

Topics: Quantum Bits

# 1 Quantum Bits

## 1.1 Introduction

As a concrete example of probability, we now take a look at the building blocks of a quantum computer, the *quantum bit*. Recall that a classical bit can be in one of two states, either 0 or 1. A quantum bit can also be in one of these two states, but it can also be in a superposition of these states as well.

Before we continue, let me introduce some notation that will facilitate our discussion. The notation  $|\psi\rangle$  is used to denote a quantum state and is called the *wave function* of the state, and the states corresponding to the classical 0 and 1 are written as  $|0\rangle$  and  $|1\rangle$ . Then a quantum bit can be in any state  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ , where<sup>1</sup>  $\alpha^2 + \beta^2 = 1$ .

Now consider a system of two bits. Classically, they can be in one of the four states 00, 01, 10, and 11. Quantumly, they can be in any of these states or in a superposition of these states,  $|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$ , where  $\alpha^2 + \beta^2 + \gamma^2 + \delta^2 = 1$ .

This is easily generalized into our first rule for quantum bits.

**Rule 1:** *A system of quantum bits can be in any (properly normalized) superposition of the classical states of the system. In other words the state of a quantum system is  $|\psi\rangle = \sum_i \alpha_i |i\rangle$ , where the  $|i\rangle$ 's are the classical states and  $\sum_i \alpha_i^2 = 1$ .*

For those of you familiar with linear algebra, the classical states form the basis of a type of vector space called a *Hilbert space*, and the state of a quantum system can be any normalized vector in this space. The classical states are thus more generally called *basis states* of the system<sup>2</sup>.

What does it mean for a quantum bit to be in a superposition of states? Physically, when you measure some physical property of a qubit, you always get a quantity that corresponds to a basis state<sup>3</sup>. For example, measuring the energy of a qubit  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  results in  $E_0$ , the energy of the state  $|0\rangle$ , with probability  $\alpha^2$ , and in  $E_1$  with probability  $\beta^2$  (hence the normalization constraint above).

Thus the second rule for quantum bits is the following.

**Rule 2:** *A measurement on a quantum system in a superposition  $|\psi\rangle = \sum_i \alpha_i |i\rangle$  results in a value consistent with state  $|i\rangle$  with probability  $\alpha_i^2$ .*

As a concrete example, consider a quantum bit implemented physically as a hydrogen atom. Let  $|0\rangle$  correspond to the atom being in the ground state, and  $|1\rangle$  correspond to the atom being in the first excited state. Then consider a qubit in the state  $|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$ . Suppose we measure the energy of this qubit. What result will we get? We will get  $E_0 = -13.6$  eV with probability  $(\frac{1}{\sqrt{3}})^2 = \frac{1}{3}$ , and  $E_1 = -3.4$  eV with

<sup>1</sup>In actuality,  $\alpha$  and  $\beta$  can be complex. Thus the normalization requirement is  $|\alpha|^2 + |\beta|^2 = 1$ . But we will ignore the possibility of complex coefficients.

<sup>2</sup>It is actually somewhat specific to qubits that the classical states are also the basis states for the system. For example, consider the  $z$ -component of the spin of an electron. Classically, it can take on any value, but quantumly, it can only be  $+\frac{\hbar}{2}$  or  $-\frac{\hbar}{2}$ . These two states are the basis states for the  $z$ -component of an electron's spin. In general, it is the *eigenstates* of a particular Hamiltonian (energy operator) that form the basis states of a system.

<sup>3</sup>It is possible for a state to be an eigenstate of one physical property but not of another. However, in our discussion we will assume that the classical states are eigenstates of all the properties that we are measuring.

probability  $\frac{2}{3}$ . Note that we will never measure anything except these two values<sup>4</sup>.

What does all this have to do with CS70? Well, notice that the state of a quantum system defines a probability space for the results of a measurement on the system. In the example above, the probability space consists of two points, measuring  $E_0$  with probability  $\frac{1}{3}$  and measuring  $E_1$  with probability  $\frac{2}{3}$ . As a result, we can do all of our probability calculations with quantum systems.

## 1.2 Conditional Probability

Suppose we have a system of two qubits  $|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$ . Suppose we measure the energy of the first qubit and get a value of  $E_0$ . Now if we measure the energy of the second qubit, what values can we get and with what probabilities?

