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**PROFESSOR:** I apologize for the delay. But we are ready for multimedia show with three different applications. One of them are the clickers. I hope you all took a clicker. It's just two questions today, but really good questions.

[LAUGHTER]

So today's actually very nice topic. I think almost every lecture we have a nice topic, but today's especially nice. It's called Unraveling Open Quantum System. That may not tell you so much. Well unravelling means we want to sort of untangle it, We want to understand what is inside.

And so we want to develop a better understanding what is inside a density matrix. How can we think about the quantum system in an even more microscopic way than the density matrix tell us? And again, this finds applications in atomic physics, because one application of it is spontaneous emission optical block equations. On the other hand, actually, this class will also teach you something very general about quantum physics.

So today's lecture is this part. We'll have three topics. One is I want to provide a motivation for single quantum systems. And you should appreciate this. A single quantum system is not what Schrodinger and Heisenberg told us about. Quantum mechanics was formulated as an ensemble average. But today we want to talk about, is there something in addition? About single quantum systems.

Part two is-- addresses the derivation of the quantum Monte Carlo wave function method. And this is a formalism, which is really simulating in quite general terms, quantum physics by following-- using quantum Monte Carlo simulations-- trajectories of individual quantum systems. So here the individual quantum system--

even if you have one, even if you don't have one-- becomes a computational tool.

And eventually in part two I want to give you another example for unraveling open quantum system, which differ from the models for dephasing. And if you remember that this was on one of your homework assignment that's correct. I sort of want to here take your homework into the classroom discussion.

Well I think it's nice to start this lecture with the quote by Erwin Schrodinger. Where he said, "We never experiment with just one electron, or atom, or molecule. In thought experiments, we sometimes assume that we do; this inevitably entails ridiculous consequences." Well today we want to talk about those ridiculous consequences, because many people in our field trap, address, and observe single electrons and single atoms.

Now this is related to quantum jumps. Quantum jumps has even made it into the popular realm. You can find lots and lots of references on quantum jumping, but I warn you this is about quantum jumping into different worlds. It's about broadening your horizon. And those authors, those people actually, sell you something by claiming that people like Einstein and Stephen Hawking would support the idea that you can jump into different universe, experience another version of yourself-- probably a better version of yourself-- and this will inspire you to change your life in the world you live.

But-- So this is quantum jumping. I'm not talking about quantum jumping, I will only talk about quantum chunks. So what you see here is really a classic experiment. One of three experiments which were done almost simultaneously. There have always been races for, you know, the first observation of something. And there was the [? Hamburg ?] group by [? Toshak ?], the Seattle group by Hunt [INAUDIBLE], and the Boulder Group by Dave Wylene, who observed the phenomenon of quantum jumps for the first time.

Let me just tell you what it is, because it's exactly what you're going to describe. Here in this situation you have a system. It's a trapped barium ion with a p and s state. And there is very fast transition where you can rapidly scatter light, and get

lots of fluorescence, at 493 nanometer. But what happened is, every once in a while, the particle has a branching ratio to decay to d state, and, well, d to s 2 units of angular momentum.

The transition here down to the ground state is very slow. It's slow because it's forbidden. It's even slower because it happens at longer wavelengths of 1,600 nanometer. And this is slow. And it has a lifetime of about 50 second.

So you-- If you think about it naively and that's probably the correct approach-- you would say the particles in the s state, it's like a light bulb. It scatters many, many photons, but then it branches to the d state. And for 50 seconds the light bulb is switched off, until the particle spontaneously goes down to the s state, and then the light bulb is switched on. And this is exactly what people observed.

But I mean I was-- This was '86. That was the time I was a graduate student, and I talked with theorists in the field, and respectable theorists told me that there was a controversy-- probably not among experimentalists, who use the naive approach-- but theorists who believed too much in what they calculate. Because if you solve it quantum mechanically, and look what you get. It's a steady state solution. Atom in steady state. Laser in steady state. And if you calculate the quantum mechanical expectation value, the expectation value is constant as a function of time.

So a simple quantum calculation would say the fluorescence is on average. Well just the time average and his constant, and his time independent. So there were some serious doubts whether you would observe this, or something which looks more like the ensemble average.

Well made all of the theorists soon realize you cannot calculate the steady state average. You have to calculate the correlation function in steady state. And the steady state correlation function has structure exactly at 50 seconds. So in a steady state system, if you're interested in fluctuations and temporal behavior, you can't just calculate quantities, you have to calculate correlation functions of quantities.

So anyway-- But then of course, if you now average over many, many realizations,

you find exactly an exponential decay of 50 seconds. And this is sort of what you would get for an ensemble average.

So this is what quantum jumps are. This is what you should always imagine when we talk about quantum jumps in the rest of this lecture. But I also want to show you more recent example from Serge Haroche, in Paris, where they observed quantum jumps. Recording a single photon in a cavity. So what happens is there's a single photon in this cavity, and they can read out whether there is a photon or not by sending Rydberg atoms through. And a single photon is never observed, but it causes a phase shift, an AC-Stark shift, on the Rydberg atom. And then they can read out with a Ramsey interferometer the AC-Stark shift.

So every atom which passes through the cavity will tell you whether there is a photon or not. And-- And this is shown here. Blue means no, there is no photon. Red means there is a photon. So here you repeatedly figure out again there is no photon. And suddenly there is a quantum jump when the cavity has absorbed a photon, or when a thermal photon was released.

