PROFESSOR: The last topic we discussed on Monday it was the situation of the Landau-Zener transition that you sweep for resonance. You've all seen the Landau-Zener formula, you all know that in crossing turns into an avoided crossing. But I tried to at least provide you additional insight by emphasizing that the whole process is absolute coherent. That it's full-phase coherent throughout.

And what happens is there is a coherent transfer of amplitude from the state 1 to the state 2. This is nothing else than Schrodinger's equation.

But I want to point out that for the short times you sweep through, there is no T2 independence here. In other words, when I discussed what is the effective time during which the transfer of population takes place, at the time here is so short that the detuning doesn't matter. Actually, the criterion which leads to this effective time during which the transfer takes place is actually exactly the time window where the detuning is small enough that-- to say it loosely, it doesn't make a difference whether your in resonance or slightly away. The atom experiences the same tri field.

And so based on this criterion, we discussed that we can understand the Landau-Zener probability in the perturbative limit as a coherent process where we transfer population, we transfer amplitude with a Rabi frequency during this effective time, delta t.

It's not the only way how we can look at it, but it's one way which I think is insightful. Any questions about this or what we discussed on Monday?

If not, I would like to take the topic one step further and discuss the density matrix formalism. So we have so far discussed purely Hamiltonian unitary evolution.

Namely, the Schrodinger equation. And of course, unitary evolution leaves the system which is in a pure state in a pure state. It's just that the quantum state evolves.

However, that means we cannot describe processes like decoherence or some losses away from the two levels we are focusing on. And so now we want to use the density operator, the density operator formalism to have a description of two-level system which goes beyond that.

So let me just-- so Schrodinger equation deals only with pure states, cannot describe loss of particles, loss of photons, and decoherence.

Well, there is one exception. If the decoherence process is merely a state-dependent loss of atoms to a third state, then you can still use the wave function formalism. So this is the exception.

If you have two states, that's the excited state. If you have two states and all of what happens is that you have some loss to some other levels and their rate coefficients, then one can still use a Hamiltonain description, but you have to replace the eigenvalues by complex numbers. In other words, you have to add an imaginary part to the energy levels. And that means the time evolution is exponentially dent. So that's as much as you can incorporate decoherence and losses into a wave function formalism.

However, many other processes require the formalism of the density matrix. And the simplest process where wave function formalism is absolutely inadequate is the process of spontaneous emission. When you have a loss in the excited state, you could still describe the excited state with a complex energy eigenvalue. But the fact that whatever is lost from the excited state is added to the ground state. There is no wave function formalism which can describe that.

So for those processes and for decoherence in general, we require the use of the density operator. So I know that most of you have seen the density operator in statistical mechanics or some advanced course in quantum mechanics. So

therefore, I only spend about five minutes on it. So I want to kind of just remind you or give you a very short introduction.

So for those of you who have never heard about it, I probably say enough that you understand the following discussion. And for those of you who know already everything about it, five minutes of recapitulation is hopefully not too boring.

So my way of introducing the density operator is first introduce it formally. Write down a few equations for pure state. But then in a moment, add something to it.

So if you have a time-dependent wave function, which we expand into eigenfunctions, then we can, in these spaces, define arbitrary operators by matrices. We want to describe our system by finding out measurable observables, expectation values of operators, which of course, depend on time.

And this is, of course, nothing else than the expectation value taken with a time-dependent wave function. But now we can expand it into the bases m, n and we can then rewrite it as a matrix, which is a density matrix. Or, simply as the trace of the density matrix with the operator.

And what I introduced here as the density matrix can be written as psi of t, psi of t. And the matrix element given by this combination of amplitudes when we expand the wave function psi into its basis.

So this density matrix his diagonal and off-diagonal matrix elements. The diagram matrix elements are called the populations, the populations in state n and the off-diagonal matrix elements are called coherences.

OK, so this is just rewriting Schrodinger's equation expectation value in a matrix formalism. Yes, please.

AUDIENCE: Why are you starring the coefficients?

PROFESSOR: Oh, there's one star too many. Thank you.

AUDIENCE: That makes sense.

PROFESSOR: But the reason why I wrote it is that we want to now add some probability to it. We do not know for sure that the system is in a pure state. We have probabilities P i that the system is in a quantum state psi i. So we add another index to it.

And when we perform the expectation value-- there's also one star too many. When we perform the expectation value, we sort of do it for each quantum state with a probability P i.

