18: Modern (Non relativistic) Quantum Mechanics

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18.1 Preamble

The early steps in quantum theory were all well and good, but there was no coherence to it. Each time a new experimental result seemed strange, physicists searched for a new ad hoc assumption to make that would somehow give the right answer. Previous results lent little insight into how the next problem should be approached. This kind of progress is good, but it has very limited predictive and explanatory power. We can answer the “what?” questions on an individual basis, but understand little of the “how?” and essentially know nothing of the “why?”. This situation was dramatically improved by the comprehensive theory put forward by Shrödinger and Heisenberg. I say dramatically improved rather than solved because the true nature of some quantum concepts is still a topic of legitimate (if not lively) debate amongst professional physicists (not to mention philosophers and confused laypeople...).

The upshot of this is that you get to ask questions to which the answer is “well, no-one really knows, but what I think is...”. I will make clear when I am expressing an opinion versus verifiable fact, and especially if I happen to hold a minority viewpoint. There are also instances of physicists being simply saying incorrect things. Your textbook, as most treatments of quantum theory at an introductory level, lies to you about a couple of things in an overzealous attempt to try and make sense of the physics. I’ll point out these lies where I notice them, because I would rather tell you true things that confuse you than lull you into a false sense of understanding. I fully expect you to leave this lecture fundamentally confused, because this stuff makes absolutely no sense from our usual perspective. I realize that, say, Gauss’s Law didn’t make a lot of sense to you either. But that was more a matter of complex new ideas that were hard to wrap your mind around. Quantum mechanics appears in many situations to be quite simple and quite simply *wrong*. Reconciling the fact that it appears obviously incorrect while being entirely verified and real is a whole new kind of confusing.

18.2 Matter Waves

The first issue to be addressed, is what in the world are these matter waves all about? We've got electron waves and they give us some predictions for the double slit experiment and so on, but what does it mean? What is an electron, or any other particle, really?

Start by considering what defines a wave. Waves have a wavelength, a frequency, and an amplitude. In the case of light the wavelength and frequency are interchangeable because the velocity is a constant, but in general they are independent properties. We've already defined the wavelength of a particle. The frequency, when combined with wavelength, tells us about velocity (sortof. Don't worry about it but its actually way more complicated than you'd expect). What about the amplitude?

In the case of light, rather than talk about the amplitude we will often talk about the *intensity*, which is the square of the wave. This weeds out pesky minus signs and simplifies interpretation. Intensity ends up being how bright the light is, or how much light passes through a point, which in the quantum picture means *how many photons* pass through a region. If my intensity is larger in a region, a larger number of photons pass through.

What about really really dim, low intensity light, such that you find that fewer than one photon passes through a given region? How can we interpret intensity then? The same way, as a number of photons. However, the interpretation of a fraction of a photon isn't necessarily entirely obvious. The entire point of a photon is that it is the smallest possible piece of light, so a fraction shouldn't be possible right? Right! So instead, we interpret the intensity as a *probability density*. If the probability density in a region is less than one, then there is some chance the photon is not there, and some chance that it is. The total of this probability over all of our space must add up to the number of photons we have. So if we have 1, the probability adds up to 1 and is less than one for any smaller region. If we have 10^{20} photons in a room (I made that number up), then any reasonably sized volume inside the room will likely have a huge number of photons in it.

We interpret the amplitude of matter waves in exactly the same way. The ("complex". Again, don't worry about it) square of the amplitude is interpreted as a probability density. Using our understanding of waves in general or later our quantum theory, we can make predictions about how the matter waves will behave. Then we square them and interpret the result as a probability density. This much of the interpretation of QM is essentially universally accepted as a practical fact of life. The big questions come in when we think about how we go from this probability wave to "oh, there it is. Right there in that single exact tiny spot which is far far smaller than the wavelength should allow me to resolve and yet somehow I can.". There are lively competing ideas about this, one of which is the Copenhagen Interpretation which the text pretends to explain and portrays as near-universally accepted. What we generally mean by the Copenhagen interpretation goes further than what I have explained so far, and states that when a "classical measurement" occurs, the probability wave (wave function) "collapses" to a single point. After this collapse to a single determined state, the system continues to evolve quantum mechanically until another "classical measurement" occurs. I put these terms in quotes because actually defining them, which we should do since this is supposed to be science, is bloody near impossible. Valiant efforts have been made by serious people, and it can be very interesting to read about. However, these questions of interpretation very rarely make anything like a measurable prediction. They all give, in the end, the same probabilistic interpretation of the wave function and the same rules for its behavior, as they must since these properties are well measured and verified. That said, the situation is somewhat dissatisfying and many physicists hope that ongoing work will result in testable predictions that lend insight into whats really going on.

