since the observable $\hat{S}_x$ must be Hermitian), setting $|S_x, -\rangle = \alpha |+\rangle + \beta |-\rangle$, we have

$$\begin{aligned} 0 &= \langle S_x, + | S_x, - \rangle \\ &= \frac{1}{\sqrt{2}} \left(\langle +| + \langle -| e^{-i\delta} \right) (\alpha |+\rangle + \beta |-\rangle) \\ &= \frac{1}{\sqrt{2}} \left(\alpha + \beta e^{-i\delta} \right) \end{aligned}$$

so $\beta = -e^{i\delta} \alpha$ and the normalized state must be

$$|S_x, -\rangle = \frac{1}{\sqrt{2}} |+\rangle - \frac{1}{\sqrt{2}} e^{i\delta} |-\rangle$$

Then $\hat{S}_x$ is given by

$$\begin{aligned} \hat{S}_x &= +\frac{\hbar}{2} |S_x, +\rangle \langle S_x, +| + \left(-\frac{\hbar}{2} \right) |S_x, -\rangle \langle S_x, -| \\ &= \frac{\hbar}{2} \left(\frac{1}{\sqrt{2}} \left(|+\rangle + e^{i\delta} |-\rangle \right) \frac{1}{\sqrt{2}} \left(\langle +| + \langle -| e^{-i\delta} \right) - \frac{1}{\sqrt{2}} \left(|+\rangle - e^{i\delta} |-\rangle \right) \frac{1}{\sqrt{2}} \left(\langle +| - \langle -| e^{-i\delta} \right) \right) \\ &= \frac{\hbar}{4} \left(|+\rangle \langle +| + |+\rangle \langle -| e^{-i\delta} + e^{i\delta} |-\rangle \langle +| + |-\rangle \langle -| - |+\rangle \langle +| + e^{i\delta} |-\rangle \langle +| + |+\rangle \langle -| e^{-i\delta} - |-\rangle \langle -| \right) \\ &= \frac{\hbar}{4} \left(2e^{-i\delta} |+\rangle \langle -| + 2e^{i\delta} |-\rangle \langle +| \right) \\ &= \frac{\hbar}{2} \left(e^{-i\delta} |+\rangle \langle -| + e^{i\delta} |-\rangle \langle +| \right) \end{aligned}$$

We could have made exactly the same arguments for $\hat{S}_y$, so with σ some other phase we may also write

$$\hat{S}_y = \frac{\hbar}{2} \left(e^{-i\sigma} |+\rangle \langle -| + e^{i\sigma} |-\rangle \langle +| \right)$$

But we also know that the x and y directions will have the same relationship to one another that they each have with the z direction, for example,

$$\begin{aligned} \left| \langle S_x, \pm | S_y, + \rangle \right| &= \frac{1}{\sqrt{2}} \\ \left| \langle S_x, \pm | S_y, + \rangle \right| &= \frac{1}{\sqrt{2}} \end{aligned}$$

Either of these relations gives:

$$\begin{aligned} \left| \frac{1}{\sqrt{2}} \left(\langle + | \pm \langle - | e^{-i\delta} \right) \frac{1}{\sqrt{2}} \left(| + \rangle + e^{i\sigma} | - \rangle \right) \right| &= \frac{1}{\sqrt{2}} \\ \frac{1}{2} \left| 1 \pm e^{i(\sigma - \delta)} \right| &= \frac{1}{\sqrt{2}} \end{aligned}$$

which happens if and only if

$$\begin{aligned} e^{i(\sigma-\delta)} &= \pm i \\ (\sigma - \delta) &= \pm \frac{\pi}{2} \end{aligned}$$

The remaining indefiniteness of the phase can be chosen by fixing the overall phase of $|S_x, +\rangle$. It is conventional to choose $\hat{S}_x$ to be real, so that $\delta = 0$ and

$$\hat{S}_x = \frac{\hbar}{2} \left(| + \rangle \langle - | + | - \rangle \langle + | \right) = \frac{\hbar}{2} \sigma_x$$

