Quantum Computing

Lecture 2 - Introduction to Quantum Mechanics

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1 Introduction: Beyond Classical Physics

At the turn of the 20th century, confidence was high that nature could be described accurately and exhaustively by classical physics. Lord Kelvin echoed a popular sentiment of the time: "There is nothing new to be discovered in physics now. All that remains is more and more precise measurement." The classical paradigm of physics can be summarized in three axioms:

1) *Once the initial state of a physical system is specified (say a point particle by its initial position and velocity), the state of that system deterministically evolves according to the laws of nature governing the system (say F=ma).*

2) *At any point in time, any physical value of that system's state space (say energy) can be measured. We can predict the result of that measurement from the governing laws of the system (say Boltzmann's Law).*

3) *Any measurement of a physical value in the system's state space (say a momentum measurement) can be made at any time without affecting the state of that physical system.*

A series of groundbreaking experiments at atomic length scales within a few years of Kelvin's proclamation showed that classical physics was an emergent phenomena of a more fundamental description of nature. They showed that nature did not obey the classical axioms at these scales. The first mathematically and physically consistent theory by Schrodinger, Heisenberg, and Bohr to accurately explain and predict the outcome of these experiments demand some odd amendments to the classical axioms. This was the beginning of Quantum Mechanics:

1) *This one is actually still correct but we need to completely rethink the concept of a physical system's state. Rather than F=ma, we have something called the Schrodinger Equation that tells us deterministically how quantum state evolves forward in time. Instead of a set of known physical values,* $\{x, p, E, V, ...\}$*, all the physical information about*

a physical state comes in the form of a wave function ψ. It will give us the probability that the physical variables of our system will take certain values when measured.

2) *The physical variables of a system can still be measured at any time, however, this cannot in general be done without dramatically affecting the state of the system. In fact, a measurement of a physical variable in general causes what is known as the 'collapse' of the wavefunction ψ non-continuously to the outcome of the measurement. Any time a measurement is made, the time evolution of the system is no longer deterministic from the time before the measurement to the time after the measurement is made. Before and after the measurement is made, the system will evolve deterministically according to the laws of quantum mechanics.*

3) *ψ is an indeterministic state that only gives probability distributions over possible values rather than the values of physical quantities. However, a measurement demands a particular real value as its outcome. When we look at a red ball on a driveway, it is in a particular position. When was the last time you saw anything on your driveway in a 46% chance of being 1 meter away from you? This means that a change must happen to ψ when a measurement is made from the indeterministic probability state to the certain value state that we actually observe in real physics. This 'collapse' is non-deterministic and occurs the same way a coin flip resolves. It has a certain probability of yielding a certain value for the physical variable measured. This is alluded to in 2) but after the measurement is made, ψ remains in the state the measurement 'collapses' ψ to. If we stop observing the state ψ it will deterministically evolve in accordance with the laws of quantum mechanics, possibly to another indeterministic state that cannot give us definite information about the values of the physical variables of state our system is in. That is, if we do not observe it, ψ can evolve back into a wave function that only gives us information about the state of our system in terms of probability distributions over the possible values of physical variables rather than definite answers like in Newtonian mechanics.*

These changes uproot the foundations of classical physics. The way nature actually works is so far beyond our intuitions and expectations that we would never have considered these possibilities theoretically were it not for undeniable experimental proof.

2 The Double-slit Experiment

Now we turn to the most damning nail in the coffin of classical physics: the Double-slit experiment. Full appreciation and understanding of how the dynamics of the electron look in the quantum reality of nature requires some forematter on how waves vs. particles would act in the same situation. Rest assured, it acts like neither one. However, the physical details of the electron mimics both at times in a way that bafflingly defy classical physics. The experimental setup of the Double-slit experiment involves a wall with two cut out windows in it, each of which can be closed at will, in between an electron gun and a back screen. The electron gun can be moved back and forth along the x axis and emits a beam of electrons or one electron at a time. The middle screen is orthogonal to both the x and y axes and the windows are cut along the z axis. The back screen has some mechanism of detecting the electrons, we can say it is a scintillating screen that lights up whenever an electron impacts it and we can record this scintillation by camera. Over a certain period of time we can count the number of scintillations and divide by the number of electrons fired by the electron gun to calculate the probability of an electron making an impact at x=x_1 along the back screen. This quantity $P(x)$, the probability of an electron impacting the back screen at a position x along the x axis is the variable of interest.

