C191 - Lecture 2 - Quantum states and observables

I. ENTANGLED STATES

We saw last time that quantum mechanics allows for systems to be in superpositions of basis states. Many of these superpositions possess a uniquely quantum feature known as *entanglement*. As an example, consider the two-qubit state

$$|\psi\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Because this is a two qubit state, I can separate the two qubits, giving one to Alice and the other to Bob. If Alice measures her qubit, she will have a 50% chance of measuring 0 and 50% chance of measuring 1. But if Alice measures a 1, then necessarily Bob will measure a 1, even if the qubits are removed from causal contact from one another (many light seconds away, for instance). Contrast this with the state

$$|phi\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|01\rangle$$

Now Alice will measure 0 with 100% probability, but Bob's measurement will still be 0 or 1 with 50% probability each. This state is called *separable* because it may be written as

$$|\phi\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|0\rangle\,1 = \frac{1}{\sqrt{2}}|0\rangle\otimes|0\rangle + \frac{1}{\sqrt{2}}|0\rangle\otimes|0\rangle = |0\rangle\otimes\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right)$$

Entangled states are those which can never be written this way. We will see later that entanglement is an extremely important resource for quantum computation.

II. DENSITY MATRICES

Quantum states are inherently probabilistic, but how do we handle situations where there is additional *classical* uncertainty? This could arise, for instance, if we were given a quantum state that, with probability p_1 was prepared in some state $|\psi\rangle$, and with probability p_2 was prepared in a state $|\phi\rangle$. The expectation value of an operator, A over some state, $|\psi\rangle$, is defined as,

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle$$

But recall what an expectation value is: it the sum of all possible measurement outcomes weighted by their probabilities. So if we have some classical uncertainty, we can just build that into the definition of the expectation value,

$$\begin{aligned}\langle A\rangle &= p_1\langle A\rangle_\psi + p_2\langle A\rangle_\phi \\ &= p_1\langle\psi|A|\psi\rangle + p_2\langle\phi|A|\phi\rangle\end{aligned}$$

At this point we introduce a mathematical object known as the *resolution of the identity*. We can take a complete set of states, $\{|n\rangle\}$ and take their outer products, $\mathcal{I} = \sum_n |n\rangle\langle n|$. This is equal to the identity. We can see this in a simple example of a two level system: multiply any two level state on the left by $|0\rangle\langle 0| + |1\rangle\langle 1|$ and you will see that you get the same state back. In matrix form, this can be written as:

$$\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix},$$

which is the identity matrix. Inserting the resolution of the identity into the above expression, we have

$$\begin{aligned}\langle A\rangle &= p_1\sum_n \langle\psi|n\rangle\langle n|A|\psi\rangle + p_2\sum_n\langle\psi|n\rangle\langle n|A|\phi\rangle \\ &= p_1\sum_n\langle n|A|\psi\rangle\langle\psi|n\rangle + p_2\sum_n\langle n|A|\phi\rangle\langle\psi|n\rangle \\ &= \sum_n\langle n|A\left(p_1|\psi\rangle\langle\psi| + p_2|\phi\rangle\langle\phi|\right)|n\rangle\end{aligned}$$

We call the quantity in the parentheses the *density matrix*

$$\rho = p_1 |\psi\rangle\langle\psi| + p_2 |\phi\rangle\langle\phi|$$

and we can interpret $\sum_n \langle n| B |n\rangle$ as the trace of the matrix B. This can be seen again by considering a two level system:

$$\begin{aligned}\sum_n \langle n| B |n\rangle &= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= b_{00} + b_{11} \\ &= \operatorname{Tr} B\end{aligned}$$

So we have

$$\langle A \rangle = \operatorname{Tr} \rho A$$

We'll see density matrices frequently when we begin to talk about errors in quantum states. These errors occur when the controls we use to create states are imperfect and introduce uncertainty into the system.

III. HERMITIAN OPERATORS

One of the axioms of quantum mechanics is that every observable corresponds to a Hermitian operator. Let's review some properties of these objects

1. By definition, a Hermitian operator is equal to its conjugate transpose. $A = A^{\mathsf{T}*} = A^\dagger$.

2. Hermitian operators have real eigenvalues. For some eigenstate, $A |u\rangle = a |u\rangle$. Multiply on the left by $\langle u|$ and we have

   $$\langle u|A|u\rangle = a \langle u|u\rangle = a$$

   Now take the conjugate-transpose of both sides.

   $$\begin{aligned}\langle u|A|u\rangle &= a^\dagger \\ |u\rangle^\dagger A^\dagger \langle u|^\dagger &= a^* \\ \langle u| A |u\rangle &= a^*\end{aligned}$$

   Which implies that $a = a^*$, so the eigenvalue must be real.