So we are actually-- and this is what I wanted to point out. This was the purpose of this short discussion, that we are now actually performing two averages. One can be regarded as the normal quantum mechanical average when you find the average value or the expectation value for quantum state. So this is sort of the statistics or the averaging, which is inherent in quantum physics.

But then in addition, there may simply be another probabilistic average because you have not prepared the system in a pure state, or the system may undergo some stochastic forces and wind up in different states. So there are two kinds of averages which are performed.

And the advantage of the density matrix formalism is that both kinds of averages can be done simultaneously in a very compact formalism. So therefore, I put this probabilistic average in now into the definition of the density matrix. Or I can write the density matrix in this way.

And with this extended definition of the density matrix, both kinds of averages are done when I determine the expectation value and operator by performing the trace with the density matrix.

A lot of properties of the density matrix, I think are-- you're familiar with many of those. For instance, that Schrodinger's equation for the density matrix becomes this following equation.

You can derive that by-- if you take the Schrodinger equation and you apply the Schrodinger equation to each state psi i. And then you do the averaging with a

probability P i. You find that the Schrodinger equation for each state psi i turns into this equation for the density matrix.

Let me just write down that the purpose now is we have two averages here. One is the quantum mechanic average and one is sort of an ensemble average with the probabilities P i.

I want to discuss in a few moments the density matrix for two-level system. So I have to remind you of two properties, that the density matrix is normalized to unity. So there's probability of unity to find the system in one of the states.

When we look at the square of the density matrix, a trace of rho square, this is simply the probability-- the sum of the probability squared. And this is smaller than 1.

And the only way that it is one is for pure state. So pure state is characterized by the fact that there is only-- that we can find the basis where only one of the probabilities, P i is non-vanishing. And then, of course, almost trivially the trace rho is 1 and the trace rho square is 1.

So, so far I've presented you the density matrix just as an elegant way of integrating the two averages into one formalism. And in essence, this is what it is. But you can now also use the density matrix if the whole system undergoes a time evolution, which is no longer unitary. No longer described by a Hamilton operator. Because you're interested in the time evolution or a small system which is part of a bigger system.

The bigger system is always described by unitary time evolution, but a smaller system is usually not described by unitary time evolution. And that's when the density matrix becomes crucial.

Of course, you can see this is just you describe the smaller system and you do some probabilistic average what the other part of the system does. And therefore, it's just another version of doing two averages. But this is sort of why we want to use the density matrix in general.

So we want to use the density matrix for non-unitary time evolution. And the keyword here is that this is often the situation for open systems where we are interested in a small system, but it is open to a bigger system. Like, we're interested to describe an atom, but the atom can spontaneously emit photons into other parts of [INAUDIBLE] space. And we're not interested in those other parts of [INAUDIBLE] space. So an open system for this purpose is where we limit our description to a small part of a larger system.

Again, an atom interacting with all the modes of the electromagnetic field, but we simply want to describe the atom. And then, we cannot use a wave function anymore. We have to use the density matrix. OK

After these preliminaries, I want to now use the density matrix formalism for arbitrary two-level systems. So what is the most general Hamiltonian for the most general two-level system?

Well, the most general Hamiltonian is the most general Hamiltonian we can construct with 2 by 2 matrices. And the base is set to expand the 2 by 2 matrices are the Pauli matrices. So if you expand the Hamiltonian into the unity matrix, sigma x, sigma y, and sigma z, we have four coefficients, four amplitudes, which are complex in general-- omega 1, omega 2, omega 3. And here is something which I've called omega bar.

By appropriately shifting what is the 0 point of energy, we can always get rid of this. So this is just this definitional character. So therefore, the most general Hamiltonian for any two-level system can be written in this very compact way that it is the scalar product of the vector omega-- omega 1, omega 2, omega 3-- with the vector sigma of the three Pauli matrices-- sigma x, sigma y, sigma z.

OK, so this is a way to write down the most general Hamiltonian for a two-level system. Now, we describe two-level systems by a density matrix, by statistical operator, which is also a 2 by 2 matrix. And the most general density matrix can also be expanded into the its four components. Sort of the basis set of matrices is

the unitary matrix and the three Pauli matrices. So 1, 2, 3.

Of course, this time we cannot throw away the unity matrix because otherwise the density matrix would have no trace and there would be no probability to find the particle.

But we can, again, write it in a compact form that it is 1/2-- yes, I'm using the fact now that the trace of rho is r0. And this is, by definition, or by conservation of probability, is 1. So therefore, r0 is not a free parameter. It's just the sum of all the probabilities to find the system in any state. And the non-trivial part is then the scalar product of this vector r-- rx, ry, rz-- with the vector of the three Pauli matrices.