2.1 How Would Particles Act?

If electrons were classical particles as was previously thought, they would act just like pellets when fired from BB guns. If we ignore the possibility of two electrons colliding with each other and scattering off one another, we obtain the pattern below. Given that the probability for an electron to impact the back screen with only window 1 open is P_1 and the probability for an electron to impact the back screen with only window 2 open is P_2, the probability for an electron to impact the back screen with both windows open is P = $P_1 + P_2$ That is, if both windows on the middle wall were open, the probability

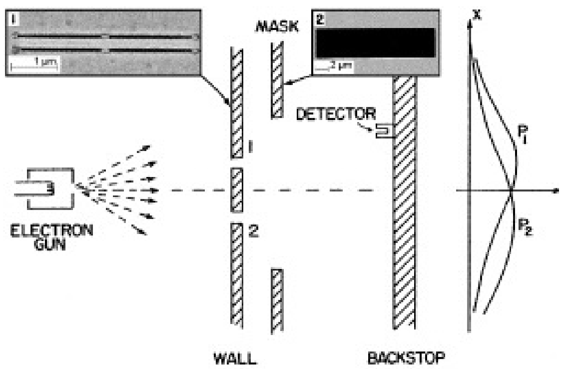

Figure 1: The results of the Double-slit experiment if electrons were classical particles

P_1 for an electron to travel through the first window and impact anywhere on the back screen would simply add with the probability P_2 that an electron would instead travel through the second window and impact anywhere on the back screen. Now let's look at how electrons would act if they were waves.

2.2 How Would Waves Act?

Let's say instead that electrons were waves. How would this experiment look then? Well, waves interfere with each other over spatial regions where they intersect. If you imagine the ocean, you can see this in your head. Two waves that meet do not just pass right through one another unscathed. Similarly, if we model a father pushing a child on a swing with the frequency ω_1 of a cosine wave $A\cos(\omega_1 t)$ and a mother pushing the same child with the frequency ω_2 of another cosine wave $B\cos(\omega_2 t)$ the maximum amplitude of the child's height modeled as a third cosine wave would be a function of the first two driving cosine waves. If both parents pushed with the same frequency ω_c the maximum amplitude would be A+B and if one parent instead pushed with the frequency ω_1 and the other pushed with the frequency $\omega_1+\pi$ the swing wouldn't go anywhere! This is called constructive and deconstructive interference, respectively. The peaks and troughs in Figure 2 below are caused by the fact that parts of the electron wave have to travel further than other parts. So when they meet at the back

