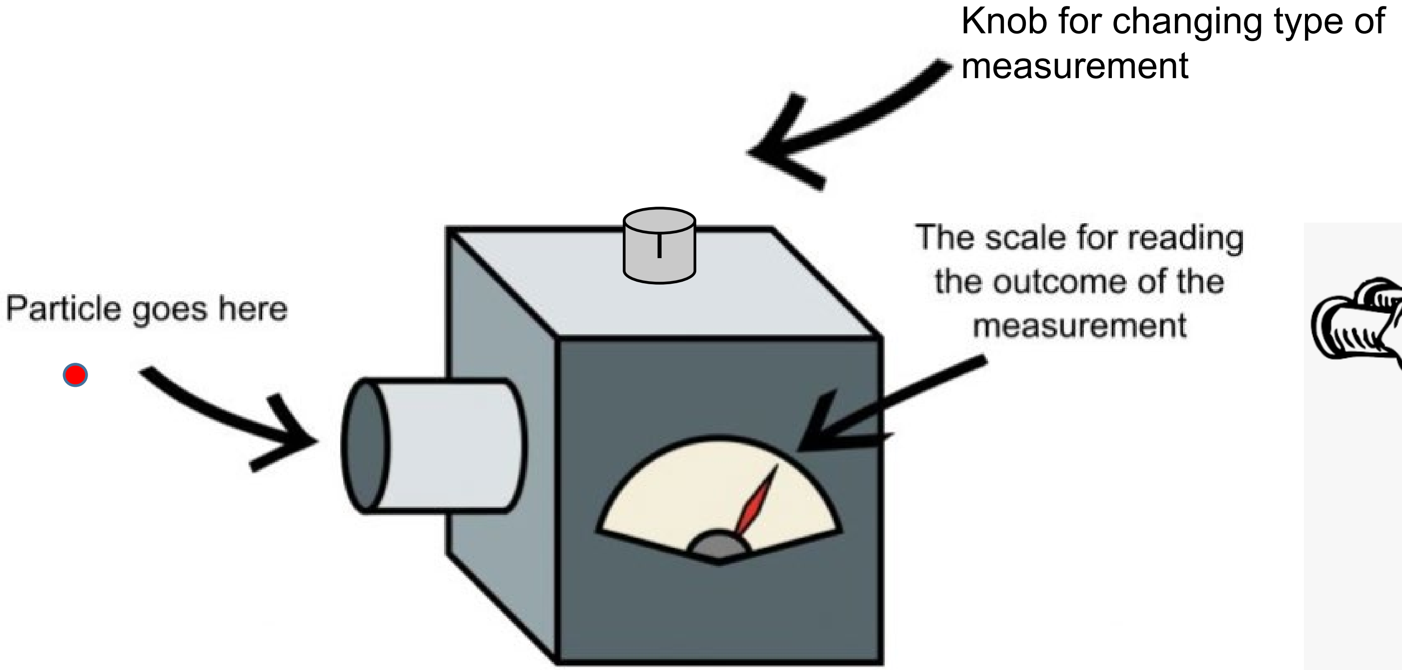
10. Observables



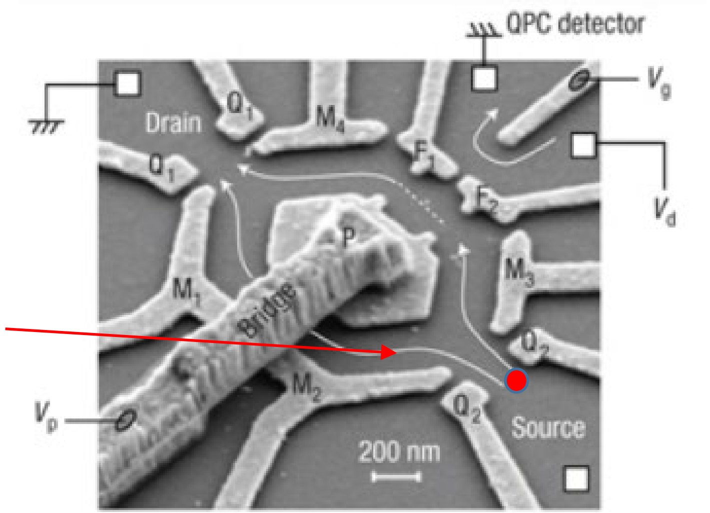
Physical quantities & the quantum state

The quantum wavefunction contains all the information about the state of the system.