This is just a conditional probability calculation<sup>5</sup>. Let  $A$  be the event that we measure  $E_0$  for the first qubit,  $B$  be the event that we measure  $E_0$  for the second qubit, and  $C$  be the event that we measure  $E_1$  for the second qubit. We want to calculate  $\Pr[B|A]$  and  $\Pr[C|A]$ .

Now we see that the states  $|00\rangle$  and  $|01\rangle$  are consistent with measuring  $E_0$  for the first qubit, so  $\Pr[A] = \alpha^2 + \beta^2$ . State  $|00\rangle$  is consistent with  $A \cap B$ , so  $\Pr[A \cap B] = \alpha^2$ . Similarly,  $\Pr[A \cap C] = \beta^2$ . Thus  $\Pr[B|A] = \frac{\alpha^2}{\alpha^2 + \beta^2}$ , and  $\Pr[C|A] = \frac{\beta^2}{\alpha^2 + \beta^2}$ . Notice that the probabilities sum to 1, as they should.

What if instead of measuring the energy of the second qubit, we had left the system alone after measuring the first qubit. What state would the system be in? Well, since  $\Pr[A|A] = 1$ , we would require it to be composed only of basis states with the first qubit being 0. And since  $\Pr[B|A] = \frac{\alpha^2}{\alpha^2 + \beta^2}$ , and  $\Pr[C|A] = \frac{\beta^2}{\alpha^2 + \beta^2}$ , we would require it to be composed of states with the second qubit 0 and 1 in such a proportion as to generate these probabilities. The state

$$|\psi'\rangle = \frac{\alpha}{\sqrt{\alpha^2 + \beta^2}}|00\rangle + \frac{\beta}{\sqrt{\alpha^2 + \beta^2}}|01\rangle$$

satisfies these requirements.

The general rule that results in the above state is the following.

**Rule 3:** A measurement on a state  $|\psi\rangle$  removes all elements of the state that are inconsistent with the result of the measurement. In other words, a measurement on a state  $|\psi\rangle = \sum_i \alpha_i |i\rangle$  results in a state  $|\psi'\rangle = \sum_j \frac{\alpha_j}{N} |j\rangle$ , where the  $|j\rangle$ 's are the states consistent with the measurement, and  $N = \sqrt{\sum_j \alpha_j^2}$  to preserve normalization.

As a simple example, suppose we have a state  $|\psi\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$ , and we measure the energy of the state to be  $E_1$ . What is the resulting state? Well, only  $|1\rangle$  is consistent with this outcome, so the final state is  $|\psi'\rangle = \frac{\sqrt{3}}{2} / \sqrt{\frac{3}{4}} |1\rangle = |1\rangle$ .

This rule has an unfortunate consequence. Suppose we have a state in an unknown superposition  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ . Can we determine the values of  $\alpha$  and  $\beta$ ? No, since a measurement would destroy the superposition<sup>6</sup>. Worse, we can't even make copies of the state and measure each one, due to the *No-Cloning theorem*. The best we can do is repeat the construction of the state from scratch many times, and the measure each one to come up with some sort of histogram from which we can extrapolate the original state.

On the other hand, the rule can be used to our advantage, and is a key part of the quantum factoring algorithm.

<sup>4</sup>Well, in this case this is a simplification, since we are ignoring the existence of the other excited states.

<sup>5</sup>Well, this is actually a bit of a stretch. We are really making two distinct measurements here. Conditional probability would only apply for a single measurement. However, it just so happens that quantum physics works in such a way that this analysis works for multiple measurements as well. In reality, this follows from rule 3, instead of rule 3 following from this fact.

<sup>6</sup>An exception to this is when we measure a property of which this superposition is an eigenstate. But it is impossible to know that it is an eigenstate beforehand.

### 1.3 Expectation

As noted above, we can reconstruct an unknown quantum state multiple times, and then measure energy, for example, in order to come up with some average. This average is called the *expectation* of the energy of the system.

For a quantum state in the superposition  $|\psi\rangle = \sum_i \alpha_i |i\rangle$ , the expectation of a quantity  $X$  is  $\mathbb{E}[X] = \sum_i \alpha_i^2 \times X_i$ , where  $X_i$  is the value of  $X$  in state  $|i\rangle$ .