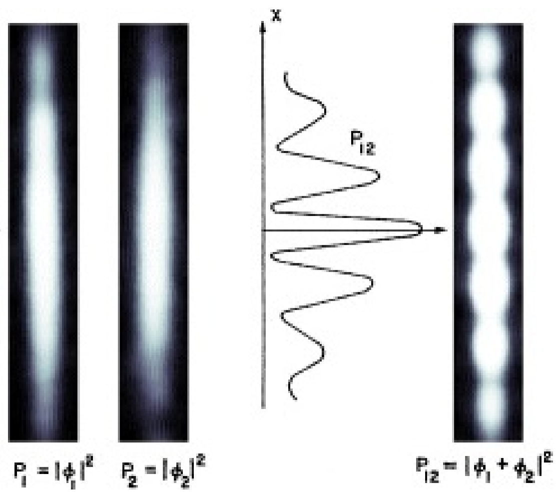

Figure 2: Caption

screen, there is a phase delay $A\cos(\omega t - \delta_1) + A\cos(\omega t - \delta_2)$ that causes the peaks and troughs in the graph. If electrons were waves, we would see this kind of wavy interference rather than the superposition of normal distributions like in the particle case. Quantitatively, if opening window 1 only resulted in a probability of P_1 for an electron to hit the back screen and opening window 2 only resulted in a probability of P_2 for an electron to hit the back screen, then opening both windows would result in the probability $P = P_1 + P_2 + P_1 P_2 \cos\delta$ where δ is the phase difference between the wavefronts at that point. In the wave case we have picked up this interference term $P_1 P_2 \cos\delta$ that isn't present in the particle case. Now let's see how electrons actually did act in the Double-slit experiment.

2.3 How Electrons Actually Act

What do we observe in the Double-slit experiment with real electrons that shook the foundations of physics so? Well, a stream of electrons do interfere with each other like waves when we are not observing them. If we do observe them, they act like particles. That's the high level experimental summary. In fact, even individual electrons act like waves *that can interfere with themselves*. If we fire a single electron at a time, and keep both windows open you still observe this wave-like interference term $P_1 P_2 \cos\delta$. It is as if a single electron was able to go through both windows simultaneously and *interfere with itself!*. If that isn't strange enough, when we check to see which window the electron actually went through, the interference disappears. Just observing to see if the electron actually went through window 1 or window 2 causes the electron interference pattern to disappear. It now looks like the particle-like situation of 2.1 rather than the wave-like situation of 2.2 if we do not make this observation. So, you see now what is meant by saying the electron is neither a particle nor a wave. This should be sufficient motivation to consider the classical notions of physics outlined in the introduction fallible. Now let's try to come up with some theory that fits our experimental results.

3 Quantum Theory

The system looks and acts like a wave, as long as no observations are being made on it. The difference between this wave and those we are used to is that this wave can't be felt like an ocean wave or seen like a light wave. Quite the opposite. If observed, it isn't there anymore. Though this wave doesn't exist in any physically observable state, it is a mathematical abstraction we fit over physically very real probability distributions. That is, the wave itself cannot be observed, but the amplitude of the wave does correspond to a physically observable reality: the probability that the electron strikes the back screen. What does this wave look like? What is it's amplitude at time t? What is its frequency? These are all questions we need to answer if a wave is governing real physical quantities.

3.1 The Wave Equation

Let's try to derive a sensible wave theoretically.

A wave, such as the one we observed experimentally, must have the mathematicaly form:

$$\psi(x,t) = Ae^{i(kx-\omega t)} \tag{1}$$

Furthermore, it must conserve energy:

$$\frac{p^2}{2m} + V(x) = E \tag{2}$$

Another experiment by Einstein on the photoelectric effect showed that light, which we thought was purely a wave, only delivers energy and momentum in discrete particle like packets called quanta[1]:

$$E = \hbar\omega \tag{3}$$

[1]Interesting to note that electrons which we thought were particles act like waves in the Double-Slit experiment and light, thought to be a wave, acts like a particle in the photoelectric effect experiment.

$$p = \hbar k \tag{4}$$

Substituting equations 3 and 4 into equation 2 gives:

$$\frac{\hbar^2 k^2}{2m} + V(x) = \hbar\omega \tag{5}$$

Multiplying equation 5 by the wave function in equation 1 yields:

$$\frac{\hbar^2 k^2 \psi(x,t)}{2m} + V(x)\psi(x,t) = \hbar\omega\psi(x,t) \tag{6}$$

Now we need to find the differential equation that will give this result when applied to the wave function in equation 1 in order to enforce the conservation of energy. Looking at equation 1 makes it clear that the two differential operators that will produce $-k^2$ and ω are $\frac{\partial^2}{\partial x^2}$ and $i\frac{\partial}{\partial t}$, respectively. This gives us the following wave equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{7}$$

This is known as Schrodinger's equation (in one space dimension - it can easily be generalized to three spatial dimensions by replacing the differential operator with the Laplacian operator). It is a second order linear partial differential equation that uniquely determines the wave function $\psi(x,t)$ for a given potential V(x) in a physical system. Well, this isn't a wave, but it's an equation that will give us one. Let's solve it!

