## Quantum Computing (CST Part II) Lecture 3: The Postulates of Quantum Mechanics

The most incomprehensible thing about the world is that it is comprehensible. Albert Einstein

## Resources for this lecture

This lecture is based on Section 2.2 of Nielsen and Chuang - p80-96.

# What is quantum mechanics?

When we speak of classical mechanics we think of Newton's laws, but *quantum* mechanics is quite different – it is not a physical theory, but rather a framework for the development of physical theories.

There are four postulates of quantum mechanics that any (quantum) physical theory must satisfy.

Quantum electrodynamics (Feynman) is an example of a successful quantum physical theory, whilst a quantum theory of gravity remains elusive, and is one of the most important open problems in theoretical physics.

# The four postulates of quantum mechanics

- 1. State space: how to describe a quantum state.
- 2. Evolution: how a quantum state is allowed to change with time.
- 3. **Measurement**: the effect on a quantum state of interaction with a classical system that yields classical information.
- 4. Composition: How to compose multiple quantum systems.

# State space

#### Postulate 1

Associated to any isolated physical system is a complex vector space with an inner product (that is, a Hilbert space) known as the *state space* of the system. The system is completely described by its *state vector*, which is a unit vector in the system's state space.

In this course, we consider only qubits, quantum states with space  $\mathbb{C}^2$ , and compositions thereof (i.e., according to postulate 4), although higher dimensional "qudit" states are sometimes considered in quantum computing literature, and indeed physically there may be infinite dimensional systems.

Examples of physical realisations of qubits:

- The spin of an electron.
- The polarisation of a photon.
- The current in a superconducting circuit.

## Evolution

#### Postulate 2

The time evolution of the state of a closed quantum system is described by the *Schrödinger equation*:

 $i\hbar\frac{\mathrm{d}\left|\psi\right\rangle}{\mathrm{d}t}=\mathrm{H}\left|\psi\right\rangle$ 

where  $\hbar$  is the physical constant, *Planck's constant* and H is a fixed Hermitian operator known as the *Hamiltonian* of the closed system.

# Evolution - simplified

In computer science, we are typically interested not in continuous time evolution, but the state at discretised time intervals. It follows that postulate 2 can thus be simplified

#### Postulate 2'

The change in the state of a closed quantum system from  $t_0$  to  $t_1$  is described by the unitary transformation:

 $\left|\psi_{t_{1}}\right\rangle = U\left|\psi_{t_{0}}\right\rangle$ 

- This expression follows directly from the Schrödinger equation.
- The unitary operator U depends only on the underlying Hamiltonian and the times  $t_0$  and  $t_1$ .
- In quantum computing we are generally treat postulate 2' as the fundamental expression of state evolution.

# The significance of unitarity

The solution to the Schrödinger equation is:

$$|\psi_{t_1}\rangle = \exp\left(\frac{i\mathbf{H}(t_1-t_0)}{\hbar}\right)|\psi_{t_0}\rangle$$

From which we define the unitary, U:

$$U(t_0, t_1) = \exp\left(\frac{i\mathbf{H}(t_1 - t_0)}{\hbar}\right)$$

The unitary nature of the discrete time evolution follows directly from the Hermitian nature of the continuous time evolution, and furthermore unitary operators are the unique linear maps that preserve the norm:

 $|| |\psi_{t_1}\rangle || = ||U |\psi_{t_0}\rangle || = || |\psi_{t_0}\rangle || = 1$ 

# The Pauli matrices

The Pauli matrices X, Y and Z are important one-qubit unitary matrices.

 $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ 

Which has the following effect on the computational basis states:  $X |0\rangle = |1\rangle$ ;  $X |1\rangle = |0\rangle$ .

Y = i	0	-1
	1	0

Which has the following effect on the computational basis states:  $Y |0\rangle = i |1\rangle$ ;  $Y |1\rangle = -i |0\rangle$ .

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Which has the following effect on the computational basis states:  $Z |0\rangle = |0\rangle$ ;  $Z |1\rangle = -|1\rangle$ .