Then $\hat{S}_y$ must be pure imaginary. With $\sigma = \frac{\pi}{2}$ we have

$$\begin{aligned} \hat{S}_y &= \frac{\hbar}{2} \left(e^{-\frac{i\pi}{2}} | + \rangle \langle - | + e^{\frac{i\pi}{2}} | - \rangle \langle + | \right) \\ &= \frac{\hbar}{2} \left(-i | + \rangle \langle - | + i | - \rangle \langle + | \right) \\ &= \frac{\hbar}{2} \sigma_y \end{aligned}$$

3 The algebra of spin

The essential properties of angular momentum are implicit in the products of these spin operators. Most importantly, we have the commutators,

$$\left[\hat{S}_i, \hat{S}_j \right] = i\hbar \varepsilon_{ijk} \hat{S}_k$$

We also have the anticommutators,

$$\left\{ \hat{S}_i, \hat{S}_j \right\} = \frac{1}{2} \hbar^2 \delta_{ij}$$

It will be useful to define the combinations

$$\hat{S}_\pm = \hat{S}_x \pm i \hat{S}_y$$

and the squared sum,

$$\begin{aligned} \hat{\mathbf{S}}^2 &= \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} \\ &= \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 \\ &= \frac{3}{4} \hbar^2 1 \end{aligned}$$

since each Pauli matrix squares to the identity. Since $\hat{\mathbf{S}}^2$ is proportional to the identity operator, we have

$$\left[\hat{\mathbf{S}}^2, S_i \right] = 0$$

4 Quantum vs. classical conditional probability: Bell's Theorem

Consider three measurements, with corresponding operators A, B and C, performed in order. Classically, let

$$P_{a \to b}$$

be the probability of the B measurement giving b when the A measurement has given a. This is called a *conditional probability*. Then, performing C, we have

$$P_{b\to c}$$

for the conditional probability of c given b, and the joint probability of measuring b then c, given a is the product:

$$P_{a\to(b,c)} = P_{a\to b}P_{b\to c}$$

If we sum over all possible outcomes, b_i, for B, we must get the conditional probability of c, given a,

$$P_{a\to c} = \sum_{b_i} P_{a\to b_i}P_{b_i\to c}$$

because we have accounted for all possible intermediate routes from a to c.

Quantum mechanically, we may write each of the conditional probabilities as:

$$\begin{aligned} P_{a\to b} &= \left|\langle b\,|a\rangle\right|^2 \\ P_{b\to c} &= \left|\langle c\,|b\rangle\right|^2 \\ P_{a\to c} &= \left|\langle c\,|a\rangle\right|^2 \end{aligned}$$

Now expand the last,

$$\begin{aligned} P_{a\to c} &= \left|\langle c\,|a\rangle\right|^2 \\ &= \langle a\,|c\rangle\langle c\,|a\rangle \\ &= \sum_i \langle a\,|b_i\rangle\langle b_i\,|a\rangle\langle c\,|a\rangle \\ &= \sum_i \langle a\,|b_i\rangle\langle b_i\,|a\rangle\sum_j \left\langle c\,\middle|b_j\right\rangle\left\langle b_j\,|a\right\rangle \end{aligned}$$

where we have inserted two copies of the identity operator. As in the classical case, the joint probability of measuring b then c, given a is now

$$\begin{aligned} P_{a\to(b,c)} &= \left|\langle b\,|a\rangle\langle c\,|b\rangle\right|^2 \\ &= \left(\langle a\,|b\rangle\langle b\,|c\rangle\right)\left(\langle b\,|a\rangle\langle c\,|b\rangle\right) \\ &= \left(\langle a\,|b\rangle\langle b\,|a\rangle\right)\left(\langle c\,|b\rangle\langle b\,|c\rangle\right) \\ &= P_{a\to b}P_{b\to c} \end{aligned}$$

However, if we sum over all intermediate states b_i we do *not* get $P_{a\to c}$! Instead, we have the *single* sum

$$\sum_i \langle a\,|b_i\rangle\langle b_i\,|a\rangle$$

$$\begin{aligned} \sum_i P_{a\to(b_i,c)} &= \sum_i \langle a\,|b_i\rangle\langle b_i\,|a\rangle\left(\langle c\,|b_i\rangle\langle b_i\,|c\rangle\right) \\ &= \sum_i P_{a\to b_i}P_{b_i\to c} \end{aligned}$$

This is an extremely important difference between classical and quantum physics!