3.2 Solving the Wave Equation

To solve our new wave equation, let's try separation of variables, the first line of offense in solving partial differential equations. Let's check for a solution of the form $\phi(x)\Psi(t)$:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\phi(x)\Psi(t)}{\partial x^2} + V(x)\phi(x)\Psi(t) = i\hbar\frac{\partial\phi(x)\Psi(t)}{\partial t} \tag{8}$$

$$\frac{-\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}\frac{1}{\phi(x)} + V(x) = i\hbar\frac{\partial\Psi(t)}{\partial t}\frac{1}{\Psi(t)} \tag{9}$$

Since the right side now does not depend on x, changing x cannot affect the right side. However, the left side of the equation can change when x is changed. Because both sides are equal, they must change together. This seems to imply that the right side must also

This synthesis of light and matter under one physical model of wave-particle duality was a silver lining of the early break with classical physics.

change when x changes apparently contradicting the equation. The only way to reconcile this apparent paradox is to have both the left side and right side equal to constants.

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\phi(x) = E\phi(x) \tag{10}$$

$$i\hbar\frac{\partial\Psi(t)}{\partial t} = E\Psi(t) \tag{11}$$

The solution to equation 11 is:

$$\Psi(t) = e^{\frac{-iEt}{\hbar}} \tag{12}$$

Equation 10 is known as the time independent Schrodinger equation. It should be thought of as the quantum analog of Newton's 2. The solution to equation 10 depends on the potential V(x) of the physical system under consideration. Once a solution to that equation $\phi(x)$ is found, the complete time dependent solution to the physical system is:

$$\psi(x,t) = \phi(x)e^{\frac{-iEt}{\hbar}} \tag{13}$$

In confirmation of our hypothesis that a solution of the form $\phi(x)\Psi(t)$ exists to the Schrodinger equation exists, we have found such a solution. It turns out that any solution to the Schrodinger equation can be written as a linear combination of these separable solutions. A quick example is called for to show more concretely how the wave function is found in typical quantum mechanics problems.

Example 2.2.1 Particle in a Box

Imagine a finite region of one dimensional space where V(x)=0 bounded by infinitely long regions where V(x)=∞. This potential is called the infinite potential well. Setting out to solve the Schrodinger equation for the finite region, we set V(x)=0:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x) \tag{14}$$

$$\frac{\partial^2\psi(x)}{\partial x^2} = -\frac{2Em}{\hbar^2}\psi(x) \tag{15}$$

The solutions to this differential equation are the sinusoidal functions Acos $\frac{\sqrt{2mE}}{\hbar}$ and $B\sin\frac{\sqrt{2mE}}{\hbar}$. So the solution obtained is $\psi(x) = A\cos\frac{\sqrt{2mE}}{\hbar}x + B\sin\frac{\sqrt{2mE}}{\hbar}x$.

The boundary condition of the potential well also constrains $\psi(0) = \psi(L) = 0$, where L is the length of the finite region where the potential is 0.

$$\psi(0) = 0 = A \tag{16}$$

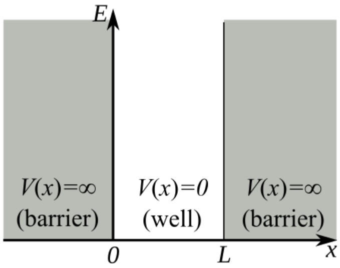

Figure 3: The infinite potential well. Beyond and at the barriers at x=0 and x=L, the potential V(x) is infinite. In between the two barriers it is 0.

