

Truths about Quantum Mechanics
St. John's College, Santa Fe, Nov. 30, 2018
Bernhardt L. Trout

Thank you to Ms. van Boxel for that thoughtful introduction and for being a most excellent host during my stay. Thank you also to Mr. Grenke for the kind invitation and to Ms. Versace for all of your help during my stay. I am guessing that it is not a coincidence that I was invited to lecture here on Quantum Mechanics not too long after I gave a lecture on the subject at your Annapolis campus, which itself was actually 364 days and 1.5 hours ago. So, I suppose that I didn't flub it up too badly then. Of course, the verdict is still out here. In particular, since I changed the title and changed the talk accordingly. In fact, the talk is rewritten, one of the major differences being that I made the jokes in it much funnier.

It does not escape me that the title smacks a bit of arrogance (especially in a college in which the period following the talk is the "question" session, whereas my title implies that I have some answers.) Certainly, I intend for the title to be provocative and both to challenge you and to spur on your challenging me. On the other hand, I have been studying quantum mechanics for over 25 years now, educated in theoretical chemistry and physics, and I am a professional quantum mechanician—yes, you can make a living by doing quantum mechanics-- so hopefully, I know something that I can share with you tonight. Still, I am well aware of Socrates' critique of the handicraftsmen (Apology 22d)—of course a quantum mechanician does not make handicrafts per se (note that MIT's motto, though, is *mens et manus*), but we tend to suffer from the same problem: indeed, we do know something, but our knowledge of our art deceives us into thinking that we know about the greatest things, about the fundamental things. Nowhere is this more evident than in the walls of physics departments, where modern mathematical physics is considered the way, the only way to understand nature. But let's set that aside for the moment. Let us embark upon understanding key concepts of quantum mechanics and with them the wonder of this great human accomplishment. Here we go.

I. Prediction and Mastery

Let's start out with a quantum mechanical calculation. <Start GaussView>. This is a program called Gaussian, which solves the Schrödinger equation for molecular systems via approximations—you may know that the Schrödinger equation can only be solved explicitly for the hydrogen atom and other simple models. It is called Gaussian because it uses sets of Gaussian functions to model the wavefunction of the system. The only parameters that it uses are: the charge of an electron, the number of electrons in the system, the nuclear charges (i.e. atomic numbers) and the universal constant called Planck's constant. <do calculation>

- NIST exp: 1594.5, 3656.6, 3755.7
- Dipole moment = 1.9 Debye
- Bond lengths 0.96 Ang. and angle 104.5 deg

Isn't it amazing that with only a few "universal" constants, we can do a calculation with experimental accuracy on a simple laptop. Of course, if we had a few more minutes, we could do a more accurate calculation, or a calculation on a larger system.

Based on knowledge of atoms and molecules, we can do much in many many fields. Take chemistry, we can make basically any molecule that we want to make:

<Examples>

Similarly, we can use knowledge of atoms and molecules to make drugs.

<example>

Note that in the above representations, we are not just speculating on the positions of atoms in the molecules, but have used x-rays and other methods to determine those positions.

We can also move around atoms on surfaces and image them directly:

<STM of IBM>

These are a couple of examples of technological applications of quantum mechanics, but we don't even need to get into the details of such examples. For applications of quantum mechanics are all around us: from the pharmaceuticals that we pretty much all use—these were designed using quantum mechanics-- to basic electronics, like the laptop here, which uses quantum mechanics to design the transistors, diodes, and other components, perhaps all of the major ones. Given these, and these are only representatives of perhaps billions of examples, all made possible by quantum mechanics, who could deny that quantum mechanics is the right approach to investigate the fundamentals of nature?

II. First-principles from Quantum Mechanics

Let's now turn to these fundamentals. In doing so, I want to leave explicitly the realm of predictions and the technical applications of those predictions, to the realm of what QM can tell us about nature. Now quantum mechanics is part of a larger field of study, modern physics, also called mathematical physics. The objective of this field is to understand everything (I was about to say everything under the sun, except that, of course, most things in the cosmos are not under the sun), at any rate, to understand everything from the utterly small to the astronomically large and from the beginning of time to its end (if there is a beginning and end); and certainly everything in between. Its aim is to find the Theory of Everything, TOE, a comprehensive and compelling statement about the world. It makes the assumption that "understanding" means to capture in a mathematics which is demonstrated to be true via experimentation. That assumption is tested by answering the question: does the posited mathematics describe the experimental results and is consistent with other mathematics describing related experimental results? And the presumption is that if the answer is "yes", then the approach of mathematical physics is correct, i.e reveals truths about nature.

Let's make that assumption and dig down in our exploration of the excitement of quantum mechanics. We are going to do this in a bit of an anachronistic way, because I want to give you a sense of the experience of quantum mechanics. Unfortunately, all I can do here is give you a whiff. And at any rate, you can only have the true experience by working these problems through yourself and actually by learning QM well enough to solve your own problems in QM, which I guess you are doing if you are seniors and will do if you are not.

The seductiveness of mathematical physics

Imagine that you are Schrödinger in 1926, or that you are you, but you are playing around with wave equations as Schrödinger did. Just for fun, you posit this equation, and then you go on to solve it using fairly recently developed mathematics. Here is a taste of what you might have done:

<SE Hydrogen atom solution>

Lo and behold, the energy levels for the H-atom pop out and compare very well to experiment.

Just by positing a form of an equation, a fairly simple one, secrets of nature pop out. What is even more bizzare is that this result, generalizable as we discussed above, leads to strange consequences, for this posited Psi function, the wavefunction, has non-intuitive properties. We will return to those shortly.

Before we do, let me give you a second example of the power of mathematical physics. You have all no doubt heard about the origin of relativity. Einstein, noticing that Maxwell's equations, the classical governing equations of electro-magnetism, are invariant to the Lorenz transformation, went about wondering what would happen if he made classical mechanics, the mechanics of Newton, invariant to the Lorenz transformation. In doing so, out popped the theory of special relativity with all of its implications of speed limited to that of light which is the same in all inertial frames, that twins will age differently relative to each other if they are traveling at different speeds, i.e. time dilation, etc.

So that was 1905, but let's return to the time of Schrodinger's equation and go a year later to 1927. You are Paul Dirac – well perhaps a bit more loquacious than Dirac, as he is known for his discourses being one word long, generally 2 or 3 letter words—“no”, “yes.” At any rate, having learned about Schrödinger's equation, you realize that it is not consistent with special relativity (which recall had been published 22 years earlier). You decide to make it consistent, and in doing so, you embark on what seems to be the simplest course: make the wavefunction a 4 dimensional vector. Then you get the following equation which came to be known as the Dirac equation:

$$\left[\left(-\frac{W}{c} + \frac{e}{c} \mathbf{A}_0 \right)^2 + \left(-\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 + m^2 c^2 \right] \psi = 0$$

Your wavefunction is now 4-dimensional, i.e. 4 non-spatial dimensions, so x , y , z , and t are each part of each of those 4-dimensions. Thus, it is unclear how to account for them. One way to do so is to interpret each dimension by each of the two spins of the electron (\uparrow, \downarrow), and each with positive and negative energies, $2 \times 2 = 4$. Fine for spins, but how do you account for negative energies? Like negative mass—“This podium weighs -20 kg” seems like nonsense. Everyone likes your equations, so they try to come up with various explanations for what a negative energy might mean, each with varying degrees of being satisfactory, but all less than 100%, that is until four years later, when the positron, the antielectron, was found experimentally. Thus, the insight gained in solving a mathematical problem led to gaining an astounding new insight into the nature of the world. Who would have imagined opposite particles that can cancel each other out. It defies common sense—what if I had an antimicrophone that could interact with this microphone, each canceling the other out in a burst of energy...

