Quantum Mechanics

Introductory Remarks
Humans have divided physics into a few artificial categories, called theories, such as

- classical mechanics (non-relativistic and relativistic)
- electricity & magnetism (classical version)
- quantum mechanics (non-relativistic)
- general relativity (theory of gravity)
- thermodynamics and statistical mechanics
- quantum electrodynamics and quantum chromodynamics (relativistic version of quantum mechanics)

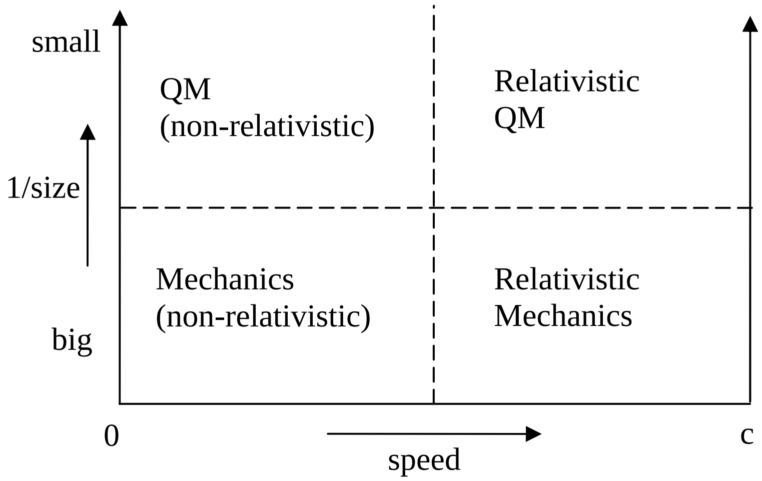
Each of these theories can be taught without much reference to the others. (Whether any theory can be *learned* that way is another question.) This is a bad way to teach and view physics, of course, since we live in a single universe that must obey one set of rules. Really smart students look for the connections between apparently different topics. We can only really learn a concept by seeing it in context, that is, by answering the question: how does this new concept fit in with other, previously learned, concepts?

Each of these theories, non-relativistic classical mechanics for instance, must rest on a set of statements called *axioms* or *postulates* or *laws*. Laws or Postulates are statements that are presented without proof; they cannot be proven; we believe them to be true because they have been experimentally verified. Newton's 2nd Law, $\vec{F}_{net} = m\vec{a}$, is a postulate; it cannot be proven from more fundamental relations. We believe it is true because it has been abundantly verified by experiment.

Actually, Newton's 2nd Law has a limited *regime of validity*. If you consider objects going very fast (approaching the speed of light) or object very small (microscopic, atomic), then this "law" begins to make predictions that conflict with experiment. However, within its regime of validity, classical mechanics is quite correct; it works so well that we can use it to predict the time of a solar eclipse to the nearest second, hundreds of year in advance. It works so well, that we can send a probe to Pluto and have it arrive right on target, right on schedule, 8 years after launch. Classical mechanics is not wrong; it is just incomplete. If you stay within its well-prescribed limits, it is correct.

Each of our theories, *except* relativistic Quantum Mechanics, has a limited regime of validity. As far as we can tell, QM (relativistic version) is *perfectly* correct. It works for *all* situations, no matter how small or how fast. Well... this is not quite true: no one knows how to properly describe gravity using QM, but everyone believes that the basic framework of QM is so robust and correct, that eventually gravity will be successfully folded into QM without requiring a fundamental overhaul of our present understanding of QM. String theory is our current best attempt to combine General Relativity and QM, but "String Theory" is not yet really a theory, since it cannot yet make predictions that can be checked experimentally.

Roughly speaking, our knowledge can be divided into regimes like so:



In this course, we will mainly be restricting ourselves to the upper left quadrant of this figure. However, we will show how non-relativistic QM is completely compatible with non-relativistic classical mechanics. We will show how QM always agrees with classical mechanics, in the limit of macroscopic objects.

The Postulates of Quantum Mechanics

The laws (axioms, postulates) of Classical Mechanics are short and sweet:
Newton's Three Laws.

The laws of classical electricity & magnetism are similarly short and sweet:
Maxwell's equations plus the Lorentz force law.