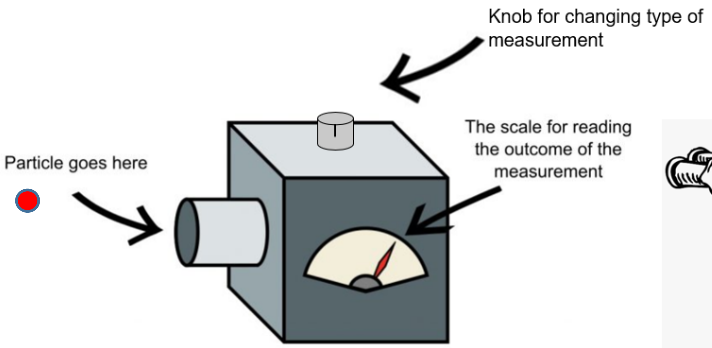
This means that any kind of physical property (e.g. position, velocity, angular momentum, energy, etc.) of the system should be relatable to the wavefunction.

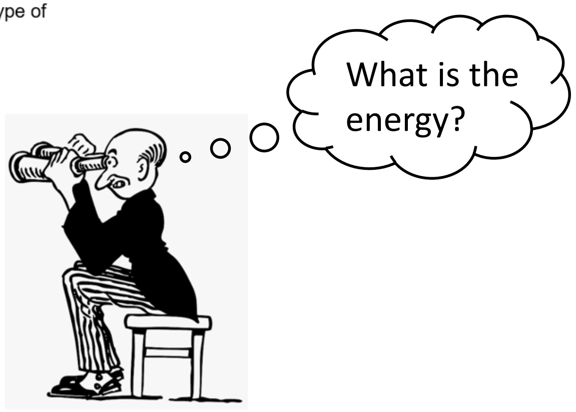
How do we relate the wavefunction to a physical property?

$$|\psi\rangle$$



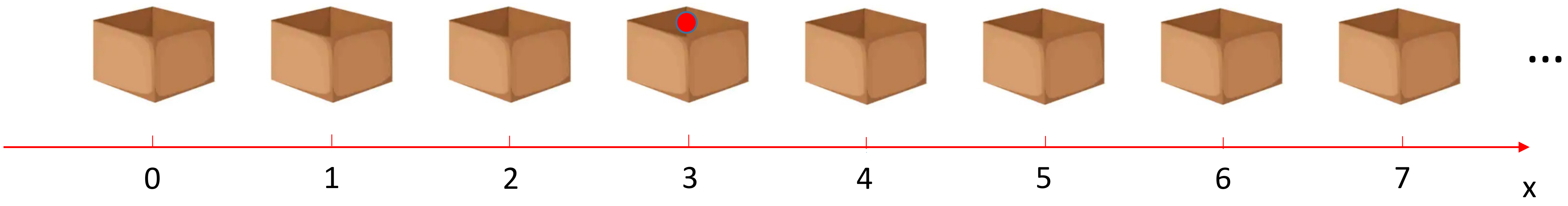
Since a physical property is generally something that we would like to attribute to the system, it is closely related to a quantum measurement.





Example: Position of a particle

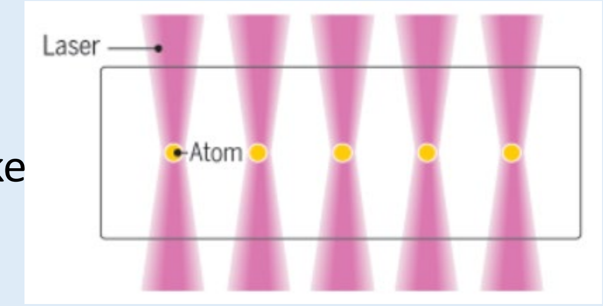
Consider a particle that could be in one of many boxes in a line.