Now, before I move to a third example, I want to pause to bring out another bizarre consequence of the two examples above. This postulated wavefunction—remember, when we discussed the H-atom, I promised to return to the wavefunction—is directly related to a probability density. That has several non-common sense implications. For example, a particle, like an electron is actually everywhere at once with some distribution of where it is randomly, and the only way in which we know where it is by performing an experiment on it, and it is the experiment itself that localizes it. But how can something be everywhere at once and only localized when it is measured. Moreover, a certain mathematical representation is correct before measurement and another one is correct after measurement. How can measuring change the mathematical representation? This impasse is known as the measurement problem, which you have no doubt heard of in the image of Schrodinger’s cat. <slide with this problem in St. John’s vs. central Santa Fe square>

A third example is the non-locality of quantum processes. <non-locality slide> For example, if you prepare two particles in random states but such that both particles have the same state, when you do an experiment to measure the state of one, the other particle instantly, i.e. non-locally adopts the same state. This is very strange, since it adds to the intrinsic randomness of quantum mechanics an intrinsic non-locality. We find this non-intuitive, and it defies common sense. (Although, I am not sure why it is less intuitive and less contrary to common sense than action at a distance, like gravity—perhaps just because we grew up with gravity, and experience it all of the time, whereas we only experience non-locality if we read about it in St. John’s seminars or if we are particle physicists.) At any rate, in this third example, the point is that this non-locality has been determined experimentally, based on a test developed from a mathematical analysis.

So far, we have been discussing QM as a description of the world around us, or more accurately, of the microscopic world. We can see its consequences in the macroscopic world through experiments certainly, but also through things like pharmaceuticals and electronic devices. At this point, I think that we have to conclude that the world exhibits patterns at all levels. QM captures those patterns it exhibits at the microscopic level.

Mathematical physics as descriptive

Let's, however, take a next step. You no doubt have noticed that my lecture tonight consists mainly of words. (It may be possible to make a mathematical text without words, but I would submit that it would not be possible to do so for a physics text, because an explanation in words is necessary for the experiments.) Given that, it seems necessary to summarize in words, as opposed to equations. Such seems to be a necessary consequence of our being human beings and desiring to understand. Let's see what conclusions we can make about the world based on quantum mechanics. (Note that in doing so, I will make one addition.):

1. The Schrödinger equation can be considered the basis of quantum mechanics; we could say a postulate of quantum mechanics; but it seems to be a true description of the world in that millions (perhaps billions) of tests have demonstrated it to be representative and predictive, and there has not been even a single case in which it is found to be wrong. (at least if applied properly)
2. There is intrinsic and irreducible randomness that simply is.
3. There is intrinsic non-locality above and beyond action at a distance that simply is.
4. Given, 1., that the Schrödinger equation is the true description of the microscopic world, we can say that each thing has a wavefunction associated with it. I will now add that this wavefunction is in an infinite dimensional complex space, called a Hilbert space, and is not itself observable. Not only is there irreducible randomness and non-locality, but we cannot even know what makes up the things of the world, for wavefunctions are not observables.
5. This wavefunction for each thing has a different mathematical form before and after a measurement. This is what we showed with the example of your location, here or in the center of old Santa Fe, and is known as "wavefunction collapse".

Another thing that I want to add here: we could do an experiment and measure everyone's height here or or some other quantifiable property, and we could develop an equation based on that. It would be probabilistic, as in a probability distribution, and with enough information, we could use it to predict the average height at any given time or some other property. The key here is "with enough information." What we have done is develop a phenomenological model, but we have not discovered anything fundamental. Quantum mechanics on the other hand is a framework that is presumed to be fundamental. For with a single equation and a few universal constants, we have found the key to everything—here you may object that we do not have a unified theory of quantum mechanics and gravity, and you would be right, but that does not make a difference with respect to the overall point. For either we eventually find that theory, the Theory of Everything, TOE, or we determine that such a theory is impossible and go back to the drawing board. Either way, we seem to have determined the foundations of nature, and frankly, I think the former more likely.

Where are we now? We have a theory of nature aimed for the microscopic that is "correct" in the sense that millions of experiments have confirmed its veracity, and when properly applied, it has never let us down. Of course, this is all within the framework of mathematical physics and according to its own criteria. To remind ourselves, those criteria are that mathematical equations are postulated and their applicability tested via experiment. If the mathematics matches the experiment then the theory is deemed correct. We can add that the more comprehensive the

better, i.e. to the extent that the theory is consistent with wide-ranging observations on phenomena, the better.

The psychology of mathematical physics

This is all very appealing—why? At a basic level, we are beings who interact with the world via patterns. We experience a stability to the world—I don't worry about falling through the floor here, but if some wind started inside the auditorium, I would get concerned. If that wind were to get warmer, I would get very concerned and run. Even then, after I relaxed, I would think that the warm wind that I experienced was a consequence of fire or some malfunction and would not be surprised that there was a casual effect.

Digging deeper into our psychology, mathematics is extremely appealing. However our levels of consciousness work, mathematics goes a level deeper than just recognizing patterns. Somehow, we are able to pull out mathematical concepts from the depths of our minds and apply them to the world, select out particular subsets of the objects of math and apply them to nature. Dirac must have been awestruck that simply making the Schrödinger equation consistent with special relativity led to a prediction of antiparticles, which were indeed found to exist. Such experiences have led not only one physicist to decide that if nature is not consistent with an elegant mathematical representation of nature, then nature is wrong.

We appreciate elegance, and a term that is often applied to modern physics (and math for that matter), beauty, that reflection of our erotic longing for completeness, for wholeness, for the cosmos to be a welcoming place for us, perhaps a cozy place, in a word, home, a completeness that we want to feel confident is there. Yet we also love the thrill of dizzying experiences, because we like novelty, even new things that pull us away from our confidence in the stability of world, but always with the expectation that we will return to that stability. Hence, the ideas of non-locality and wavefunction collapse are appealing, especially because we do not experience them directly in the patterns of the world.

Thus, we have a beautiful theory that abounds in the appeal of mathematics, and that captures patterns of nature. Our mind tends to put all of this together and conclude that we have discovered fundamentals of nature, and we are content to rest happily in our knowledge of them.