Well, so we have our most general Hamiltonian. We have our most general density matrix. And now we can insert this into the equation of motion for the density matrix. Which, as I said before, is just a reformulation of Schrodinger's equation.

And if you insert the Hamiltonian and the density matrix into this equation, we find actually something which is very simple. It says that this vector r, which we call the Bloch vector-- the derivative of the Bloch vector is given by the cross product of the vector omega, which were the coefficients with which we parametrized the Hamiltonian cross r.

The derivation is straightforward. And you will be asked to do that on your homework assignment number 1. But it has a very powerful meaning. It tells us that an arbitrary two-level system with an arbitrary Hamiltonian can be regarded as a system where we have a vector R which undergoes precession. This is the time evolution of the system. So this is a powerful generalization from the result we discussed previously where we found that if you have an arbitrary quantum-mechanical spin, the time derivative can be written in that way.

So previously, we found it for a pure state, but now we find it-- that it's even valid for a general density matrix and its time evolution. So what I've derived for you is-- Classroom Files. Is a famous theorem, which is traced back to Feynman, Vernon, and Hellwarth. It's sort of a famous paper which--

So this famous theorem-- and I've summarized it here for you-- says that the time evolution of the density matrix for the most general two-level system is isomorphic to pure precession. And that means it's isomorphic to the behavior of a classical moment, classical magnetic moment, in a suitable time-dependent magnetic field.

So when you have a Hamiltonian, which is characterized by-- the most general Hamiltonian is characterized by the three coefficients-- w1, w2, w3. But if you would create a classical system where w1, w2, and w3 are the time-dependent components, xyz-component of a magnetic field, then the precession of a magnetic moment would be exactly the same as the time evolution of a quantum-mechanical density matrix. Any question?

So in other words, we've started out with rotating frames and rotation and now we've gone as far as I will go. Namely, I've in a way told you that an arbitrary quantum-mechanical two-level system, the time evolution is just precession. It's rotation. There is nothing more complicated possible.

Well, unless we talk about decoherence. If we have such a Hamiltonian, we know, of course, that a pure state will stay pure forever. And you can immediately verify that if you look at the trace of rho square. If the trace of rho square is 1, we have a pure state. And now we have parametrized the density matrix with the Bloch vector component-- r1, r2, r3. So in those components, the trace of rho square can be written in this way.

And of course, r0 square was constant. This was our normalization of 1. So the question is now when we have an arbitrary time evolution, which we know now according to the Feynman, Vernon, Hellwarth theorem. The arbitrary time evolution of the Bloch vector can be written as omega cross r.

So this equation tells us immediately that the length of the vector r is constant because r dot is always orthogonal to r. And therefore, the lengths of the vector r is not changing. So what we have derived says that with the most general Hamiltonian, the lengths of the vector r will be constant. And therefore, the trace of rho square will be constant. This is constant because r dot is perpendicular to r. So

this will tell us that a pure state will just precess with the constant lengths of its Bloch vector forever.

However, we know that in real life some coherences are lost and now we have to introduce something else. So this does not describe loss of coherence. So now we are just one tiny step away from introducing the Bloch equations. We will fully feature the optical Bloch equations in 8.422. but since we have discussed two-level systems to quite some extent, I cannot resist to show you now in three, four minutes what the Bloch equations are. And then when you take the second part of the course, you will already be familiar with it.

So let me just now tell you what has to be added to do this step from the previous formalism to the Bloch equations. And this is the one step you have to do. We have to include relaxation processes into the description. So my less than five-minute way to now derive the Bloch equations for you goes as follows.

I first remind you that everything has to come to thermal equilibrium. In other words, if you have an atomic system, if you have a quantum computer, whatever system you have and you prepared in a pure state, you know if you will wait forever, the system will be described by a density matrix, which is the density matrix of thermal equilibrium, which has only diagonal matrix elements. The populations follow the [INAUDIBLE] factor. And everything is normalized by the partition function.

So we know that this will happen after long, long times. So no matter with what density matrix we start out, if we start with a density matrix rho pure state, for instance, there will be inevitably some relaxation process which will restore rho to rho t, to the thermal equilibrium.

Now, how this happens can be formulated in a microscopic way. And we will go through a beautiful derivation of a master equation and really provide some insight what causes relaxation. But here for the purpose of this course, I want to say, well, there is relaxation. And I want to introduce now, in a phenomenological way, damping and damping times.