Classically, the particle can only be in one of the boxes (e.g. $|3\rangle$), but quantum mechanically it can be in a superposition.

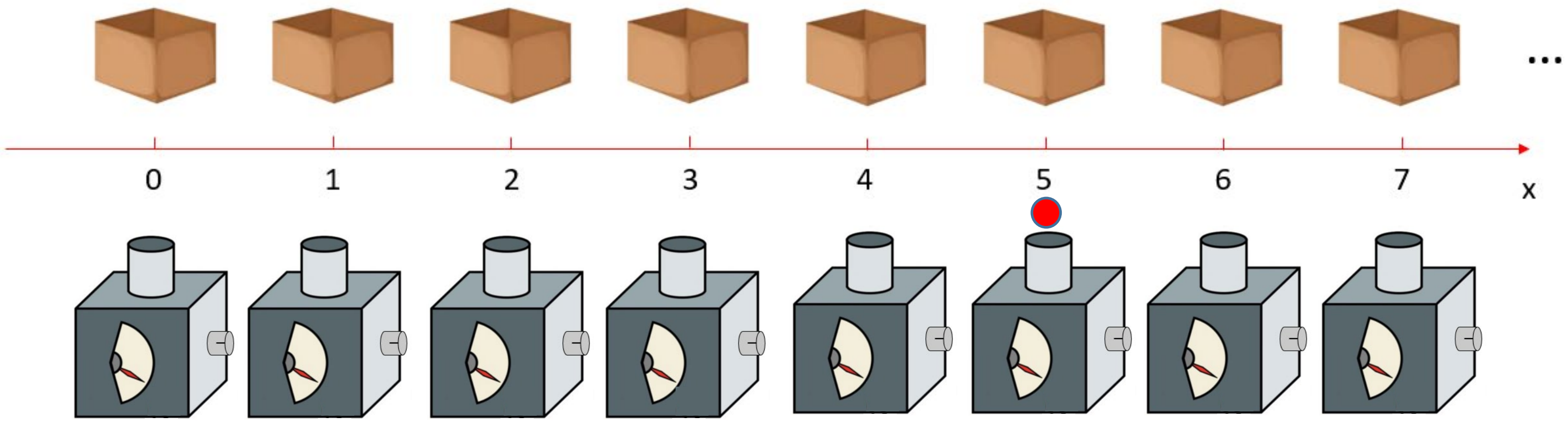
$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle + \ldots + a_N|N\rangle$$
$$= \sum_{x=0}^{N} a_x |x\rangle$$

Aside: you can do something a lot like this with atoms trapped in lasers.



Bernien et al. Nature 551, 579 (2017)