III. Problems with First-Principles from Mathematical Physics

However, let's throw a little cold water on our heated passion. Let's sober up a bit and keep front and center a few things that I stated in my lecture so far, but swept under the carpet. Maybe you heard them and were wondering why I said what I said; maybe not. Either way, let's pick up the carpet and see what we swept under it and the consequences of our doing so.

1. Remember how I kept saying things like “experimental accuracy” and “more accurate” in the very first example of the water vibrational frequencies? And for the energy levels of the H-atom, they “compare very well to experiment”. You see, QM is inexact – pretty close, but not exact—this is the problem of the mathematical; how close is good enough? In many cases, our psychology says that 999,999 in a million is good enough. We don't

worry about rounding error, and if the butcher sells us 1.000 pounds of meat weighed out on the scale to three decimal places, we don't worry that it might have been rounded up in the last decimal place. But if QM is a "true" representation, it needs to be exact, and it is not. In fact none of mathematical physics is. What we are doing is abstracting the patterns we observe in the world into a mathematical form, and then we find that form so appealing so enticing that we forget about that abstraction and the fact that it is not a perfect representation. There is always something missing. How do we judge if that missing part is important?

2. In case you think I quibble (and even if you don't), there is a more serious defect. According to QM, the world has an intrinsic randomness – I convinced you of that above in talking about the wavefunction and its relationship to a probability distribution. However, mathematics cannot generate random numbers. (Tale of RAND corporation, 1955.) Computers by the way cannot either, and so the best way to generate them is via observations of what we presume to be random natural occurrences, like radioactive decay. Probability distributions are perhaps the only mathematical way to capture randomness, but they are clearly removed from what happens in nature, even according to practitioners of quantum mechanics, who need to rely on something else to generate random numbers. At any rate, probability distributions presume an infinite number of identical experiments and say nothing about the individual.
3. Problem of the observer: we have discussed wavefunction collapse when an operation is performed, but who performs that operation? It can only be an experimentalist, i.e. a person. That person's observation is imposed on the system studied, but isn't that person a quantum system too? Let's just say yes for the sake of argument and put a box around the person and the system. Who observes what is going on in the system? Maybe another person, fine, but then that person is outside of the system. Any way we look at it, the observer is imposed into a quantum mechanical experiment, but outside of it; in other words, QM is incomplete.
4. So far, in the above 3 points, I have criticized QM via its own criteria. Let me clarify that before moving on to a criticism that comes from outside of QM. Remember in the first part of the talk, when I discussed a range of impressive examples that QM captures and can make accurate predictions about? There I said that if those are what QM does, captures patterns and makes predictions then it is successful via its own criteria. But then I moved on to the second part, in which I said that practitioners of quantum mechanics consider QM as revealing truths about nature. But it is more than just to these practitioners, since human psychology is such that we tend to absorb such knowledge as the truth about nature. We are used to taking in patterns, while at the same time, we yearn for first-principles. That combination leads us to hold onto answers to what first-principles are, even if those answers are tenuous. Thus, it is to the claim that QM tells us about first-principles that I have leveled these three criticisms, still within the realm of QM, criticism of QM on its own terms. Now here is the one outside <slides of Nero>. Now unless you are an economist--of course economists quantify everything, so they no doubt beat me to it regarding a cuteness function and even its dollar value—you would find yourself hard pressed, I think, to assign a simple cuteness value to Nero, but even if

you were an economist, what function do you use for the cuteness of Nero in any situation or what quantum mechanics would call any Eigenstate? Could you conceive of this function and the operator of the function that would capture even the economists' cuteness index for narrow in any Eigenstate? When he is sitting next to Sancho Panza or when he is running or growling for that matter? This doesn't seem appropriate, because Nero is a natural whole and not amenable to mathematical abstraction (and don't forget that QM presumes an infinite number of Neros). On the other hand, QM tend to homogenize things, to turn natural beings in that which we cannot love. We can approaches the elegance of wavefunctions, but we cannot love them. There are key aspect of natural beings that seem to defy mathematization.

IV. Another approach

Now we are feeling a bit down. And when we are feeling down, we could do worse than turn to Shakespeare. How about his quite famous Sonnet 138

When my love swears that she is made of truth,
I do believe her, though I know she lies,
That she might think me some untutored youth,
Unlearnèd in the world's false subtleties.
Thus vainly thinking that she thinks me young,
Although she knows my days are past the best,
Simply I credit her false-speaking tongue:
On both sides thus is simple truth suppressed.
But wherefore says she not she is unjust?
And wherefore say not I that I am old?
Oh, love's best habit is in seeming trust,
And age in love loves not to have years told.
Therefore I lie with her and she with me,
And in our faults by lies we flattered be.

With our friends and lovers, we ignore their faults. Often we convince ourselves that those faults are part of their charm. If quantum mechanics is just a way of organizing data and making predictions, then, indeed, we can ignore those faults; this is what I proffered during the first part of my lecture. However, if quantum mechanics is, as many think it to be, and as our psychology directs us to believe, the true description of the world, then we cannot ignore these faults. So if QM means anything important, we are stuck. We grasp the products of quantum mechanics as true descriptions of nature, but on the other hand, we have called into question all of quantum mechanics, including all of its ramifications: atoms, molecules, fundamental constants, and fundamental particles to name a few.

Perhaps a new launching point can be now found in the writings of Francis Bacon. If we go to his *Novum Organum* Aphorism #45 (in the first part): "The human intellect is constitutionally prone to supposing that there is more order and quality in things than it actually finds." He then talks about imposing a circular motion onto the heavens and of making proportions, 10:1, for example, and imposing them nature. He may as well be talking about the H-atom energy levels

that we discussed above, imposing in this case, a $1/r^2$ relationship on our images of what part of the constituents of beings might be. Let's go a step farther, however: doesn't everyone know that atoms exist and that molecules are made of atoms? It couldn't be just that these are concepts that we are imposing on nature, could it? Yet perhaps we should consider that since those concepts are so much a part of the modern world, we are so imbued with them that perhaps it would take an extreme and long drawn out act of will to eradicate them from our minds as what we consider truths about nature.

Part of the challenge is this: There is no definitive book or Bible of quantum mechanics. And because there is no Bible of QM, there can be no Spinoza for QM. QM is something that has been built up over time by many, many extremely smart people. Perhaps if we stripped down the achievements of quantum mechanics to its backbone, we would have to say that something like 100 years maybe 200 years of very smart people have collectively developed it. Perhaps the actual number is greater, but nevertheless, it seems impossible for a single person to redo quantum mechanics (at least in a single lifetime), if redo means to develop a completely different picture of the microscopic world given the data that has been generated. On the other hand, we might note that there are different versions of quantum mechanics than what we have been discussing here, Feynman's path integral approach to name one, and Everett's many worlds theory to name another, so perhaps it is not impossible.

On the other hand, we can observe around us natural wholes that resist reduction. The wavefunction approach may be inapt to apply my dog Nero, but, nevertheless, even given that Nero is a natural whole, we can still justifiably ask: What are the first principles that govern this and other natural wholes? What is the material out of which they are composed? Quantum mechanics together with the rest of the apparatus of modern physics certainly gives an answer to those questions, and we can make use of that answer, but we must always keep in mind that that answer has defects and more importantly that our psychology is such that we tend to set those defects aside.