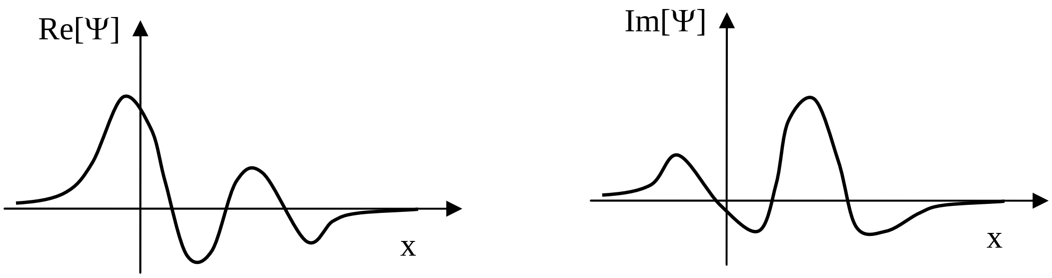
Alas, there is no agreement on the number, the ordering, or the wording of the Postulates of Quantum Mechanics. Our textbook (Griffiths) doesn't even write them down in any organized way. They are all in there, but they are not well-labeled, and not collected in any one place. (Griffiths sometimes indicates Postulate by putting the statement in a box.)

Quantum Mechanics has (roughly) 5 Postulates. They cannot be stated briefly; when stated clearly, they are rather long-winded. Compared to Classical Mechanics or E&M, quantum mechanics is an unwieldy beast – scary and ugly at first sight, but very, very powerful. I will be stating the Postulates as given in Gillespie's book. As we go along, I will write the Postulates as clearly as I can, so that you know what is assumed and what is derived. Writing them all down now will do little good, since we haven't yet developed the necessary vocabulary. I will begin by writing partially correct, but incomplete or inaccurate versions of each Postulate, just so we can get started. Later on, when ready, we will write the rigorously accurate versions of the postulates.

So let's start:

Postulate 1: The state of a physical system is *completely* described by a complex mathematical object, called the wavefunction Ψ (psi, pronounced "sigh"). The wavefunction $\Psi = \Psi(x)$ is single-valued, continuous, and normalized.

In this course, we will mostly be restricting ourselves to systems that contain a single particle (like one electron). In such a case, the wavefunction can be written as a function of the position coordinate $\vec{r}$ of the particle, $\Psi = \Psi(\vec{r})$. Often, we will simplify our lives by considering the (rather artificial) case of a particle restricted to motion in 1D, in which case we can write $\Psi = \Psi(x)$. In general, this is a complex function of x; it has a real and an imaginary parts. So when graphed, it looks something like.



In fact, it can look like *anything*, so long as it is continuous and normalized. Definition: A wavefunction is *normalized* if $\int\limits_{-\infty}^{+\infty} \left|\Psi(x,t)\right|^2 dx = 1$.

Actually, there are many different ways to write the wavefunction describing a single spinless particle in 1D: $\Psi(x)$, $\Phi(p)$, $\left|\Psi\right\rangle$, and others, to be explained later. (Here x is position, and p is momentum).

If the particle has spin, then we have to include a spin coordinate m, in addition to the position coordinate in the wavefunction $\Psi = \Psi(\vec{r}, m)$. If the system has 2 particles, then the wavefunction is a function of two positions: $\Psi = \Psi(\vec{r}_1, \vec{r}_2)$.

Postulate 2 has to do with operators and observables and the possible results of a measurement. We will skip that one for now.

Postulate 3 has to do with the results of a measurement of some property of the system and it introduces indeterminacy in a fundamental way. It provides the physical interpretation of the wavefunction.

Postulate 3: If the system at time t has wavefunction $\Psi(x,t)$, then a measurement of the position x of a particle will not produce the same result every time. $\Psi(x,t)$ does not tell where the particle is, rather it give the probability that a position measurement will yield a particular value according to

$$|\Psi(x,t)|^2\,dx = \text{Prob(particle will be found between x and x+dx at time t)}$$

An immediate consequence of Postulate 3 is

$$\int_{x_1}^{x_2} |\Psi(x,t)|^2\,dx = \text{Prob(particle will be found between } x_1 \text{ and } x_2\text{)}$$

Since the particle, if it exists, has to be found somewhere, then Prob(particle will be found between –∞ and +∞) = 1. Hence the necessity that the wavefunction be normalized, $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\,dx = 1$

This QM description is very, very different from the situation in classical mechanics. In classical mechanics, the state of a one-particle system at any given instant of time is determined by the position and the momentum (or velocity) : $\vec{r},\ \vec{p}$. So, a maximum of 6 *real numbers* completely describes the state of a classical single-particle system. Only 2 numbers, x and p, are needed in 1D. In contrast, in QM, you need a *function* $\Psi(x)$. To specify a function, you need an *infinite* number of numbers. (And it's a complex function, so you need 2 × ∞ numbers.)

In classical mechanics, the particle always has a precise, definite position, whether or not you bother to measure its position. In quantum mechanics, the particle *does not have a definite position*, until you measure it.