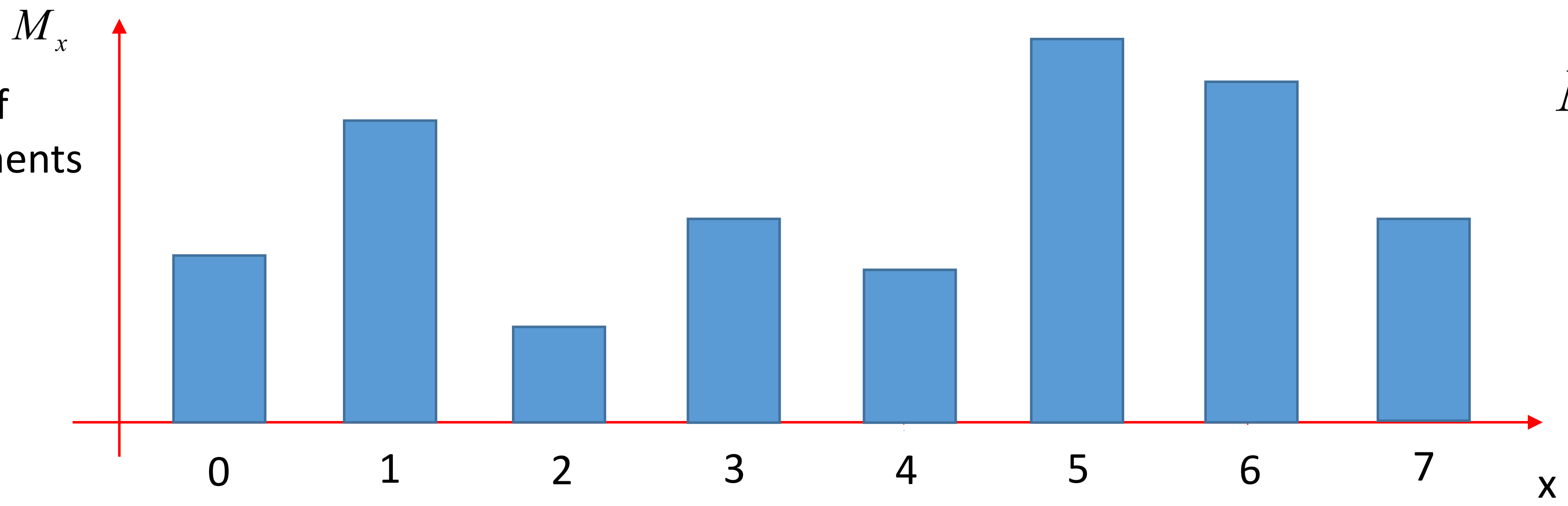
Now if we try to measure where the particle is, we find it is one of the boxes, randomly.



$$|\psi\rangle = \sum_{x=0}^{N} a_x |x\rangle$$

If we repeat the experiment many times, we will get a histogram of where the particle ends up

Number of measurements in xth box



$$M_x = p_x M_{tot} = |a_x|^2 M_{tot}$$

$M_{tot} =$ Total number of measurements

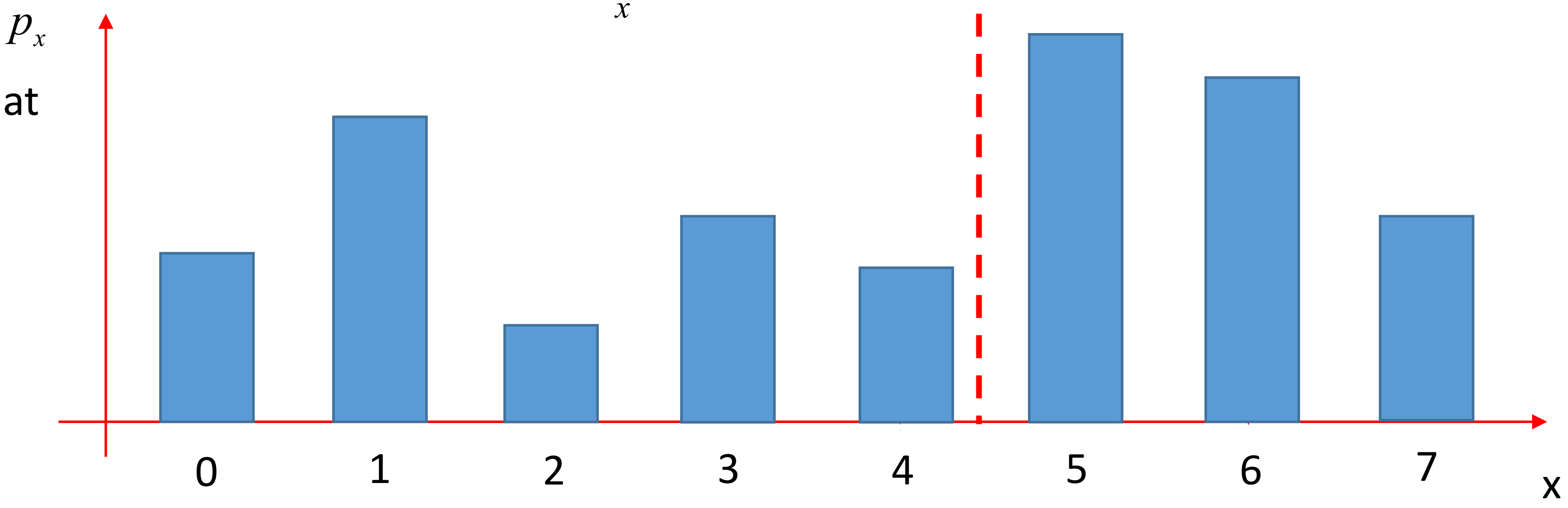
Now suppose we ask the question "Where is the particle?"