You may say, what happened here? Well no measurement is perfect. There is some noise. But by seeing that these are outliers, you clearly see that here is a photon in the cavity, and here where the red read out of the atom overwhelms the blue readout here you have no photon. And then as time goes by, you can observe the death and birth of micro-cavity photons. So these are now quantum jumps in the-- not in atomic population, but quantum jumps in the photon number in a cavity.

**AUDIENCE:** What's the time scale on that? Seconds?

**PROFESSOR:** Yeah, time is second. So what is shown here is-- I think what is shown is here are 300 milliseconds, and this is 2.5 second element.

**AUDIENCE:** What was the density of each line mean?

**PROFESSOR:** Each line is a Rydberg atom, which has been readout with a Ramsey interferometer. And--

**AUDIENCE:** So that means that they're leaving no, like between--

**PROFESSOR:** I think that means there was a Rydberg atom in state e, which means there is a photon. And blue means, the blue bar means, there was a Rydberg atom in state g. These are two highlighting states of the rubidium atom. Sort of each spike here is one readout of the microchannel plate. So these are detector clicks. You can say, yes. You can sort of say, blue is yes, and red is no. And these are the two clicks.

**AUDIENCE:** Yeah, but, like the separation between two clicks is not uniform.

**PROFESSOR:** No, because if you're an atomic beam the atoms come not equally spaced out. There's a randomness when the atom comes. I think it's posed only in statistics in this experiment. It's a real experiment. It's amazing. Other questions? Team One.

**AUDIENCE:** So one more question. So the, for example, the first bit of blue is all measurements for the same state of the cavity. I know blue means photon or no photon, but if it does mean photon, that means it's the same photon interacting with--

**PROFESSOR:** Yes.

**AUDIENCE:** OK.

**PROFESSOR:** Yes, because, I mean, this is something people know that the photon number in this cavity only changes over very long time scales. And you sort of see, kind of, exactly hear how-- You see here two quantum jumps. One from blue to red, and one from red to blue in this cavity. Yes?

**AUDIENCE:** I don't if this is maybe just my accent's not very good, but in the bottom left graph-- Right? Or on the bottom graph, in sort of the left corner, it looks like there's some overlap between the dark blue and the dark red. Yeah.

**PROFESSOR:** You mean here?

**AUDIENCE:** Yeah, like right there. Is that like sort of there is a photon in that [INAUDIBLE] simultaneously?

**PROFESSOR:** I think, to the best of my knowledge, I haven't really looked-- I've heard wonderful talks about it. You can go back and read the paper, but this probably means in the atom number in the cavity, and the algorithm they have used to analyze the data says that here the photon number was 0, jumped to 1, and jumped back again. So you-- If you see here, for instance, there is some overlap, but you would still say, since either there is a photon or not a photon, as long as you have a-- as you have a higher number of red clicks than blue clicks, you would say there is a photon.

And the little overlap, there is maybe a little bit of time where you don't know whether there is a photon or not. But this really-- This is real, because every measurement takes a certain amount of time. Since you have a few random clicks, if they are a few random clicks, you do not know yet if the system has jumped, you have to wait a little bit. But this is really also showing how our knowledge about the quantum system comes with time. And therefore, the wave function, or the statistical operator changes with time, because of wave function and statistical operator are simply a description of our knowledge about the quantum system.

**AUDIENCE:** [INAUDIBLE] is too dense

**PROFESSOR:** You could have a situation, for instance, you could prepare the cavity, that it has an equal probability foreseeable in one. And then what you would read out may just be completely random. So that may be possible, but in their experiment, I think, the nature here is that you have most of the time stable photons, because the cavity is cooled to very low temperature, and only occasionally does the thermal distribution, the Bose-Einstein distribution of photons in the cavity have a one. And what we observe are the thermal fluctuations between mainly 0 and occasionally a 1.

If you would make the cavity and little bit hotter, it would have maybe half of the time a 1 and half of the time 0. But that wouldn't mean that you have completely randomness in your results, because there is a thermal relaxation time over which a photon is created, and a photon goes back. The photon would not jump back and forth from the cavity to the walls of the cavity in microseconds. It would probably

have an exchange time, and you could sort of measure the thermal correlation time of photons in a cavity.

It's a really good experiment. OK. So in that sense I think I showed you that what Schrodinger said is ridiculous is real, is the subject of current research, and since for quantum information processing in quantum computers, we need single quantum system is at the heart of quantum information processing.

So therefore, we want to now describe single quantum systems.

But when I do that, I-- come very -- It will become clear at the end of this unit, but I want to give you the warning right away. The way how I describe now a single quantum system may not be unique. There will be, there is actually, an infinite number of ways.

And I've already mentioned that to you, that there is an infinite number of ways to unravel a density matrix. I mentioned that you can write every density matrix as a probability of pure states. Weighted probability of being in pure states, but there's always different choices. You can get an infinite number of different combinations of pure states, and construct your density matrix. So, so this was sort of in at the level of the density matrix, but similarly-- and this will come out of this discussion today-- there is also an infinite number of ways to unravel the dynamics-- the dynamics involved in the evolution of an open quantum system.

So-- so with that I want to describe the quantum Monte Carlo wave function method. So in the quantum Monte Carlo wave function method, we perform-- We don't need an experiment. We don't need sophisticated experiments to observe a single quantum system. It's a theoretical method, but we perform thought, or gedanken experiments.

So our gedanken experiments is that we perform measurements. So we assume-- we have-- When we want to describe an ensemble of atoms, we assume we have a single atom. We assume it emits photon, and then we assume that the photon is

detected. And the moment-- So the moment the photon is detected we know, for instance, that the atom is in the ground state.