Equation 16 means A must be 0. The wave function is further constrained to be 0 at length L:

$$\psi(L) = 0 = \sin \frac{\sqrt{2mE}}{\hbar} L \tag{17}$$

This gives a condition on the argument of the sin and thus on the allowed energies the wave function can take:

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \tag{18}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \tag{19}$$

The wave function for the infinite potential well is then: $\psi(x) = \sin k_n x$ where $k = \frac{\sqrt{2mE_n}}{\hbar}$ and the allowed energies of the system are $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$. Figure 4 below shows what this wave function looks like for the first four values of n:

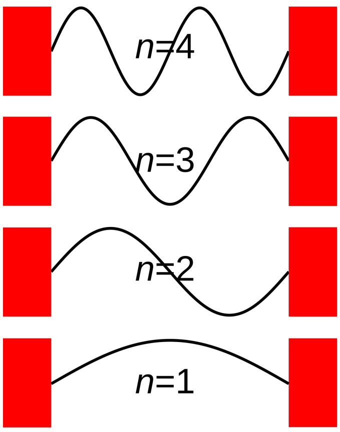

Figure 4: $\psi(x) = \sin k_n x$ graphed over the region of the infinite potential well where V(x)=0 for the first four energy values.

As this is not a quantum mechanics course, the focus will not be on solving problems like this. Nonetheless, a short problem set with problems like these will be assigned to give the student more of a quantitative intuition for the differences between quantum and classical physics.

4 Quantum State

It may not look this way at first, but the wave function $\phi(x)$ is a vector like the classical state vectors we saw in the last lecture. There are also significant difference between ψ and these classical vectors which lie at the heart of quantum computing. However, it is mathematically a vector. It satisfies all the mathematical axioms of a vector just like any other. You can add wave functions and the operation is commutative, multiply them by constants, and even take the inner product of two of them to calculate their length just like classical vectors. However, there are two big distinctions between Euclidean vectors and wave functions.
1) The entries of wave functions can be complex numbers. They are not restricted to be real numbers like in the case of Euclidean vectors.
2) The length of wave functions and their inner product with each other is calculated in a different way that Euclidean vectors.
Wave functions are vectors over Hilbert space rather than Euclidean space like the vectors we are used to. The metric of these two vector spaces is different. That means that the length of vectors over Hilbert space like our wave function is calculated in a different way. In Euclidean space, we calculate the length of a vector with the Pythagorean theorem:

$$|\vec{X}| = \vec{X} \cdot \vec{X} = \sqrt{X_x^2 + X_y^2 + X_z^2} \tag{20}$$

This is not how length is calculated in Hilbert space. Instead we use the following metric, where X^* denotes the complex conjugate of X:

$$|\vec{X}| = \sqrt{X_x^* X_x + X_y^* X_y + X_z^* X_z} \tag{21}$$

To join our intuition for vectors to $\phi(x)$, we can think of it as an infinitely long column vector with one entry for each space coordinate:

$$\phi(x) = \begin{pmatrix} \phi(x_1) \\ \phi(x_2) \\ \phi(x_3) \\ ... \end{pmatrix} \tag{22}$$

The physical interpretation of these wave function, as alluded to earlier, is that the complex norm of each column entry is the probability that the particle is in the position represented by that row. For example, $|\psi(x_1)|$ is the probability that the particle will be in the position x_1 when measured. The norm of any wave function must be one since the particle has to be somewhere. If the norm is not one, it is acceptable to normalize the wave function to a norm of one by multiplying it by an overall constant since this constant does not physically change the state represented by the wave function. The wave vectors of quantum mechanics that we get by solving the Schrodinger equation represent quantum state and information the same way the classical vectors we looked at in the last lecture represent classical state and information. However, there are key mathematical differences we can use to make new algorithms, logic gates, states of information, and ultimately quantum computers.