Classically this is a well-defined question with a definite answer, but quantum mechanically it is not quite so simple because the particle is "in many places at once", and each time we measure it, it randomly emerges at different locations.

But we already know how to deal with such randomness already from probability theory. We **can** say on average, the particle is at position

$$\langle x \rangle = \sum_x x p_x$$

Probability at position x



e.g. the "expectation value" of the position is

$$\langle x \rangle = 4.3$$

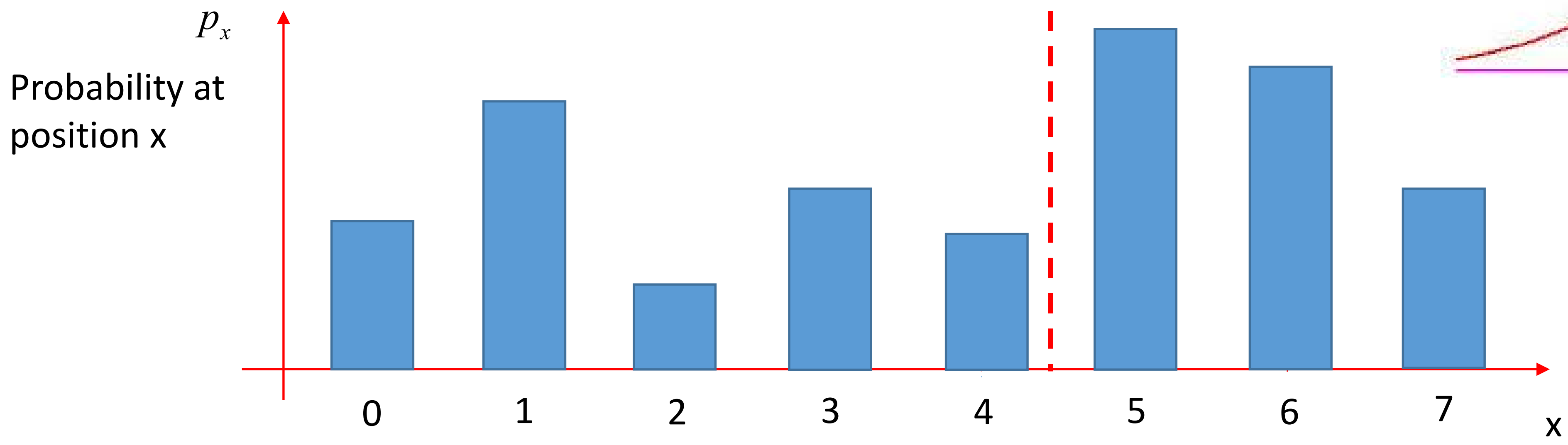
We can apply all the methods from probability theory, since we have a probability distribution.

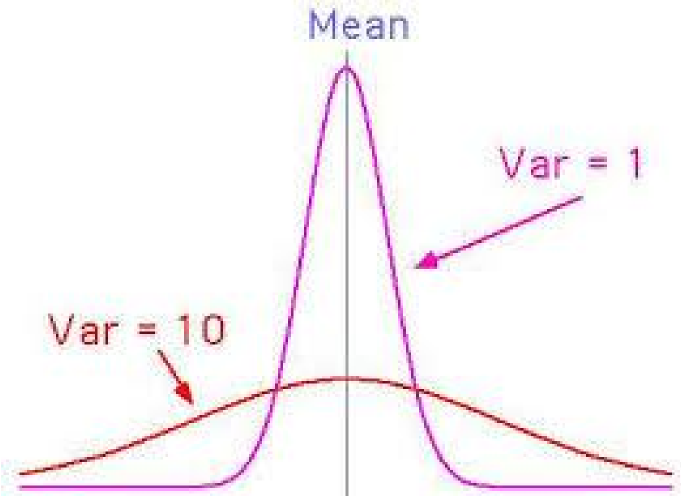
Another quantity to characterize the probability distribution is variance, which is how spread out the probability distribution is.