18.3 Heisenberg Uncertainty Principle

The uncertainty principle is the most lied about concept in physics, as far as I can tell. The principle itself is almost always stated more or less correctly:

It is impossible to measure both the position and momentum of a particle perfectly simultaneously Heisenberg Uncertainty Principle

But this expression implies a different, more restricted emphasis than the true meaning. Yes, it is true that such measurements cannot be made. But it has *nothing to do* with the process of measurement itself, and is not restricted to measurement. The more correct statement, which is fundamentally different when you think about it for a while, is:

The position and momentum of a particle ARE NOT simultaneously DEFINED perfectly Heisenberg Uncertainty Principle

The difference is illustrated by the red herring which is almost ubiquitously used to explain the uncertainty principle. It is generally stated that if you try and measure the position of something by hitting it with a photon, you'll change its momentum and thus not be able to know both at the same time. This is a complete crock and you should avoid letting it shape your understanding of the uncertainty principle in the slightest. The process described is in a sense real and true (it is, in fact, hard to make precise measurements because of this effect) but:

1. It has nothing to do with quantum mechanics and would be just as true if we were talking about tiny billiard balls.

2. It is actually possible to make certain measurements in a fashion which doesn't involve any sort of interaction or "destruction" of the initial state, completely avoiding this effect. Even when this is done, the uncertainty principle is just as valid as ever. This is often called "Interaction Free Measurement" and is delightfully weird.

3. The "you can't help but jostle the electron" problem implies that the uncertainty principle has to do with the measurement of a state/object rather than the condition of the object itself. Even if an electron had

> a precisely defined position and momentum at all times, the jostling problem would exist. The uncertainty principle tells us something different. It tells us that the electron simply *doesn't have* both a precise position and momentum at the same time. Even if you could magically measure it without jostling it, the uncertainty principle would apply.

OK, I'll drop the wrench and leave the horse alone now.

The precise mathematical expression of the uncertainty principle is given by

$\Delta x \Delta p_x \geq \frac{\hbar}{2} = \frac{h}{4\pi}$ Uncertainty Principle

There is no "approximately" as implied by the $\gtrsim$ in the text. This product of uncertainties absolutely cannot be even a little smaller than this. This result can be derived from more fundamental principles that are too mathematical in nature for us to delve into here, but suffice it to say that it is exact (and has nothing to do with the horse I beat to death earlier). The kernel of weirdness is that, in quantum mechanics, $xp \neq px$. That's right, it matters which order you multiple things together in (sometimes!). Suddenly algebra gets that much more annoying.

There are lots of combinations of variables for which an analogous relationship holds. The next most commonly used relates time and energy:

$\Delta E \Delta t \geq \frac{h}{4\pi}$

Like most things quantum, these effects are tiny and we never notice them on macroscopic scales, but at atomic scales this all becomes very relevant.

I should note that despite the fact that I spent a long time tearing apart the book's explanation of uncertainty, his point about the wavelength of the electron being relevant is correct and relevant. This point essentially equates quantum uncertainty with diffraction effects in optics and other situations with waves. This is another, entirely valid way of looking at the uncertainty principle.

18.4 The Schrödinger Equation

We aren't going to be solving Schrödinger's equation, but I want to show it to you and present a few solutions to give a feel for what the quantum world “looks” like. While it is possible to make a much more compelling argument for the existence of Schrödinger’s equation than your text presents, the central point that it is a made-up law is still true. In a modern perspective quantum mechanics is based on just 4 assumptions, of which Schrödinger’s equation (in a more general form) is one. It is very analogous to Newton’s Second Law ($\vec{F} = m\vec{a}$) for classical mechanics, in terms of importance.

$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\psi(x)$ Schrödinger’s Equation

This equation describes with great precision the behavior of the wave function ψ in the presence of some potential U such as the electrostatic potential. Solving it can be anywhere from relatively trivial (as second order differential equations go...) to truly impossible. I am just going to state some standard results to show you what they look like:

Free Particle $\psi(x) = A\sin(kx) + B\cos(kx)$ $\qquad k = \sqrt{\frac{2mE}{\hbar^2}}$

Infinite Square Well $\psi(x) = \sqrt{\frac{2}{\ell}}\sin(kx)$ $\qquad k_n = \sqrt{\frac{2mE_n}{\hbar^2}} = \frac{n\pi}{\ell}$

Finite Square Well See figure 38-13, the equations are meaningless to us.

A few facts about these:

- Free particles are actually *wave packets* constructed by adding up many different solutions like the one shown. This process reduces the uncertainty in position (the equation shown exists for *all* x and so position is maximally unknown) at the expense of uncertainty in momentum (if we add up solutions with different energies, which one is *really* the energy, and thus what is the real momentum? No answer exists, its uncertain)

- The new element in the infinite square well is that ψ must be 0 where the potential is infinite: it forms an infinitely strong barrier. This forces the solution to 0 on the edges, so we only get the sin solution, and specific values of k.

- The finite square well starts to show the complexity possible in solutions. The particle still can’t escape if its energy is less than the depth of the well, but now QM uncertainty lets it go “part way” into the wall.