Having said that, let's go back to the excitement that we were sharing earlier on. Studying quantum mechanics is fascinating because of its elegance and beauty. It reveals things to us that are thrilling and awe-inspiring about the power of mathematical physics. Perhaps it even addresses our longing for transcendence, since the wavefunction is everlasting; it is immortal. Thus, it seems justified to wallow for a while in intellectual joy of QM, and in doing so, perhaps then we can also better understand the meaning of its limitations. QM is important to clarify our understanding of the atomic hypothesis that is omnipresent in the world in which we inhabit. Perhaps it is also an antidote for other dogmatisms that might emerge and that our mind might grasp and not want to let go of. I am thinking, for example, of Ch. 7 of Descartes' *Treatise on Light*, when Descartes explains his abjuration of his schooling by criticizing the contentlessness of Aristotle's definition of motion: *motus est actus entis in potentia, prout in potentia est*. (Of course, we must appreciate the irony in his quote: being in Latin, it is really a praise of Aristotle's genius in anticipating the formation of the Scholastic Latin language.) At any rate, the point is that even if we dig up things from the layers of history that have covered them in order to free ourselves from the present, don't we subject ourselves to the risk of just settling on a new dogmatism?

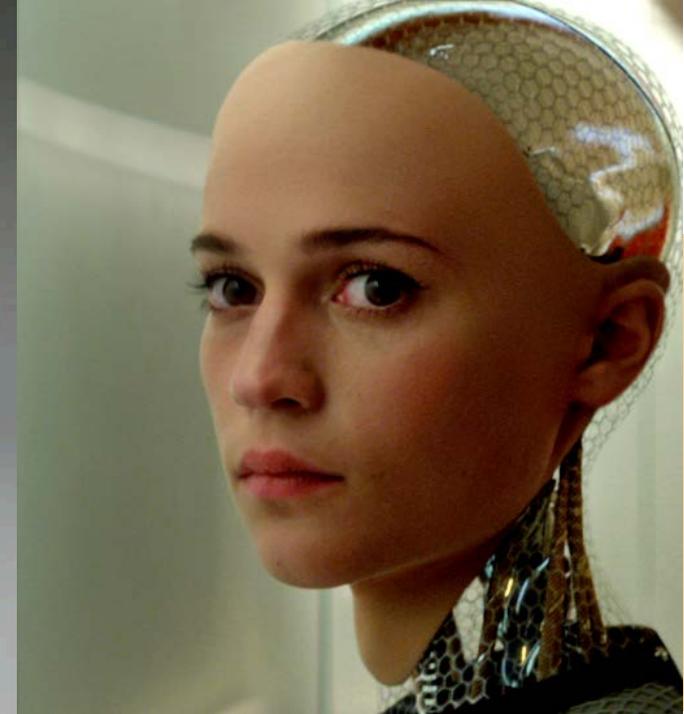
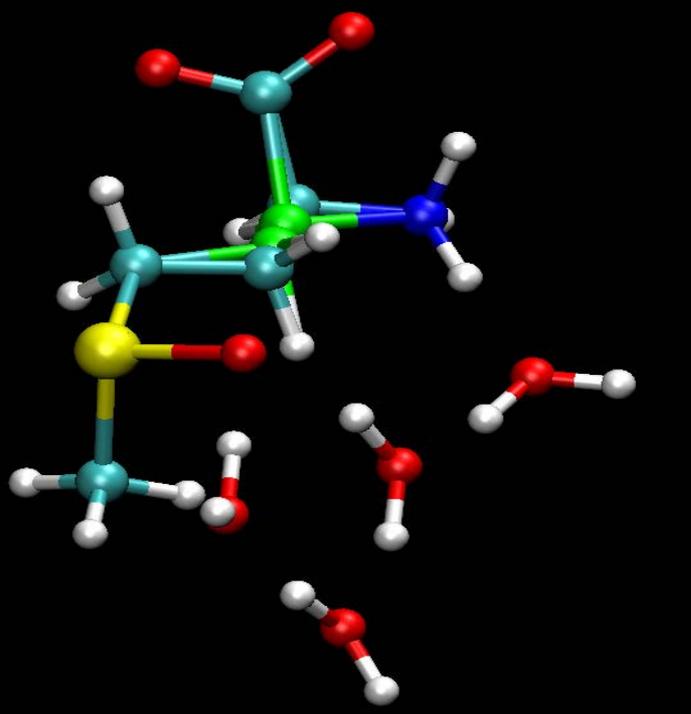
I would like to finish by reminding you of the Sirens' song from Book 12 of the Odyssey. <show vase> You no doubt remember Odysseus putting beeswax in the ears of his comrades and having them tie him to the mast, so that he could hear the Siren's song without suffering the fate of all those others who heard it and therein were seduced into a horrible fate. Remember what the Siren's sang? It is revealing about what is most seductive to us. (Latimore, ll. 184-191)

Come this way, honored Odysseus, great glory of the Achaians, and stay your ship, so that you can listen here to our singing; for no one else has ever sailed past this place in his black ship until he has listened to the honey-sweet voice that issues from our lips; then goes on, well pleased, knowing more than ever he did; for we know everything that the Argives and Trojans did and suffered in wide Troy through the god's despite. Over all the generous earth, we know everything that happens.

Let us listen to the seductive songs in our midst that attract us by the promise of knowledge, even of knowledge of everything, but fortified against their seduction, let us keep on sailing, changed, stronger and better by what we have learned, and let's sail on towards more knowledge.

Thank you!

<Eos and Kephalos>



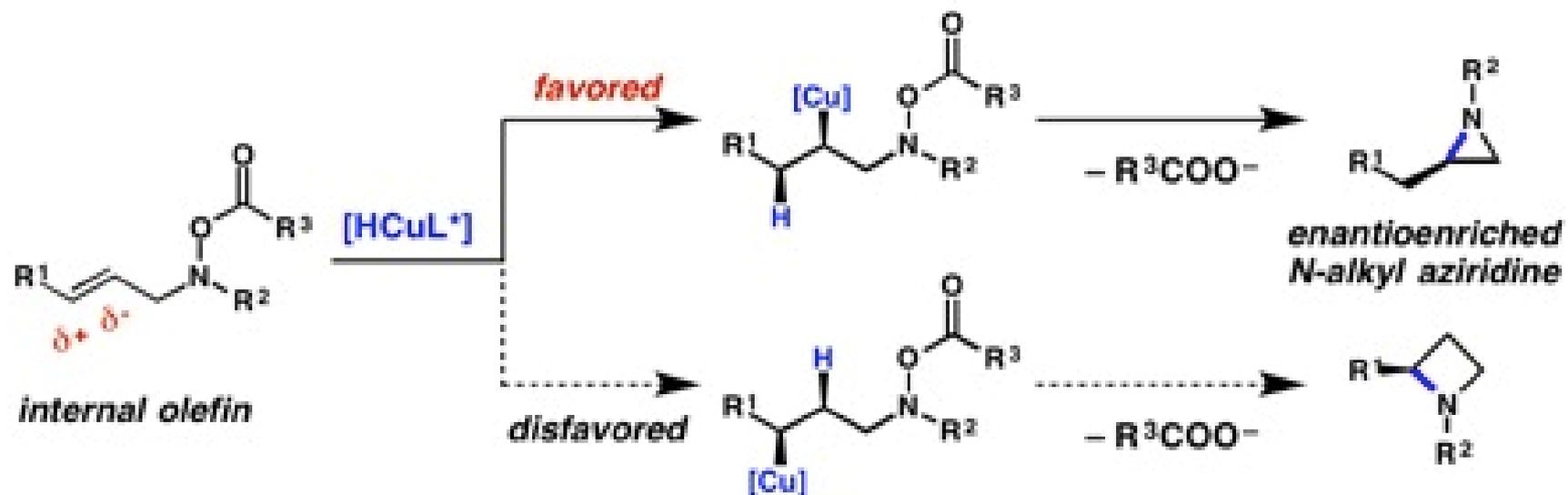
Truths About Quantum Mechanics St. John's College, Santa Fe