And so our quantum Monte Carlo simulation follows now the trajectory of the single quantum system by saying, I toss a coin, there's a certain probability for detecting the photon. If I detect the photon, the system I know is in the ground state. If I don't detect the photon, it's not in the ground state, and such. And these probabilistic approach is just simulated in the quantum Monte Carlo sense.

So-- So what is in essence-- what is the essence of the quantum Monte Carlo method is that we allow a small time step  $\Delta t$ . It's a real time simulation. And there is a small probability that the system has decayed in that time. So we may now toss a coin-- use a random function generator-- and ask, has spontaneous emission taken place?

And then the two possibilities are yes, and we continue whatever the outcome, whatever the quantum state is. Or we say no, and then with the probability-- with a-- so with a probability,  $p$ , we say yes. With a probability  $1 - p$  we say no, and then we continue the simulation accordingly.

So this will become much, much clearer when I write down the formalism for you, but there is one important aspect, which I really want to discuss with you. And this is the essence of the method. Namely, how does the wave function change by your measurement?

So-- so this is the essential, the only conceptual part for the quantum Monte Carlo wave function. Afterwards I just show you. Once you have this, once we have cleared up this conceptual part, the rest is just a few equations. And we immediately show that the quantum Monte Carlo wave function method is equivalent to the optical Bloch equation. But let's really feature and take some time for discussing the concept, namely, the change over wave function by a quantum measurement.

And maybe what this carries home to you is that the nature of an open system-- we

have a quantum system, which interacts with the environment-- is, actually, that the environment permanently performs measurements. And you will actually see that the idea of performing measurements, formalized in the quantum Monte Carlo sense, gives us an equation for the density matrix, which is identical to the optical Bloch equation.

So in other words, you can say I am re-deriving for you master equation now, but from a very, very different perspective. From the perspective of an environment which constantly performs measurement.

OK. So let's go through that. How-- What happens in a measurement? Well if our initial state is the ground state-- starting very in trivial ways-- well there is no measurement, because the particle will stay in the ground state forever.

OK. Now let's go to the next situation that our atom starts out in the excited state. Now in a time step  $\Delta t$ , we have two possibilities. A photon can be observed, or no photon is observed. When the photon is observed, we know for sure that the system is now projected into the ground state. If no photon is observed, well the system is still in the excited state.

OK. So we've discussed what happens when the system is initially in the ground, and when the system is initially in the excited state. But now comes the following question. We prepare the system in a superposition of ground and excited state. And we want to discuss what happens when the photon is observed? What happens when no photon is observed? I think if you observe the photon it's pretty clear we have to assume after photon emission the system is in the ground state.

But if no photon is observed, I want to give you three choices, and you should address them with the clicker. One choice is that the particle stays in the same state. The second choice is that the particle stays in a superposition state, but the probability to be in the excited state decays. Also no photon has been emitted, or no photon has been observed. And the third possibility is something else.

So in other words, assume you're an observer, and you know with 100% detection probability-- let's not discuss technical issues-- you have completely surrounded your system with perfect detectors. And you know in the time step  $\Delta t$ , in the time  $t$ , no photon was observed. And now you should make a prediction what happens next to the quantum system. And you make the prediction by assuming that the system is described by a wave function or density matrix. And I'm asking you, which of the three choices correctly describes what the system will do afterwards? What the system will do next?

Is the question very clear? Good.

[TAPPING]

OK. All right. Pretty good. A lot of people when I taught the class before said it's A, the wave function is not changing, because no photon has been emitted. Now in-- For those people, but there only few among those, I would have now asked the next question.

If you have-- If you have a 50-50 superposition, of ground and excited state-- And let's say the spot time for spontaneous emission is 10 nanoseconds-- But now you wait one second, and after 1 second, no photon has been observed. What is your prediction? In what state is the system at this point? Is the system in the ground state? Or is the system in, still in, a superposition of ground and excited state? Well since we have to clicker, you can tell me. Is it-- Is it still a superposition state, or is the system in the ground state?

OK. So now you have to help me out, because the people who said B, if they would go back to here-- And most people said it is B. If you put in  $\gamma = 10$  nanoseconds, the inverse of 10 nanosecond, and the time is 1 second, the excited state amplitude, the excited state mixture, is  $10^{-10}$ . So-- OK. If you want to be a mathematician and say--

[LAUGHING]

--there is epsilon 10 to the minus 10, yes. Then you can say there is still a small admixture to the excited state. But by making it so extreme-- 10 nanoseconds versus a second-- at least in all practical terms, the system is in the ground state. And I think this should teach you what it means if you have a system which is in the superposition of ground and excited state, and after 1 second it has not emitted a photon. I mean--

Then you would say, it had its chance. It had plenty of chances to emit, but it decided it doesn't want to emit. And that would mean your 50/50 superposition of ground and excited state means the atom decided that it's in the ground state. You should also realize a 50% superposition of ground and excited state means in half, in 50% of the cases there will never be a photon emitted.

So in other words, what you should realize is if your 50-50% superposition of ground and excited state, that the quantum evolution of this system is-- after a long time the system is definitely positively, absolutely in the ground state. It's always in the ground state after a long time. In 50% of the cases with emission of a photon, in 50% of the cases without emission of a photon.

If you have a radioactive-- ensemble of radioactive nuclei-- and let's say half of the atoms are in the excited state and [INAUDIBLE] and half are in the ground state-- and you send the sample to your friend, and your friend waits many, many, many half times, common sense tells you that all the particles are now in the ground state. Also only half of them have decayed, because the other half were in the ground state to begin with. I mean this is what quantum physics tells us. This is what a 50/50 superposition is.