$$Var(x) = \langle x^2 \rangle - \langle x \rangle^2 = \sum_x x^2 p_x - \left(\sum_x x p_x \right)^2$$

The standard deviation is the square root and is how broad the distribution is.

$$\sigma_x = \sqrt{Var(x)}$$





Finding observables from a measurement

Let us make this a bit more general, with a general observable Q

This observable has some definite values in the $|n\rangle$-basis. Let us call these definite values q_n

For example: if the states $|n\rangle$ are in definite positions, then the q_n are the numerical values of the position.
if the states $|n\rangle$ are in definite energies, then the q_n are the numerical values of the energy.

Now if we have the state $$|\psi\rangle = \sum_{n=0}^{N} a_n |n\rangle$$

And measure the states we get the probabilities like $$p_n = |a_n|^2 = |\langle n|\psi\rangle|^2$$

Then if we want to take the average for an observable Q, we have $$\langle Q\rangle = \sum_{n=0}^{N} p_n q_n = \sum_{n=0}^{N} |a_n|^2 q_n$$

Observable operators

There is a neat way to write the average of an observable that makes everything automatic.

First define the observable operator

$$Q = \sum_{n=0}^{N} q_n |n\rangle\langle n|$$

Outer product of the state with itself.

The value of each state

Then we can write the expectation value of Q as

$$\boxed{\langle Q \rangle = \langle \psi | Q | \psi \rangle}$$

Because $Q|\psi\rangle = \left(\sum_{n=0}^{N} q_n |n\rangle\langle n| \right) \left(\sum_{n'=0}^{N} a_{n'} |n'\rangle \right) = \sum_{n=0}^{N} a_n q_n |n\rangle$

Then $\langle \psi | Q | \psi \rangle = \left(\sum_{n'=0}^{N} a_{n'}^* \langle n'| \right) \left(\sum_{n=0}^{N} a_n q_n |n\rangle \right) = \sum_{n=0}^{N} a_n a_n^* q_n |n\rangle = \sum_{n=0}^{N} |a_n|^2 q_n |n\rangle = \sum_{n=0}^{N} p_n q_n |n\rangle$

Same as 2 pages ago!

Observables in other bases

The previous case was quite easy because the observable Q and state $|\psi\rangle$ were written in the same basis.

If the observable R has some definite values for some other basis $|m\rangle$

Then we would have to convert the state to be written in the basis of Q first.

$$|\psi\rangle = \sum_{n=0}^{N} a_n |n\rangle \to \sum_{m=0}^{N} b_m |m\rangle$$

Then the rest is the same. We measure the states and get the probabilities $p_m = |b_m|^2$

Then if we want to take the average for an observable R , we have $\langle R\rangle = \sum_{m=0}^{N} p_m r_m = \sum_{m=0}^{N} |b_m|^2 r_m$

Observable operators for other bases

Ok that is neat to write it that way, but what about for operators where Q and the state are not written in the same basis?

Answer: It's the same!

$$\boxed{\langle R \rangle = \langle \psi | R | \psi \rangle}$$

$$R = \sum_{m=0}^{N} r_m |m\rangle\langle m|$$

Proof:

First evaluate as before

$$R|\psi\rangle = \left(\sum_{m=0}^{N} r_m |m\rangle\langle m| \right)\left(\sum_{n=0}^{N} a_n |n\rangle \right) = \sum_{m=0}^{N}\sum_{n=0}^{N} \langle m|n\rangle a_n r_m |m\rangle$$

$$\langle \psi | R | \psi \rangle = \left(\sum_{n'=0}^{N} a_{n'}^* \langle n'| \right)\left(\sum_{m=0}^{N}\sum_{n=0}^{N} \langle m|n\rangle a_n r_m |m\rangle \right) = \sum_{m=0}^{N} \left(\sum_{n'=0}^{N} a_{n'}^* \langle n'|m\rangle \right)\left(\sum_{n=0}^{N} a_n \langle m|n\rangle \right) r_m$$

$$= \sum_{m=0}^{N} \left| \sum_{n=0}^{N} a_n \langle m|n\rangle \right|^2 r_m$$

Meanwhile, from 3 pages ago we know that
$$\langle R \rangle = \sum_{m=0}^{N} |b_m|^2 r_m$$

What are the coefficients b_m ?