Let's look at an example. Let the three operators be the spin operators in the z, x and y directions, respectively, and let's work as usual in the z basis. Start with a general spin state,

$$|\psi\rangle = \alpha\,|+\rangle + \beta\,|-\rangle$$

where normalization requires $\alpha\bar{\alpha} + \beta\bar{\beta} = 1$. Then the probability of measuring spin up in the x and then spin up in the y directions is

$$\begin{aligned} P_{\psi\to((x+),(y+))} &= \left(\langle\psi\,|S_x,+\rangle\langle S_x,+\,|\psi\rangle\right)\left(\left\langle S_y,+\,|S_x,+\right\rangle\left\langle S_x,+\,\middle|S_y,+\right\rangle\right) \\ &= \alpha\bar{\alpha}\left(\frac{1}{\sqrt{2}}\times\frac{1}{\sqrt{2}}\right) \\ &= \frac{\alpha\bar{\alpha}}{2} \end{aligned}$$

Summing $P_{\psi\to((x\pm),(y+))}$ over both possible intermediate x states gives

$$\begin{aligned}
\sum_{(\pm,x)} P_{\psi\to((x\pm),(y+))} &= \left(\langle\psi|S_x,+\rangle\langle S_x,+|\psi\rangle\right)\left(\langle S_y,+|S_x,+\rangle\langle S_x,+|S_y,+\rangle\right) \\
&\quad +\left(\langle\psi|S_x,-\rangle\langle S_x,-|\psi\rangle\right)\left(\langle S_y,+|S_x,-\rangle\langle S_x,-|S_y,+\rangle\right) \\
&= \frac{\alpha\bar{\alpha}}{2}+\frac{\beta\bar{\beta}}{2} \\
&= \frac{1}{2}
\end{aligned}$$

Now consider

$$\begin{aligned}
P_{a\to c} &= |\langle c|a\rangle|^2 \\
&= \left(\langle a|+\rangle\langle +|c\rangle+\langle a|-\rangle\langle -|c\rangle\right)\left(\langle c|+\rangle\langle +|a\rangle+\langle c|-\rangle\langle -|a\rangle\right) \\
&= \left(\bar{\alpha}\gamma+\bar{\beta}\delta\right)\left(\bar{\gamma}\alpha+\bar{\delta}\beta\right) \\
&= \alpha\bar{\alpha}\gamma\bar{\gamma}+\beta\bar{\beta}\delta\bar{\delta}+\bar{\alpha}\beta\gamma\bar{\delta}+\alpha\bar{\beta}\bar{\gamma}\delta
\end{aligned}$$

$$\begin{aligned}
P_{a\to c} &= |\langle c|a\rangle|^2 \\
&= \langle\psi|S_y,+\rangle\langle S_y,+|\psi\rangle \\
&= \frac{1}{\sqrt{2}}\left(\bar{\alpha}+i\bar{\beta}\right)\frac{1}{\sqrt{2}}\left(\alpha-i\beta\right) \\
&= \frac{1}{2}\left(\alpha\bar{\alpha}+\beta\bar{\beta}+i\left(\alpha\bar{\beta}-\beta\bar{\alpha}\right)\right)
\end{aligned}$$