# Wolfgang Pauli

Wolfgang Pauli was a pioneer in quantum physics, notable for the Pauli exclusion principle and coining the phrase "not even wrong" (in scientific argument), amongst many other things.



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## The Hadamard matrix

Another important one-qubit unitary is the Hadamard matrix:

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}$$

Which has the following effect on the computational basis states:

$$H |0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \equiv |+\rangle$$
$$H |1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \equiv |-\rangle$$

i.e., it puts the computational basis states in superposition. H is self-inverse, therefore:

$$H \left| + \right\rangle = \left| 0 \right\rangle \qquad H \left| - \right\rangle = \left| 1 \right\rangle$$

i.e., it interferes the superposition to recover the original computational basis states.

## Measurement

#### Postulate 3

Quantum measurements are described by a collection  $\{M_m\}$  of *measurement operators*. These are operators acting on the state space of the system being measured. The index m refers to the measurement outcomes that **may** occur in the experiment.

If the state of the quantum system is  $|\psi\rangle$  directly before the measurement, the probability of the *m*th outcome is given by:

 $p(m) = \langle \psi | M_m^{\dagger} M_m | \psi \rangle$ 

and the state of the system after the measurement is

 $\frac{M_m \left|\psi\right\rangle}{\sqrt{\left\langle\psi\right| M_m^{\dagger} M_m \left|\psi\right\rangle}}$ 

# Measurement (continued)

It is necessary that the probabilities of all possible outcomes sum to one, that is

$$\sum_{m} p(m) = \sum_{m} \left\langle \psi \right| M_{m}^{\dagger} M_{m} \left| \psi \right\rangle = 1$$

as  $|\psi\rangle$  is arbitrary and not dependent on the index m, we can see that this is satisfied by the *completeness equation*,

$$\sum_{m} M_m^{\dagger} M_m = I$$

That is, because:

$$\sum_{m} p(m) = \sum_{m} \langle \psi | M_{m}^{\dagger} M_{m} | \psi \rangle$$
$$= \langle \psi | \left( \sum_{m} M_{m}^{\dagger} M_{m} \right) | \psi \rangle$$
$$= \langle \psi | I | \psi \rangle$$
$$= \langle \psi | \psi \rangle$$
$$= 1$$

### Measurement in the computational basis

In computer science, we often implicitly assume that by *measurement* we mean single qubit measurement in the computational basis. In this case, our measurement operators are

$$M_0=\left|0
ight
angle \left\langle 0
ight|=\left[egin{matrix} 1&0\0&0 \end{bmatrix}
ight
angle$$
 and  $M_1=\left|1
ight
angle \left\langle 1
ight|=\left[egin{matrix} 0&0\0&1 \end{bmatrix}
ight
angle$ 

which we can verify satisfies the completeness equation:

 $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}^{\dagger} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}^{\dagger} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$ 

Now let  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ , we have that:

 $p(M_0) = |\alpha|^2$   $p(M_1) = |\beta|^2$ 

which you are asked to verify in the exercise sheet.

# Measurement in the $|+\rangle$ , $|-\rangle$ basis

Consider the state  $|+\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$ . If we measure this in the computational basis, we get either outcome  $M_0$  or  $M_1$  each with probability 1/2. However, if we measure in the  $|+\rangle$ ,  $|-\rangle$  basis (recall  $|-\rangle = (1/\sqrt{2})(|0\rangle - |1\rangle)$ ), which has measurement operators

$$M_+ = \left|+\right\rangle \left\langle+\right| = \frac{1}{2} \begin{bmatrix} 1 & 1\\ 1 & 1 \end{bmatrix} \text{ and } M_- = \left|-\right\rangle \left\langle-\right| = \frac{1}{2} \begin{bmatrix} 1 & -1\\ -1 & 1 \end{bmatrix}$$

then we get state  $M_+$  with probability 1:

$$p(M_{+}) = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$
$$= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$
$$= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$
$$= 1$$