Recall that the identity matrix on any vector gives the same vector

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$I|\psi\rangle = |\psi\rangle$$

We can always make an identity operator in any basis:

$$I = \sum_{n=0}^{N} |n\rangle\langle n| = \sum_{m=0}^{N} |m\rangle\langle m|$$

Then multiply the state by the identity operator using the $|m\rangle$ basis

$$|\psi\rangle = I|\psi\rangle = \left(\sum_{m=0}^{N} |m\rangle\langle m| \right)\left(\sum_{n=0}^{N} a_n |n\rangle \right) = \sum_{m=0}^{N} \left(\sum_{n=0}^{N} a_n \langle m|n\rangle \right)|m\rangle$$

$$\boxed{b_m = \sum_{n=0}^{N} a_n \langle m|n\rangle}$$

So then we have $$\langle\psi|R|\psi\rangle = \sum_{m=0}^{N}\left|\sum_{n=0}^{N} a_n \langle m|n\rangle\right|^2 r_m = \sum_{m=0}^{N}|b_m|^2 r_m = \langle R\rangle$$

Since $$b_m = \sum_{n=0}^{N} a_n \langle m|n\rangle$$

These are the same, so this proves $$\langle R\rangle = \langle\psi|R|\psi\rangle$$

This makes clear why we have the bra-ket notation, we can make averages just by "sandwiching" the observable operator by the states.

Variances then follow from this

$$Var(R) = \langle R^2\rangle - \langle R\rangle^2 = \langle\psi|R^2|\psi\rangle - \left(\langle\psi|R|\psi\rangle\right)^2$$

Qubit observables: The Pauli operators

For a qubit, there are 3 commonly used observables, called the Pauli operators.

These are defined according to which basis they use, and the values that they take are +1 or -1, for each of the two qubit states.

Pauli operator	Basis state 1	Value of basis state 1	Basis state 2	Value of basis state 2
Z	$\|0\rangle$	$+1$	$\|1\rangle$	-1
X	$\|+\rangle = \frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$	$+1$	$\|-\rangle = \frac{1}{\sqrt{2}}(\|0\rangle - \|1\rangle)$	-1
Y	$\|+y\rangle = \frac{1}{\sqrt{2}}(\|0\rangle + i\|1\rangle)$	$+1$	$\|-y\rangle = \frac{1}{\sqrt{2}}(i\|0\rangle + \|1\rangle)$	-1

Rationale of the Pauli operator

Why define it in this way? Taking the example of the Pauli Z-operator, this corresponds to performing measurements from which we get probabilties

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Measurement apparatus

$$|\psi_0^{meas}\rangle = |0\rangle \qquad p_0 = |\alpha|^2$$

$$|\psi_1^{meas}\rangle = |1\rangle \qquad p_1 = |\beta|^2$$

Then we take these probabilities and calculate $\langle Z\rangle = |\alpha|^2 - |\beta|^2$

Since $|\alpha|^2 + |\beta|^2 = 1$, we can only have $-1 \le \langle Z\rangle \le 1$

This is a measure of how much the probabilities are biased towards $|0\rangle, |1\rangle$

Matrix form of the Pauli operators

We can write the matrix forms of the Pauli operators according to the definition

$$Z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$Q = \sum_{n=0}^{N} q_n |n\rangle\langle n|$$

$$X = |+\rangle\langle +| - |-\rangle\langle -| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Y = |+y\rangle\langle +y| - |-y\rangle\langle -y| = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$|-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$$

$$|+y\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right)$$

$$|-y\rangle = \frac{1}{\sqrt{2}}\left(i|0\rangle + |1\rangle\right)$$

These can be used to simply evaluate the expectation values.