So the phenomenological way to introduce damping goes as follows. Our equation of motion for the density matrix was that this is a unitary evolution described by-- the Schrodinger equation was that the density matrix evolves according to the commutative with the Hamiltonian.

But now-- and I have to pick big quotation marks around it because this is not a mathematically exact way of writing it. But now I want to introduce some term which will damp the density matrix to the thermal equilibrium density matrix with some equilibration time, Te. I mean, this is what you can always do if you know the system is damped. You have some coherent evolution, but eventually you added a damping term and you make the damping term-- you formulate in such a way that asymptotically the system will be damped to the thermal equilibrium. In other words, the damping term will have no effect on the dynamics once you've reached equilibrium. So it does all the right things.

Of course, we have to be a little bit careful because everything is either an operator or matrix. And I was just adding the damping term as you would probably do it to a one-dimensional equation. So therefore, let me be a little bit more specific.

In many cases, you will find that there are two distinctly different relaxation times. In other words, the system will have usually at least two physically distinct relaxation times. They are traditionally called T1 and T2. T1 is the damping time for population differences.

So this is the damping time to shovel population from some inverted state or some other state into the equilibrium state. That usually involves the removal of energy out of the system. So it's an energy decay time.

And if you would inspect our parameterization of the Bloch vector, population or population differences are described by the z-component, the third component of the Bloch vector.

Well, we have other components of the Bloch vector which correspond to coherences. The off-diagonal matrix element of the density matrix. And they're only

nonzero if you have two states populated with a value-defined relative phase.

When the system, quantum mechanical system, loses its memory of the phase, the r1 and r2 component of the Bloch vector go to 0. So therefore, the time T2 is a time which describes the loss of coherences, the dephasing times. And in most situations, well, if you lose energy, you've also lost-- if you lose energy because you quench a quantum state, you've also lost the phase. So therefore in general, T2 is smaller than T1. Often by a lot.

So with those remarks about the two damping times, I can now go back to the equation at the top, which was sort of written with quotation marks, and write it in a more accurate way as a matrix equation for the damping of the components of the density matrix expressed by the Bloch vector.

In other words, the equation of motion for the z-component of the Bloch vector, which is describing the population, has a coherent part, which is this generalized precession. And then, it has a damping part, which damps the populations to the equilibrium value with a damping time T1.

And then we have the corresponding equations for the x and y, or the 1 or 2 component of the optical Bloch vector. We just replace the z index by x and y from the equation above, but then we divide by a different relaxation time, T2.

So what we have found here, these are the famous Bloch equations, which were introduced by Bloch in 1946. Introduced first for magnetic resonance, but they're also valid in the optical domain.

For magnetic resonance, you have a two-level system, spin up and spin down. In the optical domain, you have a ground and excited state. In the latter case, they're often referred to as the optical Bloch equations. Any questions about that? Yes, please.

AUDIENCE: So what determines [INAUDIBLE]?

PROFESSOR: Well, that's a long discussion. We spent a long time in 8.422 discussing various

processes. But just to give you an example, if you have a gas of atoms and there are slightly inhomogeneous magnetic field, that would mean that each atom, if you look at it as precession motion, precesses at slightly differently rates. And the atoms will decohere. They all will eventually wind up with a different phase, that if you look at the average of coherence, it's equal to 0.

So any form of inhomogeneity, which is not quenching a quantum state, which is not creating any form of de-activation of the excited state, can actually decohere the phase. And these are contributions to T2. So often, contributions to T2 come from inhomogeneous environment, but they are not changing the population of states.

Whereas, what contributes to T1 are often collisions. Collisions which, when an atom in an excited state collides with the buffer gas atom, it undergoes a transition from the excited to the ground state. So these are two distinctly different processes. One is really a collision and energy transfer. Each atom has to change its quantum state. Whereas, decoherence can simply happen that there is a small pertubation of the energy levels due to external fields. And then, the system as an ensemble loses its phase.

In the simplest way, you can assume inhomogeneous broadening. But you can also assume, if the whole ensemble is subject to fluctuating fields, then since you don't know how the fields exactly fluctuate after characteristic time, you no longer have a phased coherent system. Rather, phase at a later time is deterministically related to the phase at which you prepared it. And that would mean the system has dephased. And this dephasing time is called the T2 time. Nancy.

AUDIENCE: I think I have two things. First, you said that it's generally true that T2 is less than T1. Is it ever true that it's not the case?