Bernhardt L. Trout

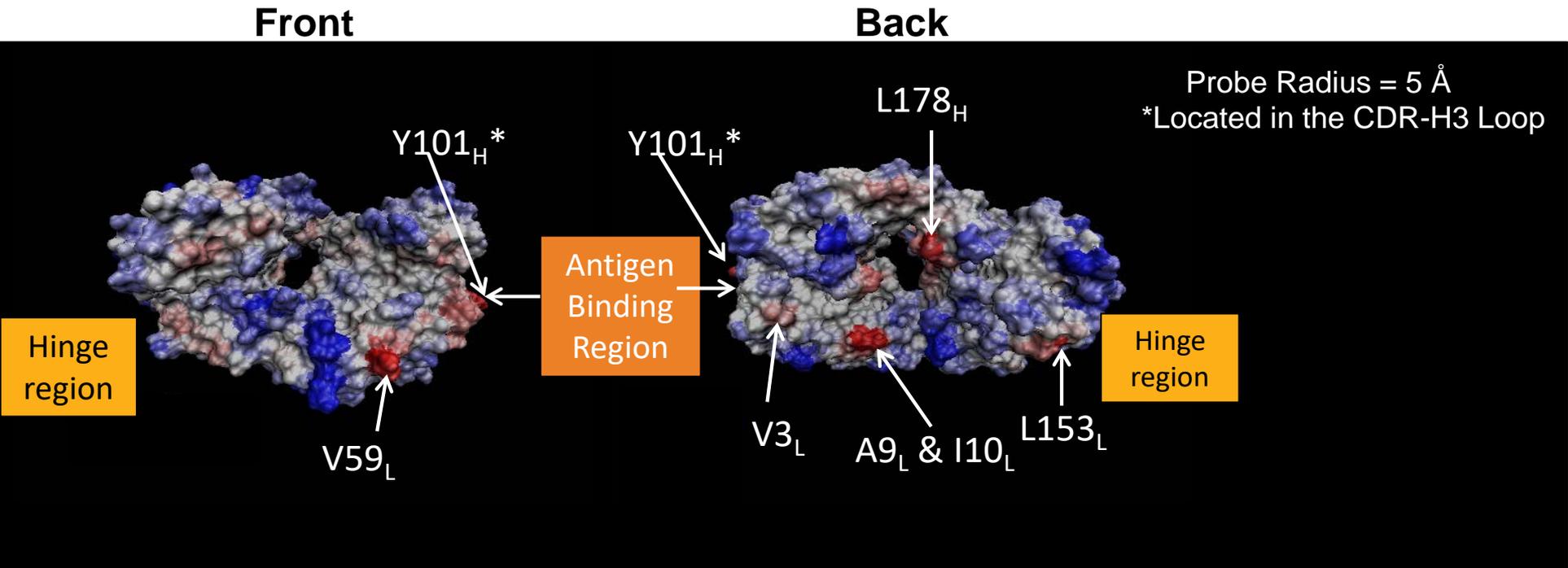
Raymond F. Baddour, ScD, (1949) Professor of Chemical
Engineering, MIT