The Conventional Umpire:	"I calls 'em as I see 'em."
The Classical Umpire:	"I calls 'em as they <u>are</u>."
The Quantum Umpire:	"They ain't <u>nothing</u> till I calls 'em."

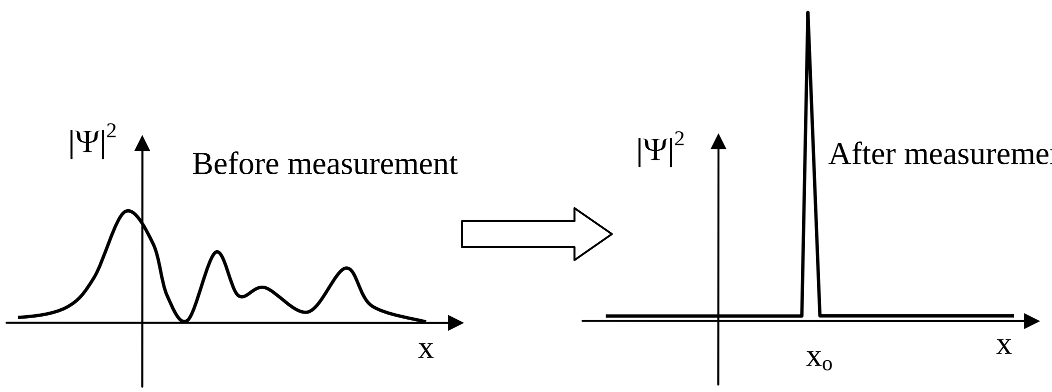
In quantum mechanics, we are not allowed to ask questions like "What is the particle doing?" or "Where is the particle?" Instead, we can only ask about the possible results of measurements: "If I make a measurement, what is the probability that I will get such-and-such a result?" QM is all about measurement, which is the only way we ever truly know anything about the physical universe.

Quantum Mechanics is fundamentally a probabilistic theory. This indeterminacy was deeply disturbing to some of the founders of quantum mechanics. Einstein and Schrödinger were never happy with this postulate. Einstein was particularly unhappy and never accepted QM as complete theory. He agreed that QM always gave correct predictions, but he didn't believe that the wavefunction contained <u>all</u> the information describing a physical state. He felt that there must be other information ("hidden variables"), in addition to the wavefunction, which if known, would allow an exact, deterministic computation of the result of any measurement. In the 60's and 70's, well after Big Al's death, it was established that "hidden variables" theories conflict with experiment. Postulates 1 and 3 are correct. The wavefunction really does contain everything there is to know about a physical system, and it only allows probabilistic predictions of the results of measurements.

The act of measuring the position changes the wavefunction according to postulate 4:

Postulate 4: If a measurement of position (or any *observable property* such as momentum or energy) is made on a system, and a particular result x (or p or E) is found, then the wavefunction changes instantly, discontinuously, to be a wavefunction describing a particle with that definite value of x (or p or E). We say that the wavefunction *collapses* to the eigenfunction corresponding to the eigenvalue x.

If you make a measurement of position, and find the value x_o, then immediately after the measurement is made, the wavefunction will be sharply peaked about that value, like so:



(The graph on the right should have a much taller peak because the area under the curve should be the same as before the measurement. The wavefunction should remain normalized.)

Postulate 1 states that the wavefunction is continuous. By this we mean that $\Psi(x,t)$ it is continuous in space. It is not necessary continuous in time. The wavefunction can change discontinuously in time as a result of a measurement.

Because of postulate 4, results of rapidly repeated measurements are perfectly reproducible. In general, if you make only one measurement on a system, you cannot predict the result with certainty. But if you make two identical measurements, in rapid succession, the second measurement will always confirm the first.

QM is infuriatingly vague about what exactly constitutes a "measurement". How do you actually measure position (or momentum or energy or any other observable property) of a particle? For a position measurement, you could have the particle hit a fluorescent screen or enter a bubble chamber. For a momentum or energy measurement, it's not so clear. More on this later. For now, "measurement" is any kind of interaction between the microscopic system observed and some macroscopic (many-atom) system, such as a screen, which provides information about the observed property.

Postulate 5, the last one, describes how the wavefunction evolves in time, in the absence of any measurements.

Postulate 5. The wavefunction of an isolated system evolves in time according to the Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

where V = V(x) is the potential energy of the particle, which depends on the physical system under discussion.

One's first reaction to Postulate 5 is "Where did <u>that</u> come from?" How on earth did Schrödinger think to write that down? We will try to make this equation plausible, and show the reasoning that lead Schrödinger to this Nobel-prize-winning formula. But, remember, it's a *Postulate*, so it cannot be derived. We believe it is true because it leads to predictions that are experimentally verified.