PROFESSOR: Oh. There is one exception. And that's the following. Let me put it this way, every process which contributes to T1 will also contribute to T2. But there are lots of processes which only contribute to T2. So therefore, in general, T2 is much faster because many more processes can contribute to it.

However, now if you ask me, is it always true? Well, there is one glitch. And this is the following. T1 is the time to damp populations. And that's the damping of psi square. T2 is due to the damping of the phase. And this is actually more a damping time of the wave function itself.

And if you have a wave function psi which is damped with a damping time tau. Psi square is damped with twice the damping time. So if the only process you have is, for instance, spontaneous emission, then you find out that the damping rate for population is gamma. This is the definition of the spontaneous emission rate. But the damping rate 1 over T2 is 1/2 gamma. But because simply the way how we have defined it, one involves the square of the wave function. The other one involves simply the wave function. So there is this factor of 2 which can make-- by just a factor of 2-- T1 faster than T2.

But apart from this factor of 2, if T2 would be defined in a way which would incorporate the factor of 2, then T2 would always be faster than T1.

AUDIENCE: Yeah, it makes sense [INAUDIBLE]. I can't imagine if the system has a smaller T1, then it still has any coherence left in it.

PROFESSOR: So maybe to be absolutely correct, I should say this. T1 is much larger than-- is larger or equal than T2 over 2. In general, we have even the situation that T1 is much, much larger than T2.

But with this factor of 2, I've incorporated this subtlety of the definition. Other questions? Yes.

AUDIENCE: Just a question about real motivation of using Bloch equation [INAUDIBLE]. I understand that [INAUDIBLE]. But you mentioned before that you can't describe spontaneous emission with a Hamiltonian formalism.

PROFESSOR: Yes.

AUDIENCE: But couldn't you use-- [INAUDIBLE]. Don't you still get spontaneous emission out of the coupling into the continuum? The emission into the different modes? You don't

necessarily need [INAUDIBLE].

PROFESSOR: Yes, but let me kind of remind you of this. If you are interested in a quantum state and it decays to a level. But we're not really interested what this level is and we're not keeping track of the population here, when we can describe the time evolution of the excited state with a Hamiltonian because of the imaginary part, the Hamiltonian is no longer imaginary.

And this is what Victor Weisskopf theory does. It looks at a system in the excited state and looks at the time evolution of the excited state.

But if you want to include in this description what happens in the ground state, you are not having this situation. You have this situation. And what eventually will happen is you can look at a pure state which decays. And this is what is done in Victor Weisskopf theory. But if you want to know now what happens in the ground state, well, I'm speaking loosely, but that's what really happens. Every spontaneous emission adds something to the ground state, but in incoherent way.

So what is being built up in the ground state is not a wave function. It's just population which has to be described with a density matrix. Or in other words, if you have a coherent superposition between excited and ground state, you cannot just say spontaneous emission is now increasing the amplitude to be in the ground state. It really does something fundamentally different. It puts population into the ground state with-- I'm loosely speaking now, but with a random phase. And this can only be described probabilistically by using the density matrix.

But what you are talking about is actually, for the Victor Weisskopf theory, is pretty much this part of the diagram. We prepare an excited state, and we study it with all its glorious details, with the many modes of the electromagnetic field how the excited state decays.

OK. Actually with that, we have finished one big chapter of our course, which is the general discussion of resonance, classical resonance, and our discussion of two-level systems.

AUDIENCE: But [INAUDIBLE], wouldn't you have to do a sum over every single mode [INAUDIBLE]? Which would be the exact same thing you do when you do a partial trace over the environment. Isn't the end result sort of the same thing that you have to do some [INAUDIBLE] infinite sum and integral or all the [INAUDIBLE]?

PROFESSOR: You need a sum, but--

AUDIENCE: That's where the decoherence comes from?

PROFESSOR: Yes. But if you're interested in only the decay of an excited state, it can decay in many, many modes, but all these different modes provide a contribution to the decay rate gamma. So at the end of the day, you have a Hamiltonian evolution with a damping time gamma. And this damping time gamma is the sum of the other states.

So in other words, the loss of population from the excited state, you just incorporate it by adding a damping time to the Schrodinger equation because you're not keeping track of the other modes where the population goes.

You're not keeping track. You just say, excited state is lost. You're not interested whether the atoms are now in the ground state or some other state. All you are describing the loss rate from the excited state. And this is possible by simply doing-- by adding damping terms to the Schrodinger equation.