Director, MIT Benjamin Franklin Project

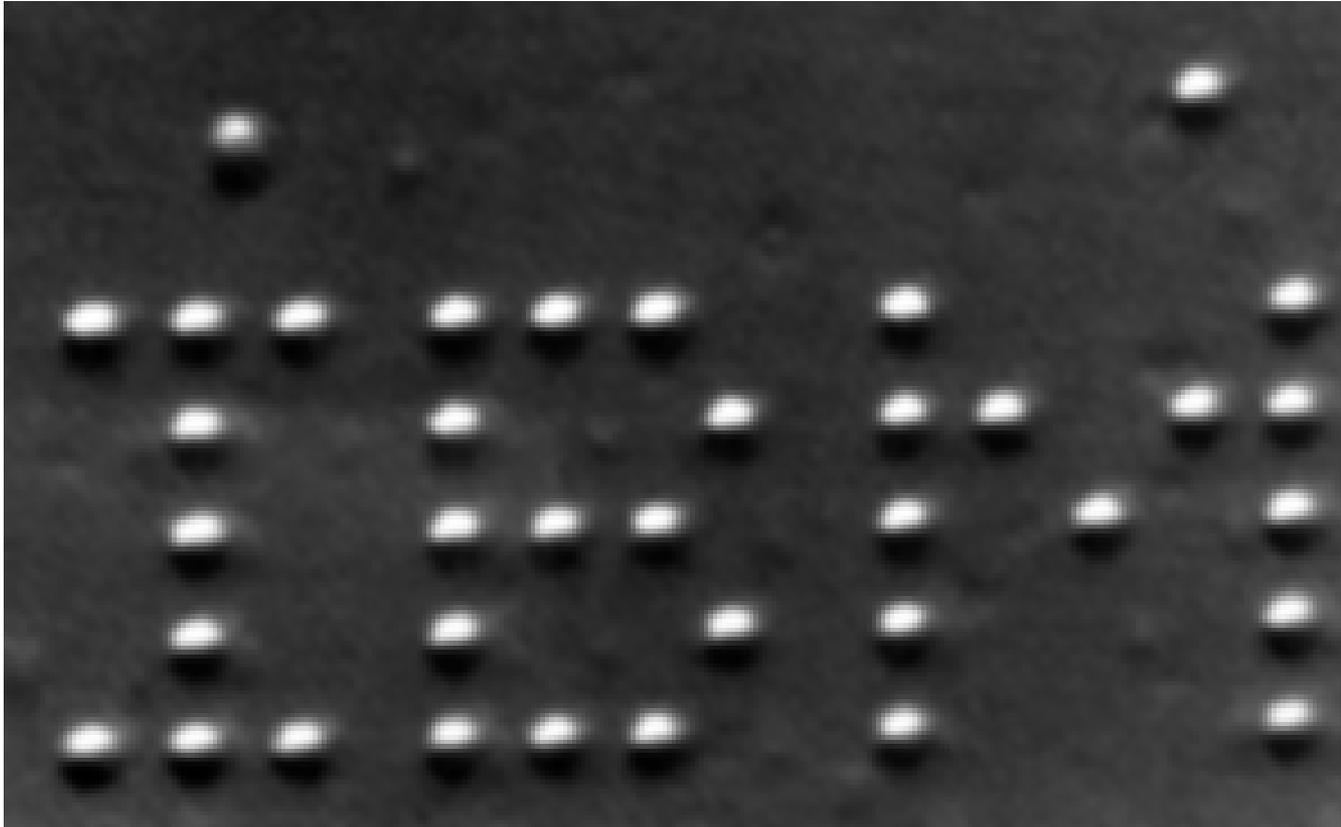
Selectively making molecules



Making biologic drugs



Visualizing atoms



Schrödinger Equation for H atom

In Chapter 4 we solved the time-independent Schrödinger equation for several one-dimensional problems. We shall now generalise our treatment to study in three dimensions the non-relativistic motion of a particle in a time-independent potential $V(\mathbf{r})$, where \mathbf{r} denotes the position vector of the particle. In fact, we can treat a slightly more general problem at no extra cost. Indeed, we have seen in Section 5.7 that the motion of two particles A and B, of masses m_A and m_B , interacting via a time-independent potential $V(\mathbf{r})$ which depends only on their relative coordinate $\mathbf{r} = \mathbf{r}_A - \mathbf{r}_B$, reduces in the centre-of-mass system to a one-body problem: the motion of a particle of mass $\mu = m_A m_B / (m_A + m_B)$ in the potential $V(\mathbf{r})$. The two problems can therefore be treated on the same footing, the time-independent Schrödinger equation to be solved being

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad [7.1]$$

This is a second-order partial differential equation, in contrast to the one-dimensional case, where the time-independent Schrödinger equation [4.3] is a second-order ordinary differential equation. As a result, the solution of the three-dimensional Schrödinger equation [7.1] can only be obtained exactly and explicitly in a few simple cases. In particular, the potential may be such that the technique of *separation of variables* may be used. The original three-dimensional problem then reduces to simpler problems of lower dimensionality.

Let us now consider a hydrogenic atom containing an atomic nucleus of charge Ze and an electron of charge $-e$ interacting by means of the Coulomb potential

$$V(r) = -\frac{Ze^2}{(4\pi\epsilon_0)r} \quad [7.91]$$

where r is the distance between the two particles. We denote by m the mass of the electron and by M the mass of the nucleus. Since the interaction potential [7.91] depends only on the relative coordinate of the two particles, we may use the results of Section 5.7 to separate the motion of the centre of mass. Thus, working in the centre-of-mass system (where the total momentum \mathbf{P} of the atom is equal to zero), the Hamiltonian of the atom reduces to that describing the relative motion of the two particles

$$H = \frac{\mathbf{p}^2}{2\mu} - \frac{Ze^2}{(4\pi\epsilon_0)r} \quad [7.92]$$

where \mathbf{p} is the relative momentum and

$$\mu = \frac{mM}{m+M} \quad [7.93]$$

is the reduced mass of the two particles. The corresponding one-body Schrödinger equation describing the relative motion is

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 - \frac{Ze^2}{(4\pi\epsilon_0)r} \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad [7.94]$$

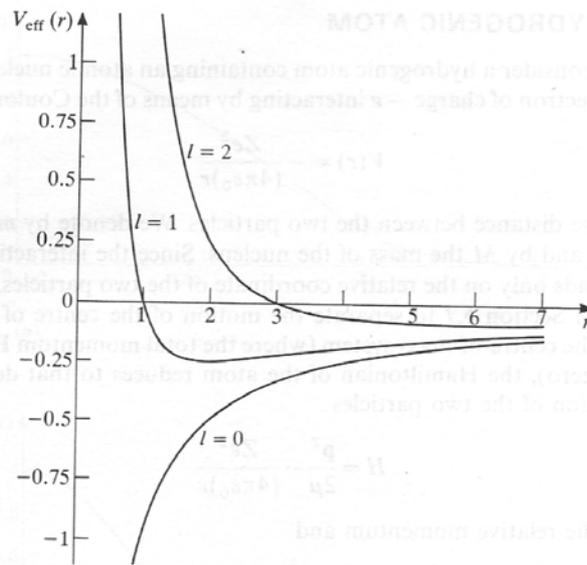
Since the Coulomb potential is central, this equation admits solutions of the form $\psi_{Elm}(\mathbf{r}) = R_{El}(r) Y_{lm}(\theta, \phi)$. Writing $u_{El}(r) = rR_{El}(r)$ and using [7.52] and [7.53], we see that the functions $u_{El}(r)$ must satisfy the equation

$$\frac{d^2 u_{El}(r)}{dr^2} + \frac{2\mu}{\hbar^2} [E - V_{\text{eff}}(r)] u_{El}(r) = 0 \quad [7.95a]$$

where

$$V_{\text{eff}}(r) = -\frac{Ze^2}{(4\pi\epsilon_0)r} + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad [7.95b]$$

is the effective potential. Figure 7.7 shows this effective potential for the case $Z = 1$ and for the values $l = 0, 1, 2$ of the orbital angular momentum quantum number. Because $V_{\text{eff}}(r)$ tends to zero for large r , the solution $u_{El}(r)$ for $E > 0$ will have an oscillatory behaviour at infinity and will be an acceptable eigenfunction for any positive value of E . We therefore have a *continuum spectrum* for $E > 0$. The corresponding unbound (scattering) states play an important role in the analysis of collision phenomena between electrons and ions



7.7 The effective potential $V_{\text{eff}}(r)$ given by [7.95b] for the case $Z=1$ and for the values $l=0, 1, 2$. The unit of length is $a_\mu = (m/\mu)a_0$ where a_0 is the Bohr radius [1.66]. The unit of energy is $e^2/(4\pi\epsilon_0 a_\mu)$.

In what follows, however, we shall focus our attention on the *bound states*, for which $E < 0$.