But quantitatively this is, of course, included in this result-- which magically that almost all of you got right-- namely there is a superposition of ground and excited state, but the excited state amplitude decays. And to the limit, in the limit that the time is much longer than the decay time, no matter what the coefficient initially was in front of the excited state, this coefficient has decayed to 0.

Any question about that? Let me just emphasize that, again in giving you also an example in the reference, a 0 measurement.

A 0 measurement modifies the wave function. You can also put it like this, what the wave function is is the best knowledge you would have about this system. The wave function is a way to predict what happens next, and it's the most precise way to predict it. More accurate predictions than the wave function always cannot be made, because of Heisenberg's uncertainty relation.

But what happens is, if you have a 50/50% superposition of ground and excited state, and the system has not emitted, then you would say initially my guess was half of the atoms were excited, half of the atoms are in the ground state. But if none of them has decayed for awhile, you would say I revise my estimate now. Now I have to assume that more are in the ground state. Because having not decayed means there is a higher probability that the system has actually-- is in the ground state to begin with. So this is how this way of dealing with a wave function automatically adjusts for the knowledge you have gained about the system.

Let me give you another example which carries home the same message, and I take it from a pedagogical paper from Dickey, from American Journal of Physics, 49, 926, 1981. And what he discussed is the following. You have a box and originally your atomic wave function is completely localized. Your Bose-Einstein condensate if you want in this box, or let's just assume one atom to be more precise, and it's completely delocalized.

But now you focus a laser beam into the system. And the laser beam would ionize your atom, and you could count the ion with 100% probability. And for a short moment, you flash on the laser and the result is yes, you count. You get a count.

In that moment you would say my wave function is more localized. I revise my estimate. Well maybe I shouldn't say ionized. If it's ionized you destroy the atom. Let's just say you observe fluorescence so the atom is still alive. But now you have to say that the atom is localized in that region.

However, if you don't observe anything, you would say, well now it's actually more probable that the atom is outside. Because if it had been in the laser beam, with a certain probability, I would have detected a photon. But the non-detection of a photon means that I revise my estimate. And I say it's much more probable that the atom is outside the laser beam than inside the laser beam.

So this here is exactly how a non-observation of anything, a 0 measurement, modifies your wave function. And the formalism to incorporate that is what we have discussed before.

Yes? Cody?

**AUDIENCE:** So your arguments here so far work the same way as if it's in a wave function, you have just an entire Pascal probability, and we're updating our understanding of probability. Like you haven't included anything about the relative phase between these two--

**PROFESSOR:** I want to do that now. I mean, I-- This is sort of just to address the basic concepts about what does a measurement mean, what does a 0 measurement mean. But now I want to write down everything for you in amplitudes. We want to do exactly the time evolution of the system. Nancy?

**AUDIENCE:** Is this, like, inconsistent with [INAUDIBLE] quantum equation? Like especially the [INAUDIBLE], because when you are saying that it is admixture of the ground and excited state, and we did not observe--

**PROFESSOR:** Then the superposition say that ground and excited state. We are not starting out in an energy heightened state, so therefore, we-- what we have is not a sharp value of the energy, but an expectation value. And also if you repeat the measurement many, many times, the average energy is conserved, and this is exactly what energy conservation in quantum physics says.

**AUDIENCE:** [INAUDIBLE]

**PROFESSOR:** Well if your particle, if your system, is not in an eigenstate of the Hamiltonian. It doesn't have a sharp energy. And that would mean that when you measure the energy now, you have fluctuations. Sometimes you measure higher, sometimes you measure lower. It's only when you're in eigenstate that you measure a sharp value.

And therefore you know from the beginning that you will measure an energy distribution. And sometimes you measure higher, and sometimes you measure lower than the average value. There's nothing wrong about it, but your question is a very good one. You should-- I mean those examples are really-- On the one hand they are trivial, but on the other hand, it's very profound what they tell us about quantum physics and how to apply conservation laws and such.

OK. I think-- Let's-- Let me now formalize exactly how this is done with all the bells and whistles. We assume we have an initial wave function, which is now an arbitrary superposition state of ground and excited state. And we have the environment, which, in this case, we assume is the 0 photon state. It's a vacuum.

And we want to exactly solve the Schrodinger equation for that system. But we restrict ourselves too much, to a very small time step. The small time step is smaller than, you know, anything else. Than the natural decay time. Maybe the inverse [INAUDIBLE] frequency if you drive the system. You're not doing it here, but I will later show how you can add a laser beam and drive the system. Or it should also be smaller than the inverse tuning.

So what is very important here is that we want to deal only with simple cases, namely one photon has been emitted or not photon. So you want to make sure that there is, at most, one spontaneous emission event during the time delta t. So what I'm writing down now is the total wave function of the system plus the environment.

And now we can evolve it. We can ask what happens? What is the wave function time later? This can be exactly done by time-dependent perturbation theory. And the result is that the system will be in a superposition of ground and excited state. And we want to calculate the coefficients alpha prime and beta prime.

And we still have the vacuum state. But then we have the possibility that a photon has been emitted. In that case we are in the ground state. And the direct product with the environment involves now the photon emitted into a certain direction with wave vector  $k$ , with the polarization  $\epsilon$ . And we have coefficients  $\beta$ ,  $k$   $\epsilon$ , and we have to sum over all possibilities for the photon to be emitted.

So we call this-- So the wave function of the total system has now two parts. It's a wave function, which I call  $\psi_0$ . This is a wave function which involves no photon in the environment. And the wave function  $\psi_1$  involves one photon in the environment.