In other words, what I'm saying is actually fairly simple. If you have a coherent state and you lose it, you just lose amplitude. what is left is coherent. When it's gone, it's gone. You have a smaller amplitude, smaller probability. And that's simple to describe.

What is harder to describe is if you accumulate population in the ground state and the population arrives in incoherent pieces. How to treat that, this is more complicated. But simply the decay of a pure state, it's just-- you have e to the i omega t, which is a coherent evolution, and then you add an imaginary part and this is a damping time. So what I'm saying, it's sort of subtle but it's also very trivial. I don't know if this addresses your question.

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In the end, in general you need a density matrix. I just wanted to sort of emphasize that there is a little bit of decoherence where you can still get away with a wave function description. And actually, Victor Weisskopf theory is the wonderful example.

OK, so we have discussed resonance. Arizonans have discussed in particular two-level systems. And if I wanted, we could now continue with two-level systems and talk about the wonderful things you can do with two-level systems. Absorbing photons, emitting photons, and all that. But let's put that on hold for a few weeks. And I think what we should first do is realize, where do those levels come from?

And we discuss where those levels come form in our discussion of atoms. So our big next chapter is now atoms or atomic structure. And we build it up in several stages.

Well, first things first. And the first things are the big chunks of energy which define the electronic structure. We discuss electronic structure for one electron and two electron atoms, hydrogen and helium. We don't go higher in the periodic table.

But then we talk about other contributions to the energy of atoms, other contributions to the level structure of atoms. And this will start with fine structure, the Lamb shift. We bring in properties of the nucleus by discussing hyperfine structure. And then as a next big chapter, we will learn how external fields, magnetic fields, electric fields, and electromagnetic fields will modify the level structure of atoms. So by going through all those different layers, we will arrive at a rather complete description. If you have an atom in the laboratory, what determines its energy level and the transitions between those energy levels? So this is our agenda for the next few lectures.

Today, we start with single electron atom with a hydrogen atom. And I cannot resist to start with some quotes from Dan Kleppner, who I sometimes call Mr. Hydrogen.

So there is some beautiful piece of writing in a reference frame in *Physics Today,* "The Yin and Yang of Hydrogen."

I mean, those of you who know Dan Kleppner know that he's always said hydrogen is the only atom, other atom he wants to work with. Other atoms are too complicated. And he studied-- actually, hydrogen was-- he did a little bit on alkali atoms, of course, but hydrogen was really the central part of his scientific work. Whether he studied Rydberg states in hydrogen or Bose-Einstein condensation in hydrogen.

And this column in *Physics Today*, he talks about the yin and yang. The simplicity of hydrogen. It's the simplest atom. But if you want to work with hydrogen, you need vacuum UV because the step from the 1s to the 2p transition is-- Lyman-alpha is vacuum UV at 121 nanometer. So it's simple, but challenging.

And hydrogen is the most pristine atom. But for those of you who do Bose-Einstein condensation, it's the hardest atom to Bose condense. Because the physical properties of hydrogen, it's simple in its structure. But the properties of hydrogen, in particular the collision cross-section, which is important for evaporative cooling, is very, very unfavorable. So that's why he talks about the yin and the yang of hydrogen.

Let me just show you the first sentence of this paper, of this reference frame. Oops. Just a technical problem to make this fit the screen. I think I select it.

What's going on? Yep. So now it's smaller. I can move it over there. Well, why don't we read it together? It's a tribute to hydrogen, a tribute to famous people.

Viki Weisskopf was on the faculty at MIT. I met him, but he was already retired at this point. But then, Kleppner interacted with him. And you see the first quote, "To understand hydrogen is to understand all of physics."

Well, it simply says that if you understand some of this paradigmatic systems in physics, you understand all of physics. I would actually say, well, you really have to understand the harmonic oscillator, the two-level system, and hydrogen. And maybe a little bit about three-level systems. But if you understand, really, those simple systems-- they're not so simple. But if you understand those so-called simple

system very well in all its glorious detail, then you have really understood, maybe not all of physics, but a hell of a lot of physics.

And this quote goes on that, "To understand hydrogen is to understand all of physics." But then Viki Weisskopf said, "Well, I wish I had understood all of hydrogen." And this is sort of Dan's Kleppner's wise words. For me, hydrogen holds an almost mystical attraction. Probably because I'm among the small band of physicists who actually confront it, more or less, daily.