18.4.1 Tunneling

Square Barrier

Nucleus

18.5 Quantum Solutions of Atomic Systems

Now that we have a real theory for quantum mechanical objects, we can see what it tells us about some real systems.

18.5.1 Electron Wavefunctions in Atoms

We've decided that wavefunctions tell us where particles have a high probability to exist in a system. Drawing this is tough in 3 dimensions, but the general idea is that any given electron will be "spread out" in a probabilistic sense throughout the region of the atom. They aren't at specific places going in specific directions, there is just some probability that you'll find an electron at a given location if you look there. This is sometimes called an electron "cloud", tho I don't entirely like the term since it implies many electrons are present but spread out, when really each wavefunction corresponds to one electron.

18.5.2 Hydrogenic Atoms

The only atoms that can be solved exactly are still hydrogenic atoms. However, Schrödinger's equation is perfectly happy to tell us the wave functions of more complex atoms so long as we make appropriate approximations or plug it into a big enough computer, and in fact can be used to solve for the wavefunctions of entire molecules.

For the hydrogen atom, we get for the ground state:

$\psi(r) = \frac{1}{\sqrt{\pi r_0^3}} e^{-\frac{r}{r_0}}$ The S1 Orbital of Hydrogen

This is the shape of the hydrogen S1 electron orbital. Easier than deriving this result is plugging it into Schrödinger's equation and seeing that it does in fact work. You don't need to, but it can add some insight if you are comfortable with derivatives. The fundamental point is that we are now entirely capable of calculating the shapes and other properties of the electron orbitals which define the chemical properties of the various elements on the periodic table. We just plug in

$U = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$

to Schrödinger's Eq (this is just the coulomb electrostatic potential of a single proton) and solve! This, incidentally, is the part that gets crazy complicated for other atoms. When you have multiple electrons, you have to worry about how they interact with each other. Even in simple Newtonian gravity, it is impossible to exactly solve a general system of 3 bodies. Doing so in a quantum system with electrostatics isn't going to be easier even if we ignore magnetic effects due to the moving charges.

When we solve schrödinger's equations, we always end up "finding" quantization conditions along the way. These are the analogues to Bohr's ad hoc search for an assumption that gave the correct result, except now they fall out of the math rather than having to be guessed. Every time you impose one of these conditions, you place a restriction on the solution and pick up a new "quantum number" that describes some quantized aspect of your solution. For the hydrogen atom, we have:

- n is the principle quantum number and labels the energies (which are thus now quantized)
- ℓ labels the orbital angular momentum and ranges from 0 to n
- m_ℓ labels the direction of orbital angular momentum of the electron and ranges from $-\ell$ to ℓ
- m_s labels the direction of "spin" angular momentum and is either $-\frac{1}{2}$ or $\frac{1}{2}$

Spin is really strange and is a result of the relativistic quantum theory of electrons. If you thought quantum was confusing so far, just try the relativistic version!

See Figure 39-8 and 39-9 for more hydrogen solutions. These are the shapes of the orbitals you may have learned about in chemistry.

18.5.3 Pauli Exclusion Principle

The Pauli Exclusion Principle states simple that no 2 particles (actually a subclass called fermions but don't worry about that for now) can have the same quantum numbers. This has to do with symmetries of the wavefunction and isn't ad hoc but we won't explain it. The upshot is that it tells you how many electrons can sit in each kind of orbital.

18.5.4 Magnetic Moments

There are 2 magnetic moments for an electron in a hydrogen atom. The orbital moment is a simple result of treating the electron as a classically moving charge which thus represents some current. The book calculates this but I'm not particularly interested in that. he cool part is that the even outside of an atom an electron has a magnetic moment due to its "spin", and this property lets us perform the Stern-Gerlach experiment (Fig 39-14). This is a great testbed for some very quantum ideas.

Incidentally, this inherent magnetic moment is one of the most precisely and accurately measured quantities ever. The most precise is in fact the magnetic moment of the electron's heavier cousin, the muon. This number is known to agree with experiment to something like 10 significant figures.

18.6 Einstein-Pedolsky-Rosen

The spookiest thing about Quantum Mechanics is what we call "entanglement". The best example of quantum entanglement is the EPR "paradox". I put paradox in quotes because it was originally proposed as a thought experiment by Einstein (and 2 other guys) to demonstrate an "obviously" preposterous result predicted by quantum mechanics. The purpose was to demonstrate that clearly something was wrong with the theory as formulated at the time by making a patently absurd prediction. This is often a great way to make your point: find a logically consistent conclusion that everyone can agree is incorrect starting from the premise you wish to disprove. In this case, however, it served instead to just demonstrate clearly how bizarre quantum theory is, because the EPR "paradox" as then observed in experiment despite being patently absurd.

EPR is what Einstein had in mind when he referred to "spooky action-at-a-distance" with regards to quantum mechanics and reasons he thought it wasn't correct. The idea of a quantum mechanical universe struck Einstein as deeply wrong, and he spent a decent amount of time trying to find some way around in.