Measurement in the  $|+\rangle$ ,  $|-\rangle$  basis (continued)

We could get the same result more quickly using Dirac notation:

 $p(M_{+}) = \langle +|(|+\rangle \langle +|)^{\dagger}(|+\rangle \langle +|)|+\rangle = (\langle +|+\rangle)^{3} = 1$ 

Similarly, if instead  $|\psi\rangle = |-\rangle$  then we get outcome  $M_{-}$  with probability 1:  $p(M_{-}) = \langle -|(|-\rangle \langle -|)^{\dagger}(|-\rangle \langle -|)|-\rangle = (\langle -|-\rangle)^{3} = 1$ 

Whereas if we measure in the computational basis, we still get each outcome with probability 1/2. This is an example of the significance of relative phase.

### Global and relative phase

We can write any one-qubit state as:

$$\left|\psi\right\rangle = e^{i\theta}(\alpha\left|0\right\rangle + \beta e^{i\phi}\left|1\right\rangle) \equiv e^{i\theta}\left|\psi'\right\rangle$$

where  $\alpha$  and  $\beta$  are positive real numbers.  $\theta$  is known as the global phase, and has no observable consequences because:

$$U\left|\psi\right\rangle = Ue^{i\theta}(\alpha\left|0\right\rangle + \beta e^{i\phi}\left|1\right\rangle) = e^{i\theta}U(\alpha\left|0\right\rangle + \beta e^{i\phi}\left|1\right\rangle) = e^{i\theta}U\left|\psi'\right\rangle$$

and for any measurement operator  $P_m$ ,

$$\left\langle \psi \right| P_{m}^{\dagger} P \left| \psi \right\rangle = \left\langle \psi' \right| e^{-i\theta} P_{m}^{\dagger} P e^{i\theta} \left| \psi' \right\rangle = \left\langle \psi' \right| P_{m}^{\dagger} P \left| \psi' \right\rangle$$

Thus we typically neglect global phase. The same cannot, however be said for the *relative phase*,  $\phi$ . For example, in the previous slide  $|+\rangle$  and  $|-\rangle$  both have  $\alpha = \beta = 1/\sqrt{2}$ , but in the former  $\phi = 0$ , whereas in the latter  $\phi = \pi$ , and we saw that measurement in the  $|+\rangle$ ,  $|-\rangle$  basis could distinguish these two 100% of the time.

# Composition

#### Postulate 4

The state space of a composite physical system is the tensor product of the state spaces of the component physical systems. Moreover, if we have systems numbered 1 through n, and system number i is prepared in the state  $|\psi_i\rangle$ , then the joint state of the total system is  $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$ .

We can now see the significance of the fact that:

 $(U_1 \otimes U_2)(|\psi_1\rangle \otimes |\psi_2\rangle) = (U_1 |\psi_1\rangle) \otimes (U_2 |\psi_2\rangle)$ 

 $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$  is what is known as a separable state. Let  $|\psi'\rangle = (U_1 \otimes U_2)(|\psi_1\rangle \otimes |\psi_2\rangle)$ ,  $|\psi_1'\rangle = U_1 |\psi_1\rangle$  and  $|\psi_2'\rangle = U_2 |\psi_2\rangle$ , we have that:

 $|\psi'
angle = |\psi_1'
angle \otimes |\psi_2'
angle$ 

i.e., single qubit unitary matrices applied to a separable state leads to a separable state.

### Entangled states

As we shall see, quantum computing draws its advantage from the fact that not all quantum states are separable. Consider the *two qubit unitary* 

$$\mathsf{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

applied to the state  $|+\rangle \otimes |0\rangle$ :

$$CNOT(|+\rangle \otimes |0\rangle) = \begin{bmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}$$
$$= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

an entangled state which cannot be separated as tensor product.

Quantum mechanics specifies four postulates to which a physical theory must adhere. You should be familiar with these, and we have also introduced the following important concepts in this lecture.

- The Pauli matrices
- The Hadamard matrix
- The significance of global and relative phase
- The existence of entangled states