So that's what we are starting out now to talk about hydrogen. I know that a discussion of the hydrogen atom, the solution of the Schrodinger equation for the hydrogen atom is in all quantum mechanics textbooks. I'm not doing it here. I rather want to give you a few insightful comments about the structure of hydrogen, some scaling of length scales and energy levels, because this is something we need later in the course. So in other words, I want to highlight a few things which are often not emphasized in the textbook.

So let's talk about the hydrogen atom. So the energy levels of the hydrogen atom are described by the Rydberg formula. This actually follows already from the simple Bohr model. But of course, also from the Schrodinger equation.

And it says that the energy levels-- let me write it in the following way. It depends on the electron mass, the electron charge, h bar square. It has a reduced mass correction. And then, n is the principal quantum number. It scales as 1 over n squared. So this here is the reduced mass factor.

This here is called the Rydberg constant R, sometimes with the index infinity because it is the Rydberg constant which describes the spectrum of a hydrogen atom where the nucleus has infinite mass.

If you include the reduced mass correction for the mass of the proton, then this factor which determines the spectrum of hydrogen is called the Rydberg constant with an index H for hydrogen.

You find the electronic eigenfunctions as the solution of Schrodinger's equation. And

the eigenfunctions have a simple angular part, which are the spherical harmonics. We are not talking about that. But there is a radial part, radial wave function.

So if you solve it, if you find those wave functions, there are a number of noteworthy results. One is in short form the spectrum is the Rydberg constant divided by n squared.

I want to talk to you about your intuition for the size of the hydrogen atom, or for the size of hydrogen-like atoms. So what I want to discuss is several important aspects about the radius or the expectation value of the position of the electron. And it's important to distinguish between the expectation value for the radius and the inverse radius.

The expectation value for the radius is, well, a little bit more complicated. 1/2 1 minus l times l plus 1 over n squared. Whereas, the result for the inverse radius is very simple.

What I've introduced here is the natural length scale for the hydrogen atom which is the Bohr radius. And just to be general, mu is the reduced mass. So it's close to the electron mass.

Well, the one thing I want to discuss with you-- we will need leader for the discussion of quantum defects, for field ionization and other processes, we have to know what the size of the wave function is. And so usually, if you wave your hands, you would say the expectation value of 1/r is 1 over the expectation value or r. But there are now some important differences.

I first want to sort of ask you, why is the expectation value of 1/r, why does it have this very, very simple form?

AUDIENCE: Virial theorem?

PROFESSOR: The Virial theorem. Yes. We know that there is a fairly simple form for the energy eigenvalues. It's 1 over n squared.

Well, Coulomb energy e square over r. So if the only energy of the hydrogen atom were Coulomb energy, it's very clear that 1/r, which is proportional to the Coulomb energy, has to have the same simple form as the energy eigenvalue.

Well, there is a second contribution to the energy in addition to Coulomb energy. This is kinetic energy. But due to the Virial theorem, the kinetic energy is actually proportional to the Coulomb energy. And therefore, the total energy is proportional to 1/r. And therefore, 1/r has to scale exactly as the energy. Since the energy until we introduce fine structure is independent of l, only depends on the principal quantum number n, we find there's only an n-dependence. But if you would ask, what is the expectation value for the radius?

You find an l-dependence because you're talking about a very different quantity. So let me just summarize what we just discussed.

We have the Virial theorem, which in general is of the following form. If you have potential energy which is proportional to radius to the n, then the expectation value for the kinetic energy is n/2 times the expectation value for the potential energy.

The most famous example is n equals 2, the harmonic oscillator. You have an equal contribution to potential energy of the spring and kinetic energy.

Well, here for the Coulomb problem, we discuss n equals minus 1. And therefore, the kinetic energy is minus 1/2 times the potential energy. So this factor of 2 appears now in a number of relations and that's as follows.

If you take the Rydberg constant, the Rydberg constant in CGS units is-- well, that's the Coulomb energy at the Bohr radius. But the Rydberg constant is 1/2 of it. So the Rydberg constant is 1/2 of another quantity, which is called 1 Hartree. We'll talk, probably not , today, but on Monday about atomic units, about sort of fundamental system of units. And the fundamental way-- the fundamental energy of the hydrogen atom, the fundamental unit of energy is whatever energy you can construct using the electron mass, the electron charge, and h bar. And what you get is 1 Hartree.

If you ever wondered why the Rydberg is 1/2 Hartree, what happens is in the ground state of hydrogen, you have 1 Hartree worth of Coulomb energy. But then because of the Virial theorem, you have minus 1/2 of it as kinetic energy. And therefore, the binding energy in the n equals 1 ground state, which is 1 Rydberg, is 1/2 of the Hartree. So this factor of 1/2 of the Virial theorem is responsible for this factor of 2 for those two energies.