3. Eigenvectors are orthogonal if they possess different eigenvalues. Now additionally assume we have another eigenvector with a different eigenvalue, $A |v\rangle = b |v\rangle$. Then with A acting to the right, we have

   $$\langle v| A |u\rangle = a \langle v|u\rangle$$

   but with A acting to the left we have

   $$\langle v| A |u\rangle = b \langle v|u\rangle$$

   this means that $a \langle v|u\rangle = b \langle v|u\rangle$. If $a \neq b$, then $\langle v|u\rangle = 0$, so the vectors are orthogonal.

4. Hermitian operators may be expressed in terms of their *spectral representation*:

   $$A = \sum_n a_n |n\rangle\langle n|$$

   Where $A |n\rangle = a_n |n\rangle$. This is called a spectral representation because the collection of eigenvalues is often referred to as the *spectrum* of an operator.

5. Commuting observables possess a simultaneous eigenbasis. This proof has two parts: i) Two operators that share an eigenbasis must commute, and ii) two operators that commute must share an eigenbasis. I'll do the first one here, the second one is worth working out yourselves. Assume we have two operators which share an eigenbasis, $A |n\rangle = a_n |n\rangle$ and $B |n\rangle = b_n |n\rangle$. Then

   $$AB |n\rangle = A(b_n |n\rangle) = b_n A |n\rangle = a_n b_n |n\rangle$$

   $$BA |n\rangle = B(a_n |n\rangle) = a_n B |n\rangle = a_n b_n |n\rangle$$

   So if $AB |n\rangle = BA |n\rangle$ on every state $|n\rangle$, then $AB = BA$, and we say that the operators commute.

A. Commutators

The commutator of two hermitian operators, A, B is defined as $[A, B] = AB - BA$. Here are some of their properties,

1. The are linear in both elements

$$[c_1 A_1 + c_2 A_2, B] = c_1[A_1, B] + c_2[A_2, B]$$
$$[A, c_1 B_1 + c_2 B_2] = c_1[A, B_1] + c_2[A, B_2]$$

2. The are antisymmetric

$$[A, B] = -[B, A]$$

3. They satisfy the Jacboi identity

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$

4. They satisfy the Leibnitz identity

$$[AB, C] = A[B, C] + [A, C]B$$

$$[A, BC] = B[A, C] + [A, B]C$$

IV. TENSOR PRODUCTS OF OPERATORS

When we combine quantum systems, the state vectors live in a Hilbert space that is the tensor product of the two constituent Hilbert spaces. If each qubit is in a particular state, then the combined state is the tensor product of the individual states. And if each qubit is operated on by a particular operator, then the combined operator is the tensor product of the individual operators.

1. Tensor products are linear

$$(a_1 A_1 + a_2 A_2) \otimes B = a_1 A_1 \otimes B + a_2 A_2 \otimes B$$

2. Each term in a tensor product acts on its own component

$$(A \otimes B)(|mn\rangle) = (A \otimes B)(|m\rangle \otimes |n\rangle) = A|m\rangle \otimes B|n\rangle$$

3. Multiplication of operators

$$(A \otimes B)(C \otimes D) = AC \otimes BD$$

4. The matrix representation of tensor products is, for states:

$$\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \otimes \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} a_0 \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \\ a_1 \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}$$

For operators,

$$\begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix} \otimes \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} = \begin{pmatrix} a_{00} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} & a_{01} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \\ a_{10} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} & a_{11} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \end{pmatrix}$$
$$= \begin{pmatrix} a_{00}b_{00} & a_{00}b_{01} & a_{01}b_{00} & a_{01}b_{01} \\ a_{00}b_{10} & a_{00}b_{11} & a_{01}b_{10} & a_{01}b_{11} \\ a_{10}b_{00} & a_{10}b_{01} & a_{01}b_{00} & a_{11}b_{01} \\ a_{10}b_{10} & a_{10}b_{11} & a_{01}b_{10} & a_{11}b_{11} \end{pmatrix}$$