For example, consider the hydrogen atom state  $|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$  from above. What is the expectation of energy in this state? It is  $\mathbb{E}[E] = \frac{1}{3} \times E_0 + \frac{2}{3} \times E_1 = \frac{1}{3} \times (-13.6 \text{ eV}) + \frac{2}{3} \times (-3.4 \text{ eV}) = -6.8 \text{ eV}$ . Notice that the expectation is a different value than the actual possible outcomes of an energy measurement! This is true of expectations in general, since an average of a set of numbers may be different than the value of any number in the set.

Consider now a system of two hydrogen atoms in the state  $|\psi\rangle = \frac{1}{\sqrt{3}}|00\rangle + \frac{1}{\sqrt{6}}|01\rangle + \frac{1}{\sqrt{6}}|10\rangle + \frac{1}{\sqrt{3}}|11\rangle$ . What is the expectation of energy for this state? First note that  $E_{00} = 2 * E_0 = -27.2 \text{ eV}$ ,  $E_{01} = E_{10} = E_0 + E_1 = -17 \text{ eV}$ , and  $E_{11} = 2 * E_1 = -6.8 \text{ eV}$ . Thus the energy expectation is  $\mathbb{E}[E] = \frac{1}{3} \times E_{00} + \frac{1}{6} \times E_{01} + \frac{1}{6} \times E_{10} + \frac{1}{3} \times E_{11} = \frac{1}{3} \times (-27.2 \text{ eV}) + \frac{1}{6} \times (-17 \text{ eV}) + \frac{1}{6} \times (-17 \text{ eV}) + \frac{1}{3} \times (-6.8 \text{ eV}) = -17 \text{ eV}$ .

Notice that in this case, the expectation has the same value as the states  $|01\rangle$  and  $|10\rangle$ . Thus by using the expectation of energy alone, it is impossible to distinguish the three states  $|\psi\rangle$ ,  $|01\rangle$ , and  $|10\rangle$ . What we need is some measure of the spread in the distribution of energy measurements in order to tell which of these states it is.

### 1.4 Variance

A simple measure of the spread of a probability distribution is the *variance*. The variance is the square of a more common measure of spread, the *standard deviation*. The variance of a quantity  $X$  is defined as

$$\text{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2.$$

Consider again the system of two hydrogen atoms  $|\psi\rangle = \frac{1}{\sqrt{3}}|00\rangle + \frac{1}{\sqrt{6}}|01\rangle + \frac{1}{\sqrt{6}}|10\rangle + \frac{1}{\sqrt{3}}|11\rangle$ . Let's calculate the variance of energy in this state.

First, we calculate  $\mathbb{E}[E^2]$ . We have  $\mathbb{E}[E^2] = \frac{1}{3} \times E_{00}^2 + \frac{1}{6} \times E_{01}^2 + \frac{1}{6} \times E_{10}^2 + \frac{1}{3} \times E_{11}^2 = \frac{1}{3} \times (739.84 \text{ eV}^2) + \frac{1}{6} \times (289 \text{ eV}^2) + \frac{1}{6} \times (289 \text{ eV}^2) + \frac{1}{3} \times (46.24 \text{ eV}^2) = 358.36 \text{ eV}^2$

Then  $\text{Var}[E] = \mathbb{E}[E^2] - \mathbb{E}[E]^2 = 358.36 \text{ eV}^2 - 289 \text{ eV}^2 = 69.36 \text{ eV}^2$ , and the standard deviation is 8.328.

How does this differ from the basis states  $|01\rangle$  and  $|10\rangle$ ? In both these states,  $\mathbb{E}[E^2] = 1 \times E_{01}^2 = 289 \text{ eV}^2$ , so  $\text{Var}[E] = 0$ . Thus we can tell that the above state  $|\psi\rangle$  is not one of these basis states.

But can we differentiate  $|\psi\rangle$  from the state  $|\psi_2\rangle = \frac{1}{\sqrt{3}}|00\rangle + \frac{1}{\sqrt{3}}|01\rangle + \frac{1}{\sqrt{3}}|11\rangle$ ? It turns out that the expectation and variance of the total energy is the same in both these states. However, we can distinguish the states by measuring the energy of just the first atom.

### 1.5 Wave Functions (*Optional*)

As an interesting side note, we discuss wave functions in more detail here. What exactly is a wave function?