I usually prefer SI units for all calculations, but there's certain relations where we should use CGS units. Just as a side remark, if you want to go to SI units, you simply replace the electron charge e squared by e squared divided by 4 pi epsilon0.

OK. So I've discussed the hydrogen atom. It's also insightful and you should actually remember that or be able to re-derive it for yourself. How do things depend on the nuclear charge z?

Well, if you have a nuclear charge z, the Coulomb energy goes up by-- well, if you have a stronger attraction. If you would go to helium nucleus or even more highly-charged nucleus and put one electron in it. Because of the stronger Coulomb attraction, all the length scales are divided by z. So everything is smaller by a factor of z. So what does that now imply for the energy?

Well, you have a Coulomb field which is z times stronger, but you probe it now at a z times smaller radius. So therefore, the energies scale with z squared.

Let me formulate a question because we need that later on. So if you have a hydrogen-like atom and the electron is in a state with principal quantum number n. And let's assume there is no angular momentum. So what I'm writing down for you is the probability for the electron to be at the nucleus. This will be very important later on when ewe discuss hyperfine structure because hyperfine is responsible-- for hyperfine structure, what is responsible is the fact that the electron can overlap with the nucleus. So this factor will appear in our discussion of hyperfine structure.

And what I want to ask you is, how does this quantity depend on the principal quantum number n and on z? And I want to give you four choices.

Of course, for dimensional reasons, everything is 1 over the Bohr radius cubed because it's a density. But you cannot use dimensional analysis to guess, how do things scale with z and with n?

So here are your four choices. Does it scale with z, z squared, z cubed? Does it scale with n squared, n cubed, n to the 6?

If you don't know it, just make your best guess. OK, one part should be relatively straightforward. And this is the scaling with z. Let me just stop it.

So the exact answer is that z n 00 at the origin squared is pi a0 cubed. And its c cubed over n cubed. So the correct answer is this one.

Let me first say-- OK, I gave you four choices and it's difficult to distinguish all of them. But the first one you should have gotten rather simply, and this is the z-scaling. Because the scaling with z is the following, that everything-- if you write down the Schrodinger equation, if you have z, you replace e squared by z e squared.

And I actually just mentioned it five minutes ago, that all length scales, the Bohr radius is h bar squared over electron mass times e squared. It actually scales with 1/z. So if all length scales go as 1/z, the density goes with z cubed. So therefore, one should have immediately narrowed down the choice. It should be A or C because they have the correct scaling with z.

The scaling with n is more subtle and there was something surprising I learned about it. And this is what I want to present to you in the last three or four minutes.

So the z-scaling, just remember that the length scaling is the length scales as 1/z. Therefore, density scale was z cubed.

The interesting thing about the length scaling is-- and I just want to draw your attention to it because it can be confusing, that in high torsion we have not only one length scale, but two length scales.

We have mentioned one of it already, which is the energetic length scale 1/r. 1/r is the Coulomb energy. Because of the Virial theorem, it's proportional to the total energy. And that's what you know, what you remember when you wake up in the middle of the night out of deep sleep, that the energy of high torsion is 1 over n squared. So therefore, this is a0 over n squared.

However, if you look at the wave function of hydrogen, you factor out. When you solve the radial equation, you factor out an exponential. There's sort of polynomial and then there is an exponential decay. And the characteristic lengths in the exponential decay of the wave function is n e0 over z. So therefore, when we talk about wave functions with principal quantum number n, there are two length scale. 1 over r n l scales with n squared. But the characteristic length scale in the exponential part of the radial wave function scales with n and not with n squared.

And it is this exponential part of the wave function which scales with n which is responsible for the probability to find the electron as the nucleus. Which, as I said before, the z-scaling is simple but the n-scaling is not n to the 6. It's n cubed.

And this is really important. And this describes the scaling with n for everything which depends on the presence of the electron as a nucleus. One is the quantum defect and the other one is the hyperfine structure.

Let me just give you one more scaling. I've discussed now what happens for 0 angular momentum, for finite angular momentum states, psi is proportional to r to the l. So therefore, if you ask, what is psi square, it scales with 2l. And at least for large n, the n-scaling is, again, 1 over n cubed.

OK, that's what I wanted to present you today. Any questions?

OK, so we meet again on Wednesday next week.