So this is the [INAUDIBLE], which seems very natural, but it's also-- you could immediately prove that these are the only possibilities, how the system can evolve. And we can verify this by using time-dependent perturbation theory.

It's actually almost everyone of you has seen it in either 8.21 or in a more basic course on quantum physics. It's time-dependent perturbation theory for the emission of a photon. But usually when you see those treatments there reservoir, the environment, is not treated as explicitly as we do it here. The theory where this is treated exactly in this way, how we need it, is the Viegener Biscoff theory.

Which is nothing else in the perturbative approach, but it's really a perturbation theory. Not just for the atomic system-- how we sometimes present it in a simplified version-- it's perturbation theory for the total wave function of the complete system. Philmore?

**AUDIENCE:**

So you mentioned the time interval [INAUDIBLE] is much smaller than a lot of things. But you were ignoring, I take it, the counter rotating terms? In which case we're still at a large enough time step that's average out, so to speak? I simply say this, because I expected to be an  $e$  with a photon term. From the  $g$  going up, so to speak.

**PROFESSOR:**

Yes. Well-- The counter rotating term-- The first answer I wanted to give you, no this is exact perturbation theory. But I think I get myself in trouble if I would allow-- I

would get myself in trouble if I would allow the time step to be extremely short, because then I'm in shorter than  $1/\omega$ . Because during the time  $1/\omega$ , we have-- you can say we have counter rotating terms. Or in other words, this particle in the ground state during a time  $1/\omega$ , particle in the ground state can emit a photon and reabsorb it. These are where those weird diagrams with virtual states, which we discussed earlier in this course.

So I think I want to assume here, which I haven't done, that the time step is larger than  $\omega^{-1}$ . And as you know the counter rotating term has a detuning  $\delta$ , which is  $2\omega$ , so therefore it is excluded. Or in other words, when we talk about photons sent into the environment, we want to talk about real photons, and not virtual photons. Yes, good point.

OK. So if you do simple lowest order time dependent perturbation theory, in the Viegener Biscoff approach, you get an exact result for beta prime. You find that beta prime in this superposition is the original amplitude beta, but it has decayed with  $e^{-\gamma t/2}$ . And since we are only interested in small time steps, we can do a linear expansion of that.

The probability,  $dp$ , that a photon has been emitted is the norm of this wave function  $\psi_1$ . And this, using Viegener Biscoff perturbation theory, is  $\gamma dt$  times the amplitude squared, that the system was excited to begin with. And because of the conservation of the norm, the wave function, the norm of the wave function  $\psi_0$ -- which is a wave function without a photon being emitted-- is  $1 - dp$ .

So what I'm telling you here is that this is an exact result of time-dependent perturbation theory. Often when this-- when textbooks treat spontaneous emission, they're more interested in getting Fermi's gold rule at this rate. But the same approach-- if you just write it down-- tells you how the amplitude in the excited state evolves. So therefore, what we learn from perturbation theory, that  $\alpha'$  and  $\beta'$ , the wave, the coefficients of the wave function, without emission of a photon, this evolution of the wave function occurs with a non-emission Hamiltonian.

And this non-emission Hamiltonian is our Hamiltonian for the atomic system. But then we have to account for spontaneous decay, and this is done by this non-emission part. So occasionally you may have heard that people wave their hands and say, your system is described by a Hamiltonian, which has an imaginary part for decay. And this is sort of phenomenological.

This is definitely not the case, because, even if you have a Hamiltonian like this, a pure state would simply decay and remain a pure state. What we are doing here explicitly is we deal with probability in the correct way. Every time the system can branch out into different possibilities, two different dimensions of the density matrix-- one has probability  $\delta p$ , one has probability  $1 - \delta p$ -- and it is only the wave function associated with probability  $1 - \delta p$ , which evolves with this Hamiltonian.

So what I'm telling you is the exact solution for the evolution of the total system, in terms of a density matrix for the atomic system. And this is exact. So that means we can now-- write down the-- Just get some extra space. Oops. How does it do it?

Nope So we have to insert new page. Yep. OK.

OK. So the procedure, how we implement this exact solution of perturbation theory, is the following. We have a time step  $\delta t$ . We compute what is the probability that a photon will be emitted. Then we need a ran-- Then we need a random number generator. So we need a number  $\epsilon$ , which is a random number chosen in the interval 0 and 1.

If this random number turns out to be smaller than  $\delta p$ , then we continue our time evolution on the computer. That  $\psi$  is now in the ground state, and maybe there is a laser beam which excites it again. And such I will add a few bells and whistles later. Otherwise  $\psi$ , our wave function, is now the wave function which is the time evolution with a non-emission operator of the original wave function  $\psi$ . And since we have a real wave function now with probability 1, we have to re-normalize the wave function by this denominator.

And then we execute the next time step. This means go to 2 and do the next time step. And then you have, so to speak, if you do it many, many times, you get a time direct trajectory of, so to speak, one experiment. And then you start again with your system in a wave function  $\psi$ , and you accumulate a second experiment. And maybe you do it 10,000 times to get enough statistics. And then you sum up, you know, everything you want and calculate all the expectation values you want to know about your quantum system.

So the claim is that this method, called quantum Monte Carlo wave function method, is fully equivalent to the optical block equations. And I want to prove it to you by showing that, if I take a density matrix, which is an ensemble average, over many realizations of those quantum Monte Carlo trajectories. That then this density matrix follows the differential equation, which is your optical block equation.