We now proceed to solve equation [7.95], subject to the condition $u_{El}(0) = 0$ (see [7.54]). It is convenient to introduce the dimensionless quantities

$$\rho = \left(-\frac{8\mu E}{\hbar^2} \right)^{1/2} r \quad [7.96]$$

and

$$\lambda = \frac{Ze^2}{(4\pi\epsilon_0)\hbar} \left(-\frac{\mu}{2E} \right)^{1/2} = Z\alpha \left(-\frac{\mu c^2}{2E} \right)^{1/2} \quad [7.97]$$

where $\alpha = e^2/(4\pi\epsilon_0\hbar c) \simeq 1/137$ is the fine-structure constant and we recall that $E < 0$. In terms of the new quantities ρ and λ , [7.95] becomes

$$\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\lambda}{\rho} - \frac{1}{4} \right] u_{El}(\rho) = 0. \quad [7.98]$$

Let us first examine the asymptotic behaviour of $u_{El}(\rho)$. To this end, we remark that when $\rho \rightarrow \infty$ the terms in ρ^{-1} and ρ^{-2} become negligible with respect to the constant term $(-1/4)$. Hence for large ρ equation [7.98] reduces to the ‘asymptotic’ equation

$$\left[\frac{d^2}{d\rho^2} - \frac{1}{4} \right] u_{El}(\rho) = 0 \quad [7.99]$$

the solutions of which are proportional to $\exp(\pm \rho/2)$. Since the function $u_{El}(\rho)$ must be bounded everywhere, including at infinity, we must keep only the exponentially decreasing function, so that

$$u_{El}(\rho) \underset{\rho \rightarrow \infty}{\sim} \exp(-\rho/2). \quad [7.100]$$

This result suggests that we look for a solution of the radial equation [7.98] having the form

$$u_{El}(\rho) = e^{-\rho/2} f(\rho) \quad [7.101]$$

where we have written $f(\rho) \equiv f_{El}(\rho)$ to simplify the notation. Substituting [7.101] into [7.98], we obtain for $f(\rho)$ the equation

$$\left[\frac{d^2}{d\rho^2} - \frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + \frac{\lambda}{\rho} \right] f(\rho) = 0. \quad [7.102]$$

We now write a series expansion for $f(\rho)$ in the form

$$f(\rho) = \rho^{l+1} g(\rho) \quad [7.103]$$

where

$$g(\rho) = \sum_{k=0}^{\infty} c_k \rho^k, \quad c_0 \neq 0 \quad [7.104]$$

and we have used the fact (see [7.58]) that $u_{El}(\rho)$, and thus also $f(\rho)$, behaves like ρ^{l+1} in the vicinity of the origin. Inserting [7.103] into [7.102], we find that the function $g(\rho)$ satisfies the differential equation

$$\left[\rho \frac{d^2}{d\rho^2} + (2l+2-\rho) \frac{d}{d\rho} + (\lambda-l-1) \right] g(\rho) = 0. \quad [7.105]$$

Using the expansion [7.104] to solve this equation, we have

$$\sum_{k=0}^{\infty} [k(k-1)c_k \rho^{k-1} + (2l+2-\rho)k c_k \rho^{k-1} + (\lambda-l-1)c_k \rho^k] = 0 \quad [7.106]$$

or

$$\sum_{k=0}^{\infty} \{ [k(k+1) + (2l+2)(k+1)] c_{k+1} + (\lambda-l-1-k)c_k \} \rho^k = 0 \quad [7.107]$$

$$\frac{c_{k+1}}{c_k} \sim \frac{1}{k} \quad [7.109]$$

a ratio which is the same as that of the series for $\rho^p \exp(\rho)$, where p has a finite value. Thus in this case we deduce by using [7.101] and [7.103] that the function $u_{El}(r)$ has an asymptotic behaviour of the type

$$u_{El}(\rho) \underset{\rho \rightarrow \infty}{\sim} \rho^{l+1+p} e^{\rho/2} \quad [7.110]$$

which is clearly unacceptable.

The series [7.104] must therefore terminate, which means that $g(\rho)$ must be a *polynomial* in ρ . Let the highest power of ρ appearing in $g(\rho)$ be ρ^n , where the *radial quantum number* $n_r = 0, 1, 2, \dots$, is a positive integer or zero. Then the coefficient $c_{n_r+1} = 0$, and from the recursion formula [7.108] we have

$$\lambda = n_r + l + 1. \quad [7.111]$$

Let us introduce the *principal quantum number*

$$n = n_r + l + 1 \quad [7.112]$$

which is a positive integer ($n = 1, 2, \dots$) since both n_r and l can take on positive integer or zero values. From [7.111] and [7.112] we see that the eigenvalues of equation [7.98] corresponding to the bound-state spectrum ($E < 0$) are given by

$$\lambda = n. \quad [7.113]$$

Energy levels

Replacing in [7.97] the quantity λ by its value [7.113], we obtain the bound-state energy eigenvalues

$$\begin{aligned} E_n &= -\frac{\mu}{2\hbar^2} \left(\frac{Ze^2}{4\pi\epsilon_0} \right)^2 \frac{1}{n^2} \\ &= -\frac{e^2}{(4\pi\epsilon_0)a_\mu} \frac{Z^2}{2n^2} \\ &= -\frac{1}{2} \mu c^2 \frac{(Z\alpha)^2}{n^2}, \quad n = 1, 2, 3, \dots \end{aligned} \quad [7.114]$$

where $\alpha \simeq 1/137$ is the fine-structure constant and a_μ denotes the modified Bohr radius

$$a_\mu = \frac{(4\pi\epsilon_0)\hbar^2}{\mu e^2} = \frac{m}{\mu} a_0 \quad [7.115]$$

with $a_0 = (4\pi\epsilon_0)\hbar^2/me^2$ being the Bohr radius [1.66].

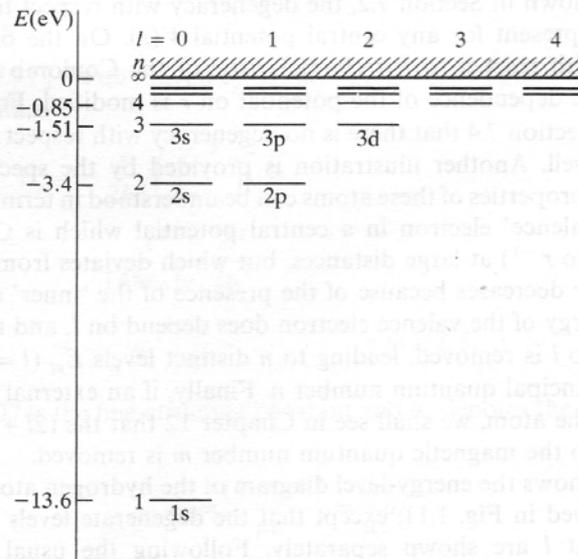
The energy levels [7.114], which we have obtained here by solving the

notation, these levels are labelled by two symbols. The first one gives the value of the principal quantum number n ; the second one is a code letter which indicates the value of the orbital angular momentum quantum number l according to the correspondence discussed in Chapter 6, namely

Value of l	0	1	2	3	4	5	...
	↓	↓	↓	↓	↓	↓	
Code letter	s	p	d	f	g	h

Looking at the hydrogen atom spectrum illustrated in Fig. 7.8, we see that the ground state ($n=1$) is a 1s state, the first excited state ($n=2$) is four-fold degenerate and contains one 2s state and three 2p states (with $m = -1, 0, +1$), the second excited state ($n=3$) is nine-fold degenerate and contains one 3s state, three 3p states (with $m = -1, 0, +1$) and five 3d states (with $m = -2, -1, 0, +1, +2$), etc.

Having obtained the energy levels of one-electron atoms within the framework of the Schrödinger non-relativistic quantum theory, we may now inquire about the *spectral lines* corresponding to transitions from one energy level to another. This problem has already been discussed in Chapter 1, where the frequencies of the spectral lines were obtained by using the Bohr model. We shall return to this question in detail in Chapter 11, where the interaction of atomic systems with electromagnetic radiation will be studied quantum mechanically. In particular, we shall re-derive in that chapter the Bohr result [1.61] giving the frequencies of the spectral lines, and we shall calculate the transition rates for the most common transitions, the so-called electric dipole transitions.