Question: Calculating expectation values

Suppose we have a general state $$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Calculate the expectation values of the Pauli X, Y, Z operators.

Question: Calculating expectation values

Suppose we have a general state $$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Calculate the expectation values of the Pauli X, Y, Z operators.

$$\langle Z\rangle = \langle\psi|Z|\psi\rangle = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ e^{i\phi}\sin\frac{\theta}{2}\end{pmatrix} = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ -e^{i\phi}\sin\frac{\theta}{2}\end{pmatrix} = \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = \cos\theta$$

$$\langle X\rangle = \langle\psi|X|\psi\rangle = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ e^{i\phi}\sin\frac{\theta}{2}\end{pmatrix} = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}e^{i\phi}\sin\frac{\theta}{2}\\ \cos\frac{\theta}{2}\end{pmatrix} = e^{i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} + e^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$
$$= \sin\theta\cos\phi$$

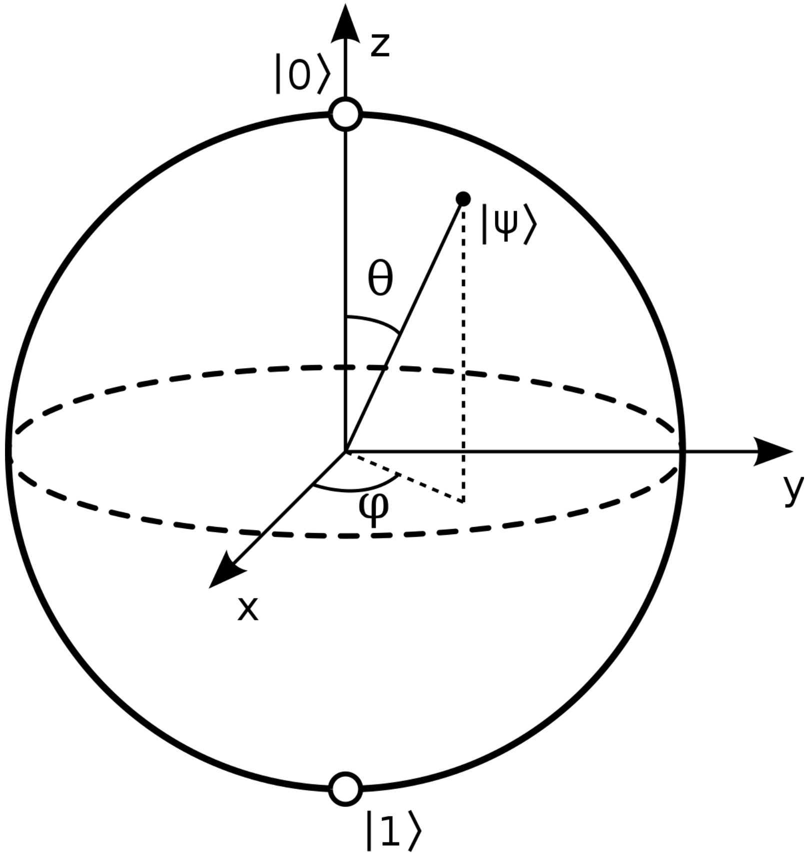
$$\langle Y\rangle = \langle\psi|Y|\psi\rangle = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ e^{i\phi}\sin\frac{\theta}{2}\end{pmatrix} = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}-ie^{i\phi}\sin\frac{\theta}{2}\\ i\cos\frac{\theta}{2}\end{pmatrix}$$

$$= -ie^{i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} + ie^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} = \sin\theta\sin\phi$$

The Bloch sphere

The expectation values of the Pauli operators look just like the coordinates of a point on the unit sphere

$$\langle X \rangle = \sin\theta\cos\phi$$
$$\langle Y \rangle = \sin\theta\sin\phi$$
$$\langle Z \rangle = \cos\theta$$



This gives a nice way of visualizing all the states of a qubit. In terms of the observables, every point on the unit sphere corresponds to a particular quantum state of a qubit.

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$