And the proof is shown here. So what I told you is the density matrix after time  $\Delta t$ , has now two matrix elements. One with probability  $\Delta p$ , and this is-- photon has been emitted. System is in the ground state, with probability  $1 - \Delta p$ . We evolve the quantum state with a non-emission Hamiltonian.

And then all what is done in the next few steps we assume that  $\Delta t$  is small. We do a Taylor expansion of the exponent. We neglect quadratic terms in  $\Delta t$ , and then we come to this line. And if we write this as  $\rho(t + \Delta t)$ , minus the original  $\rho(t)$ , we find that this follows differential equation, which is exactly the optical block equations.

So therefore what we sort of implemented as a form of doing many, many quantum measurements in the environment is a procedure, which is rigorously the same as the optical block equations, which we derived using a master equation approach.

OK. This method is very powerful for the following reasons. If you simulate a density matrix with, you know, an internal states, or external, internal states-- I should've

said with in quantum states, you need  $n$  times  $n$  matrix elements, which can become quite a memory hog for your computer. The wave function, at any given moment, has only  $n$  components. So therefore there is a computational advantage in using a stochastic wave function approach over simulation of the density matrix.

The second thing is that a lot of people, especially experimentalists, like sort of this approach, because it reflects directly what they do in the experiment. And I think it's pretty clear that with this approach you can deal with a great variety of situations. Let me just mention two obvious extensions. One is polarization.

A photon is detected. That means your random number produced a number  $\epsilon$ , which was smaller than  $\Delta p$ . At that point you can create a second random number, which determines if your photon has been detected with  $\sigma_+$ ,  $\sigma_-$ , or  $\pi$  polarization.

Or you can discuss recoil. If the photon is detected, you use-- you throw on another random function generator, which determines what the  $k$  vector of the photon is. So what direction each part  $k$  the photon has taken, and this determines now what is the recoil, the change in momentum of your atom. So you see, kind of, you can start with an atom at 0 momentum. You can see it emits a photon, and then your computer always makes a choice based on the random number. And then you say, OK my photon has now received a recoil kick at 45 degrees.

Now your wave function of the photon is such and such, and if you add a laser to the Hamiltonian, the recoil may have kicked-- may have Doppler shifted the resonance, but everything is easily taken into account. So you see this quantum Monte Carlo wave function method can easily be extended to describe external degrees of freedom, multiple laser fields, and all that. Any questions?

OK. Let me now just generalize the thought, but I think you know already everything about it. We talked about the master equation. We talked about the most general master equation in the [INAUDIBLE] platform, where those operators  $L$  are the jump operators. And the prominent example for jump operator was the signal minus

operator, which takes a particle from the excited state to the ground state. And this is the jump operator for spontaneous emission.

But you may have many jump operators. May be spontaneous emission of different photons with different polarization and such. Or the cavity may lose a photon, and then we have a jump operator for the cavity. We went through that.

Well that means now in an exact way that the non-emission Hamiltonian is the original Hamiltonian with an imaginary part, which comes because of those jump operators. And the general quantum Monte Carlo wave function procedure is that first you ask, has something happened? Has any jump happened? And this gives you the probability  $\Delta p$ .

And if-- If no jump has happened, you just do a time evolution with a non-emission Hamiltonian. But if a jump has happened, then the jump is now-- the wave function is projected by the jump operator. If you have a sigma minus operator, it takes a particle to the ground state. If you have several operators, a different jump operator may take your particle to another state. And you-- And you then have a branching ratio that you know first a jump has happened.

And then the question is, which jump has happened? And you just play the probabilities game. So that you see that the quantum Monte Carlo wave function method can be immediately be generalized.

So let me come back to the special case of spontaneous emission. In that case, we have only one jump operator, which is sigma minus. And the normalization is the square root of gamma. And that actually means that our quantum trajectory ground state, excited state, is very simple.

If you start with the system 100% in the excited state, it's very trivial what happens. Nothing happens. But if then the jump occurs, the particle is in the ground state. Then nothing happens then until infinite time.

You then have to start-- The next trajectory you start in the excited state. And this time, by chance of the random number generator, the jump happens later. Another

time the jump happens earlier. And what you then have to do is, you have to average, over all of those realizations, what is the probability for the particle to be in the excited state. And this is now your estimator for the excited state diagonal matrix element of the density matrix. And if you-- If you've written your code correctly, you will find that you get a wonderful exponential decay exactly as you have expected.

Questions? Now-- Yes? Let-- Let me now talk about dephasing. What I've shown you so far is how we can unravel the density matrix in many microscopic realizations. And I've given you a specific example. We assume probability for spontaneous emission, and with that we propagate our wave function.

But now I come to, sort of, the nitty gritty details, or the dirty truth, that what we have assumed is by no means unique. And I want to explain it to you first by reminding you of a very, very nice homework assignment you have solved. And this was about we have optical Bloch equations for the density matrix, and the dense -- and the solution of the optical Bloch equation is that we have population damping with a damping time  $t_1$ . And the off diagonal matrix elements are damped with a time  $t_2$ .

Remember if you've only spontaneous emission  $t_2$  is 2 times  $t_1$ . But we can have a lot of other processes, which can lead to much, much faster dephasing time than the population, than the time of population changes. And in your homework, you have discussed three possibilities.

One is, well, spontaneous emission is energy loss. But you have discussed three different possibilities for  $t_2$ . One-- Three different possibilities how dephasing, loss of coherence, and phase damping can happen. And in this homework assignment, you assumed either that there is a random phase, that the elastic collision which projects onto the excited state, and then you got the most crazy and artificial model. That every time, randomly, the phase of the excited state flips from plus to minus.