One interpretation of a wave function is that it contains all that we know about a particular system. We saw above that the physical significance of the wave function is that it encodes the probabilities of each of the possible outcomes of a measurement.

But this raises another question. Notice that we said a wave function contains *all that we know* about a particular system. Could there be information about the system not contained in the wave function, that we just don't know?

In particular, it seems somewhat implausible that a system could exist in a superposition state, and only make a decision on what basis state to jump into when we make a measurement. Is it possible that the

system has actually decided what basis state it is in, and that we just don't learn the result of the decision until we make a measurement?

As a concrete example, consider the state of two qubits  $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ . Suppose we make a measurement on the first qubit. If it results in a value consistent with 0, then we know the second qubit must also be 0, since the state collapses to  $|\psi'\rangle = |00\rangle$ . But if it results in 1, then we know the second qubit must be in 1. Such a state, in which measuring the value of one qubit reduces the possible values for the other qubits, is called *entangled*.

In 1935, Albert Einstein, Boris Podolsky and Nathan Rosen posed the following thought experiment, the so-called *EPR paradox*. Suppose I create a system of qubits in this state  $|\psi\rangle$ , and send one qubit off in one direction, and the other in the opposite direction. This can be done in such a way as to preserve the state of the system. Now I wait until the qubits are very far, say a light-year, apart. I measure the first qubit, and then immediately afterward, my research assistant measures the second. What possible outcomes for these measurements are there? Well, according to the wave function, the only possibilities are either both 0 or both 1.

Consider the case when both results are 0. When did the qubits decide to be in this state? Suppose that they did when the first measurement was made. But then the first qubit would have to somehow relay the fact that it chose 0 to the other qubit before the second measurement is made.

But this means that this information would have to be transmitted much faster than the speed of light! Einstein, Podolsky, and Rosen did not believe that this “spooky action at a distance” could occur, since relativistic theory restricts the speed of information to be no faster than the speed of light. This *principle of locality* dictates that one event cannot influence another simultaneous event that occurs much farther away. Thus the qubits must have decided what state to collapse into long before the measurement, perhaps when they were separated. EPR's solution to the problem was that the wave function is an incomplete description of reality, that there must be some *hidden variables* concerning the system that we just don't know.

What they did not consider, and what John Bell proposed in 1964, was what happens when you do one particular measurement on one of the qubits, and a different measurement on the other. As an example, suppose the qubits were represented by electrons. As you may recall from elementary chemistry, electrons have either spin up or spin down in the  $z$  direction, so 0 could correspond to spin up and 1 to spin down. Now suppose I measure the spin in the  $z$  direction on the first qubit, but on the second qubit, I measure the spin in the  $x$  direction? (Since there is no special direction in space, the possible results I should get are either up or down in the  $x$  direction as well. In fact, an electron with either spin up or down but not a superposition in the  $z$  axis is in an equal superposition of up and down in the  $x$  axis.)

It turns out that measuring the spins of the two electrons in different directions gives different probability distributions if you assume that the electrons decided which basis states to be in before the measurement, or if they wait until the moment of the measurement. Thus by doing this experiment and determining which of these two results the experiment obeys, we can rule out one theory or the other.

Many such experiments have been done in the past few decades. And all have been inconsistent with the decision being made before the measurement! Thus it is generally believed<sup>7</sup> that there are no hidden variables, and that the wave function is really everything there is to know about a system. The world we live in is inherently probabilistic and non-local.

## 1.6 Further Information

### 1.6.1 Courses

The quantum mechanics courses in the physics department are Physics 137A and 137B. Physics H7C also introduces quantum mechanics.

CS/Chemistry/Physics 191 is on quantum information science and technology. It teaches enough quantum physics as necessary, and introduces quantum computation.

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<sup>7</sup>Well, other interpretations to quantum mechanics have been proposed, including the somewhat implausible *many-worlds interpretation*, but none have gained much of a following among physicists.

### 1.6.2 Texts

Griffiths' *Introduction to Quantum Mechanics* is generally used in Physics 137A and 137B.

The Feynman lectures, volume three, are a good introduction to quantum mechanics, and a much easier read than Griffiths.

*Quantum Computation and Quantum Information* by Nielsen and Chuang is an extensive reference on quantum computing.