Now consider the general spin-$\frac{1}{2}$ case:

$$\begin{aligned}
P_{a\to c} &= |\langle c|a\rangle|^2 \\
&= \sum_i\langle a|b_i\rangle\langle b_i|a\rangle\sum_j\langle c|b_j\rangle\langle b_j|a\rangle
\end{aligned}$$

and

$$\sum_i P_{a\to(b_i,c)} = \sum_i\langle a|b_i\rangle\langle b_i|a\rangle\left(\langle c|b_i\rangle\langle b_i|c\rangle\right)$$

Specialize these to spin $\frac{1}{2}$, and let the middle state be in the z-basis (since we lose no generality by letting one of the directions be z):

$$\begin{aligned}
P_{a\to c} &= |\langle c|a\rangle|^2 \\
&= \sum_{\pm}\langle a|b_i\rangle\langle b_i|c\rangle\sum_j\langle c|b_j\rangle\langle b_j|a\rangle \\
&= \left(\langle a|+\rangle\langle +|c\rangle+\langle a|-\rangle\langle -|c\rangle\right)\left(\langle c|+\rangle\langle +|a\rangle+\langle c|-\rangle\langle -|a\rangle\right)
\end{aligned}$$

Set

$$\begin{aligned}
\langle +|a\rangle &= \alpha \\
\langle -|a\rangle &= \beta \\
\langle +|c\rangle &= \gamma \\
\langle -|c\rangle &= \delta
\end{aligned}$$

Then

$$\begin{aligned}
P_{a\to c} &= |\langle c|a\rangle|^2 \\
&= \left(\langle a|+\rangle\langle +|c\rangle+\langle a|-\rangle\langle -|c\rangle\right)\left(\langle c|+\rangle\langle +|a\rangle+\langle c|-\rangle\langle -|a\rangle\right) \\
&= \left(\bar{\alpha}\gamma+\bar{\beta}\delta\right)\left(\bar{\gamma}\alpha+\bar{\delta}\beta\right) \\
&= \alpha\bar{\alpha}\gamma\bar{\gamma}+\beta\bar{\beta}\delta\bar{\delta}+\bar{\alpha}\beta\gamma\bar{\delta}+\alpha\bar{\beta}\bar{\gamma}\delta
\end{aligned}$$

For the sum over intermediate states we have

$$\begin{aligned}\sum_i P_{a\to(b_i,c)} &= \sum_i \langle a|b_i\rangle\langle b_i|a\rangle(\langle c|b_i\rangle\langle b_i|c\rangle)\\ &= \langle a|+\rangle\langle +|a\rangle(\langle c|+\rangle\langle +|c\rangle)+\langle a|-\rangle\langle -|a\rangle(\langle c|-\rangle\langle -|c\rangle)\\ &= \alpha\bar{\alpha}\gamma\bar{\gamma}+\beta\bar{\beta}\delta\bar{\delta}\end{aligned}$$

So we have the difference,

$$P_{a\to c}-\sum_i P_{a\to(b_i,c)} = \bar{\alpha}\beta\gamma\bar{\delta}+\alpha\bar{\beta}\bar{\gamma}\delta$$

Write the complex numbers as

$$\begin{aligned}\alpha &= a\\ \beta &= \sqrt{1-a^2}e^{i\varphi}\\ \gamma &= b\\ \delta &= \sqrt{1-b^2}e^{i\theta}\end{aligned}$$

where the overall phase freedom allows us to choose α and γ real. Then

$$\begin{aligned}P_{a\to c}-\sum_i P_{a\to(b_i,c)} &= a\sqrt{1-a^2}e^{i\varphi}b\sqrt{1-b^2}e^{-i\theta}+a\sqrt{1-a^2}e^{-i\varphi}b\sqrt{1-b^2}e^{i\theta}\\ &= ab\sqrt{1-a^2}\sqrt{1-b^2}\left(e^{i(\varphi-\theta)}+e^{i\varphi}e^{-i(\varphi-\theta)}\right)\\ &= 2ab\sqrt{1-a^2}\sqrt{1-b^2}\cos(\varphi-\theta)\end{aligned}$$

This is a simple example of Bell's Theorem. See further detail in Notes.