So if I would implement that now, with a quantum Monte Carlo method, it would have the following effect. And I hope you enjoy, sort of, the graphical representation. You can really think about it, that this is what happens. That this is

what inside-- what is inside the density matrices described by this process.

So let's assume we have a system, which would be in a superposition of ground and excited state. And that would mean that in the left frame the dipole moment would just rotate at the resonance frequency. It rotates, and it is a rotating dipole moment, which emits coherent light.

But now you assume that you have a random phase. So if you add random phases to it, maybe because you're fluctuating magnetic fields, then the line becomes sort of-- That doesn't look random, but you know what I mean. It becomes sort of jagged. The phase distribution is still sort of there, but there is a jitter on top of it. And as a result, the light emitted by this dipole is spectrally broadened

Well in your second model you assumed that-- with a certain randomness, with a certain time constant-- there's an elastic collision in the excited state, which projects the system into the excited state. At this moment there is no superposition state anymore, and the dipole moment is 0. So that's what you assume. Or when you have random phase flips, you assumed that suddenly this kind of data to data ministic sine function suddenly jumps corresponding to a minus sign in the excited state. And depending where you are in the cycle, it creates jumps at random places.

And the question of course is, if all those three processes-- and that's what you showed in your homework-- lead to the same density matrix, which one is correct? Which one is real-- is really realized in an experiment on a system which is described by this kind of damping, or by the optical block equation?

So you can say all or none. Well you can assume what you want, it doesn't make a difference. And the reason is actually profound. The reason-- The reason is profound in that sense that the way-- our goal was to have an open quantum system, which is the atomic system, interacting with a reservoir.

But the way, how we phrase the question, we are only interested in what the atomic system does. We didn't do extra measurements on the environment. The environment was just a dump for photons; a dump for energy; a dump for whatever

we assumed in our dephasing mechanism.

So let me just take the example of putting photons into the environment. And this is described by a certain damping term, but there is an ambiguity. And this is shown here. If you evolve the system-- our, our atomic system, the density matrix evolves, but the environment sort of also evolves. And for instance here, the unitary time evolution has taken the excitation from the atom, and we have emitted a photon into the environment. And you remember we got the optical Bloch equation by doing the partial trace here, and just focusing on the atomic part.

But now wait a moment. If we trace out the environment, we can trace it out in a different basis set. Remember, I showed you the quantum Monte Carlo wave function, we emit a photon. But we can, for instance, detect the photon in our gedanken experiment. We can detect it with linear polarization or with circular polarization.

If you have a situation where you have a-- an s state, which decays to a p state,  $\sigma_+$  takes you to  $m = +1$ ,  $\sigma_-$  takes you to  $m = -1$ . So therefore, if photon is emitted in your quantum Monte Carlo procedure, you would say, now the atom mean is in the  $+1$  state, or now the atom is in the  $-1$  state.

But if you detect linearly polarized light, by just putting a polarizer here-- and this is a unitary transformation in front of your detector-- you would no longer project the atomic system on  $+1$  at  $-1$ , you would project it on  $m = 0$  or whatever is connected to the linear polarization of the measurement.

So therefore, if you simply assume that something has been dumped in the environment, and can be used for measurement, there are many ways, many unitary transformations, what you can do to the information, to the energy, to the photons, which have been dumped into the environment. And each of them will lead to a very different trajectory in your quantum Monte Carlo system.

So therefore if you just dump the photons and not measure them, you have equal

rights to assume that your quantum Monte Carlo wave function jumps to states which correspond to a circular basis, or jump to states which correspond to linear basis. And there's many, many possibilities. But each of those possibilities is 100% correct unravelling of the density matrix. And if you just do it right, assume that the measurement is done in a certain basis, and you're consistent with it, you will 100% correctly describe the time evolution of your atomic system.

Any questions? Philmore?

**AUDIENCE:** Again with the dt. I'm just curious that we take a [INAUDIBLE] very short, but why don't you run into something like the quantum Zeno effect? Where if every evolution is initially quadratic, like the [INAUDIBLE] frequency, you take very short dt-- short measuring system-- Shouldn't for a choice of sufficiently short dt you, you know the simulation would give you strange results, because of--

**PROFESSOR:** [SIGHS]

**AUDIENCE:** --some sort of quantum Zeno effect there?

**PROFESSOR:** That's a very deep question, Philmore. And I, I want to think about it more, but I think I've excluded that by saying that the time step, dt, is larger than the correlation time of the environment. So I'm doing some kind of Markov approximation with the environment, where s-- the quadratic part of the behavior is a coherent time evolution, for very short time steps a wave function evolves quadratically, but this part is a coherent evolution.

And that's related to the fact that an atom can emit a photon, but in the very first moment, before the vacuum has transported it away, it can take the photon back. And the result of that is that at very short times the exponential decay doesn't start out exponentially, it starts out a little bit flatter. We get the exponential decay, we get Fermi's golden rule, and we get optical Bloch equations only if your time step is larger than the correlation time of the reservoir.

And the fact, you remember when we derived the master equation we had to say

we do a step, which is sufficiently small for the dynamics of the atomic system, but sufficiently large, that we are not getting into any memory effects of the reservoir. And we've done the same assumption here. Other questions? Nicky?

**AUDIENCE:**

Just confused. We are not always say the environment measures the system in range at time intervals,  $\Delta t$ , which are large compared to the correlation time? What's more [INAUDIBLE] the evolution of the atom. But now everyone isn't that defected the Markov approximation we've made when we derived the master equation? And I was just wondering for just-- [INAUDIBLE] did you derive it by making the master equation? Maybe we don't actually need-- Maybe we don't need the idea of constantly measuring. Maybe a physical interpretation of the Markov approximation.