The Dirac Equation

$$\left[\left(-\frac{W}{c} + \frac{e}{c} \mathbf{A}_0 \right)^2 + \left(-\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 + m^2 c^2 \right] \psi = 0$$

Wavefunction collapse and “the measurement problem”

- Say system can be in two states:



or



Wavefunction collapse and “the measurement problem”

- Say system can be in two states

The wavefunction is

$$\frac{1}{\sqrt{2}} \Psi_{\text{billiards}} + \frac{1}{\sqrt{2}} \Psi_{\text{park}}$$
The equation shows a superposition of two wavefunctions, each with a coefficient of $\frac{1}{\sqrt{2}}$. The first wavefunction, $\Psi_{\text{billiards}}$, is associated with a circular image of a billiard table. The second wavefunction, Ψ_{park} , is associated with a circular image of a park with trees and people.

Wavefunction collapse and “the measurement problem”

The wavefunction before measurement is

$$\frac{1}{\sqrt{2}} \Psi + \frac{1}{\sqrt{2}} \Psi$$


The wavefunction after measurement is

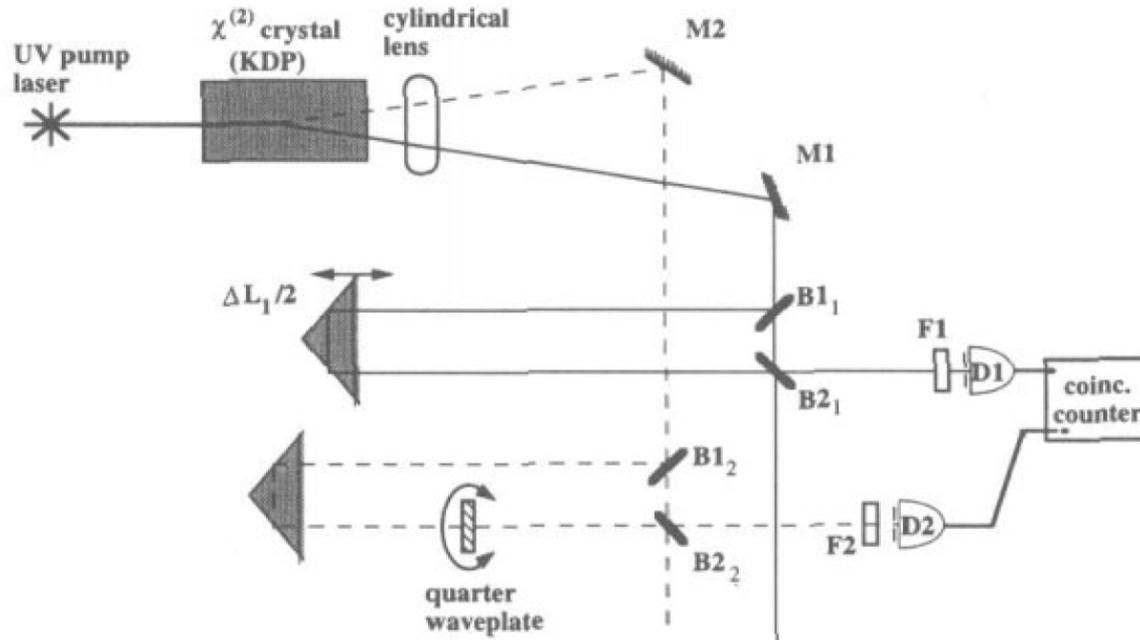
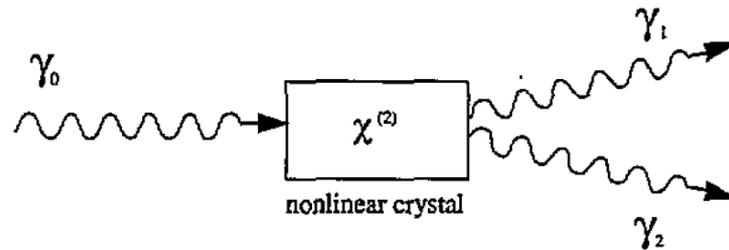
either Ψ



or Ψ



Two photon experiment demonstrating non-locality



Nero and Sancho Panza



Wavefunction of Nero



Wavefunction of Nero: momentum

$$\hat{p} \psi_{\text{Nero}} = p \psi_{\text{Nero}}$$

Wavefunction of Nero: cuteness

$$\hat{C}\psi_{\text{dog}} = \text{cuteness}_{\text{dog}}$$

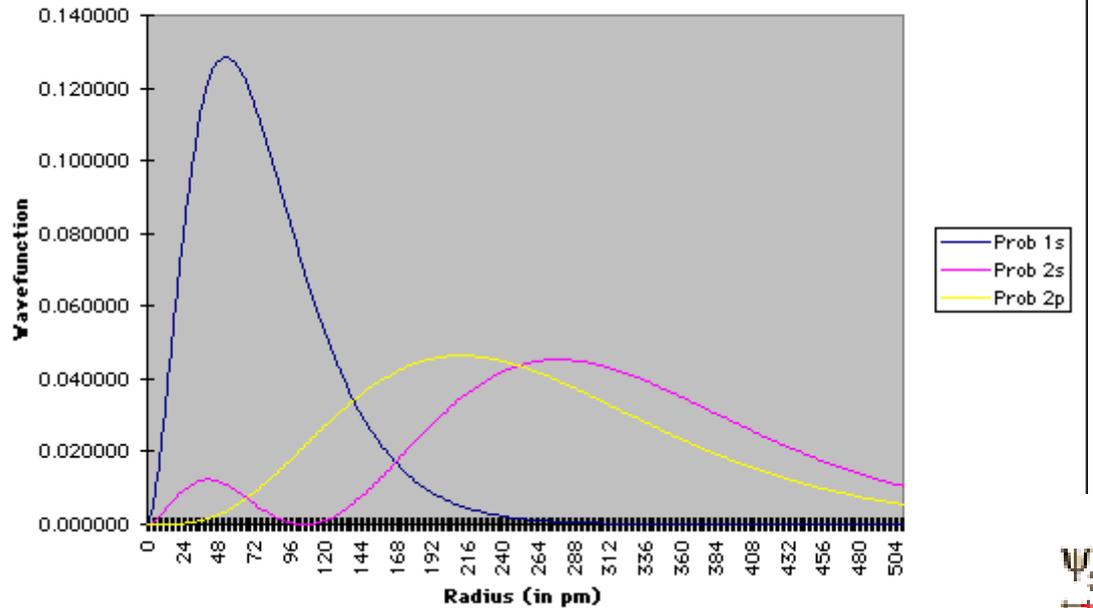
Wavefunction of ?

Ψ



Wavefunctions of electrons in different fields

Hydrogenic Wavefunctions



Particle in a box