A. Complete set of commuting observables

For any Hilbert space, we can specify a (not unique!) set of commuting observables, $\{A, B, \ldots\}$. If each eigenstate is associated with a unique set of eigenvalues over this set, the set is called a *complete set of commuting observables* or CSCO. Taking a qubit as an example, we can measure the Pauli Z operator,

$$\mathsf{Z} = \sigma_z = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

This is a somewhat trivial example, because there is only one operator in the set, but we can nonetheless associate each eigenstate, $|0\rangle$ and $|1\rangle$ with its unique eigenvalue, $+1$ and -1, respectively. For multiple qubits, we can take tensor products of the Z with the identity operator,

$$\mathcal{I} = \sigma_i = \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For example, take a six qubit system and the state $|b_1 b_2 b_3 b_4 b_5 b_6\rangle$, where b_i is a binary digit. We will consider the expectation values of the following operators:

$$\begin{aligned} \mathsf{Z}_1 &= \mathsf{ZIIIII} \\ \mathsf{Z}_2 &= \mathsf{IZIIII} \\ \mathsf{Z}_3 &= \mathsf{IIZIII} \\ &\vdots \end{aligned}$$

All of these operators commute, which can be proven by direct computation:

$$\begin{aligned} [\mathsf{Z}_1, \mathsf{Z}_2] &= \mathsf{Z}_1\mathsf{Z}_2 - \mathsf{Z}_2\mathsf{Z}_1 \\ &= (\mathsf{ZIIIII})(\mathsf{IZIIII}) - (\mathsf{IZIIII})(\mathsf{ZIIIII}) \\ &= (\mathsf{ZI} \otimes \mathsf{IZ} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I}) - (\mathsf{IZ} \otimes \mathsf{ZI} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I}) \\ &= (\mathsf{Z} \otimes \mathsf{Z} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I}) - (\mathsf{Z} \otimes \mathsf{Z} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I} \otimes \mathsf{I}) \\ &= 0 \end{aligned}$$

And their expectation values are

$$\begin{aligned} \langle \mathsf{Z}_1 \rangle &= \langle b_1 b_2 b_3 b_4 b_5 b_6 | \, \mathsf{ZIIIII} \, | b_1 b_2 b_3 b_4 b_5 b_6 \rangle \\ &= \langle b_1 | \, \mathsf{Z} \, | b_1 \rangle \, \langle b_2 | b_2 \rangle \, \langle b_3 | b_3 \rangle \, \langle b_4 | b_4 \rangle \, \langle b_5 | b_5 \rangle \, \langle b_6 | b_6 \rangle \\ &= (-1)^{b_1} \times 1 \times 1 \times 1 \times 1 \times 1 \\ &= (-1)^{b_1} \end{aligned}$$

Following the trend, we see that any eigenstate, $|b_1 b_2 b_3 b_4 b_5 b_6\rangle$ corresponds to a unique set of eiegnvalues, $\{(-1)^{b_i}\}_{i \in [1..6]}$ with respect to the CSCO listed above.

V. FUNCTIONS OF OPERATORS AND THE SCHRODINGER EQUATION

The Schrodinger equation is

$$i\hbar \frac{\partial}{\partial i} |\psi(t)\rangle = H(t) \, |\psi t\rangle$$

This looks very familiar to the ODE,

$$\frac{d}{dt} y(t) = a(t) y(t)$$

for which the solution is

$$y(t) = exp \int_0^t a(s) ds \, y(0).$$

Similarly, the formal solution to the Schrodinger equation is

$$|\psi(t)\rangle = \underset{\leftarrow}{\mathcal{T}} \exp\left(-i \int_0^t H(s) ds/\hbar\right) |\psi(0)\rangle$$

The time ordering operator $\underset{\leftarrow}{\mathcal{T}}$ is included to handle the fact the $H(t)$ might not commute with $H(t')$. But for now we will assume that $H(t) = H$ is constant, so the time ordering complication goes away and we are left with:

$$|\psi(t)\rangle = \exp\left(-iHt/\hbar\right) |\psi(0)\rangle$$

But now we must interpret this exponential of an operator,

$$\exp\left(-iHt/\hbar\right).$$

In general, functions of operators can be interpreted in terms of the spectral representation of the operators. Recall that an operator A can be written in terms of its eigenvalues and eigenvectors as

$$A = \sum_n a_n |n\rangle\langle n|$$

A function f of this operator is then interpreted as

$$f(A) = \sum_n f(a_n) |n\rangle\langle n|$$

So the solution to the Schrodinger equation may be written as

$$|\psi(t)\rangle = \sum_n \exp\left(-iE_n t/\hbar\right) |n\rangle\langle n| \, |\psi(0)\rangle$$

Where the eigenvalues of the Hamiltonian operator, H are given the special symbol E_n and are interpreted as energies.