**PROFESSOR:**

Oh yes, exactly, Nicky. I still think you said it really very, very nicely. We derived a master equation just by assuming that the system, you know, takes a photon. And past the correlation time, the photon is taken for good by the environment. And with a Markov approximation, we formalized that there is no memory effect, the photon is not stored like in a cavity. The photon has disappeared. And by saying that this time is very short, this was a Markov approximation in the derivation of the master equation.

But that also means, if the photon has disappeared, has separated from the atomic system, we are now free to make a measurement. And of course it shouldn't matter whether we make the measurement or not. But what I was able to do today is, I was making now the assumption, let's assume we make a measurement. We measure all the photons which have been emitted, and the measurement is probabilistic. And we fold this probabilistic evolution into our quantum system. And what we obtained was exactly the same time evolution for the density matrix as we got from the master equation.

So in other words, this should you that interactions with an open quantum system, where irreversibly energy, photons, angular momentum, or whatever-- flows into the environment. Once it has flown into the environment, you can measure it. And you

get all the stochastics from the measurement. But even if you don't measure it, you get exactly the same stochastics as if you had measured it. It's all the same. Jenny?

**AUDIENCE:** Now that I think about it, it seems sort of weird to me that we've-- that we're making these measurements, or lack of measurements, these interactions, at regular intervals. And not--

**PROFESSOR:** It doesn't really matter. All we-- All we have to make is-- You could actually make  $\Delta t$  a random variable. It wouldn't change anything. The only thing we have to make sure is we have to make the time interval short enough that we don't have, maybe, two photons emitted in that time. We just want to make sure that it's a simple probabilistic branching, yes or no. And that's the only requirement here.

**AUDIENCE:** Is this a formula or is it based on time? You say that would be the wave function evolving and then collapse. And that's-- This is what-- Where the measurement comes in. The equivalent, so now say, the equivalent is a wave function evolved in a collapse, when you make a measurement you say that after it evolves. So is it possible that it could also have-- like evolves some kind of formalism? Like this? Where there is an operator? Because still like even though the density matrix operator, maybe it is kind of like-- [INAUDIBLE] describes a state.

**PROFESSOR:** I haven't seen it, Mark, but I'm absolutely certain that you could describe the same physics in the Heisenberg picture, where the time evolution is with operators. Because what we have here is, we have a time step,  $\Delta t$ , where the system evolves as an isolated quantum system, and then we measure again. And so, I think if you would use operator equation, you would have an evolution of the operator with the same Hamiltonian, which is non-emission Hamiltonian. And then the measurement would do some form of projection.

I have to think about it, what the projection would be in terms of operators. But my gut feeling is, you can always take the transformation where you put the time dependence into the operators, and not in the wave function.

On the other hand, I have some little bit misgivings about that, because the quantum Monte Carlo wave function was really developed in order not to deal with matrices, not to deal with something which is dimension  $n$  times in, if  $n$  is the number of components of the wave function. It was specifically formulated to have the simpler description with  $n$  coefficients for the wave function. But conceptually, I think, it is evolution with a Hamiltonian measurement. Evolution with a Hamiltonian measurement. And I assume this could also be done with operators. Nancy?

**AUDIENCE:** Suddenly like [INAUDIBLE] but when we've-- these simulations are actively done, how important is the randomness? Like up to epsilon [INAUDIBLE] because no computer is actually emitting random numbers.

**PROFESSOR:** Well I think how random a random number has to be is really dealt with in computer science and mathematics.

**AUDIENCE:** But due to our reserves we always get this exponential behavior?

**PROFESSOR:** I don't know the answer. I mean here, conceptionally, it should be completely random number. And I think that algorithms, which even which produce pseudo random numbers, but if the pseudo is close enough, if there is a recurrence time of your random number-- if your random number-- your series of random number repeat itself after several billion random numbers, this gives you a small error bar. And if you don't-- If you'd only do a limited sampling, a limited number of time trajectories, I don't think it matters. Of course if you want to have ultimate precision, then also the precision of the random number may enter through the backdoor at some point.

**AUDIENCE:** [INAUDIBLE] lack of simulation of the photons emitted? But if we know the photons emitted, if we have that information, then we can decide [INAUDIBLE].

**PROFESSOR:** That's correct. If we-- If we would know-- If we would know more about the environment, if we would say we measured the photons in a certain basis, or when energy is dumped in the environment by a dephasing mechanism, we look at the environment. Then, of course, we would add extra information to it, and then certain

quantum trajectories would reflect the extra knowledge we have. And of course, we would then describe everything in this basis.

On the other hand, what you should learn from this is once the information, once the photon has escaped, it doesn't matter for the time evolution of your atomic system, in which basis you measure the photon. So the evolution of the atomic system itself-- at least when you averaged-- is unaffected by the basis.

However if you make a coincidence measurement, that you say your atoms which has emitted, is still flying through your vacuum chamber, and now you figure out the photon is emitted as circularly polarized light. Then of course you know that this atom, which is still available, has emitted circularly polarized light. And then you have actually obtained extra information about your atom.

In other words, the photon in the atom was entangled, like a Bell pair. And if you now do a measurement on one part of the Bell pair, you know more about the other part. But this is just how quantum physics works. If you don't use this information for anything, then you could have-- you could have as well not measured the polarization. And it would have no effect on the atomic density matrix.

OK that's it for today. We have class at the usual time on Wednesday.