ROBERT FIELD: Last lecture, I did a fairly standard treatment of the harmonic oscillator, which is not supposed to make you excited, but just to see that you can do this. And the path to the solution was to define dimensionless position coordinate, and then you get a dimensionless Schrodinger equation. And the solution of that involves two steps. One is to insist that the solutions to the Schrodinger equation have an exponentially damped form.

And then the Schrodinger equation is transformed into a new equation called the Hermite equation. You shouldn't get all excited about that-- the mathematicians take care of it. And so the solutions to this Hermite differential equation gives you a set of orthogonal and normalized wave functions. They give you the energy levels expressed as a quantum number plus 1/2, times constant.

The energy levels with the quantum number v are even or odd in v, and they're even or odd in psi. Even v corresponds to even psi. V is the number of internal nodes, and there are all sorts of things you can do to say, well, I expect if I know how to do certain things in classical mechanics, they're are going to come out pretty much the same way in quantum mechanics. So that's the standard structure, but more importantly, I want you to have in your head the pictures of the wave functions, the idea that there is a zero point energy, and that there's a reason for that-- that the wave functions have tails extending out into the non-classical, or the classically forbidden region.

And this turns out to be the beginning of tunneling. You'll be looking at tunneling more specifically. I also want you to know how the spacing of nodes is, and that involves generalization of the bright idea that the wavelength is h over p. But if the potential is not constant, then p is a function of x. This is not the quantum mechanical operator, this is a function which provides you with a lot of intuition.

And then if you know where the node spacings are, and you know the shape of the envelope, you have basically everything you need to have a classical sense of what's going on. And then-- I guess it's supposed to be hidden-- I did a little bit of semiclassical theory, and I

showed that if you integrate from the left turning point to the right turning point at a given energy of this momentum function, you get h over 2 times the number of nodes. And this is the semiclassical quantization-- it's incredibly important, and it's useful either as an exact or approximate result for all one-dimensional problems. And so it tells you how to begin.

Now, before I start talking about what we're going to do today, I want to stress where we're going. So we're going to be looking at some exactly solved problems. And so we have a particle in a box, the harmonic oscillator, the hydrogen atoms-- you have to count them-- and the rigid rotor.

Now, all of these problems have an infinite number eigenfunctions, an infinite number of energy levels, and that's intimidating, but it's true. Now, these infinite number of functions are explicit functions of the quantum number. And so we have an infinite number, but in order to describe systems, we're going to be calculating integrals.

We're going to be calculating a lot of integrals between these infinite number of functions. So we have an infinity squared of integrals. Well, that shouldn't scare you because what I'm going to show you is that all of the integrals that we are going to encounter are explicit functions of the quantum numbers, and they have relatively selection rules. In other words, which integrals are non-zero based on the difference in quantum numbers between the left-hand side and the right-hand side?

So we're collecting these things in order to calculate a whole bunch of stuff. Now, I told you that this is a course for use rather than philosophy or history. And so if you encounter any quantum mechanical problem, you'd like to be able to describe what you could observe with it. And so if you're armed with the infinite number of energy levels and eigen solutions for our problem, you can calculate any property.

So you define some property you're interested in-- there is a quantum mechanical operator that corresponds to that property. And in order to be able to describe observations of that property, you need to calculate integrals of that operator. Well, la dee dah.

That should be intimidating, but it's not because almost all of these integrals can be expressed as a simple constant times a function of the quantum numbers or the difference of quantum numbers, and that's a fantastic thing. So we have any operator-- suppose the Hamiltonian is an exactly solved problem plus something else, which we'll call h1. And this is a complexity in the-- or it's the reality in the problem.

And in order to deal with this, again, you're going to need to calculate integrals of this operator. And the last thing that's really going to be exciting is once we look at the time dependent Schrodinger equation, we're going to get wave packets. And these are functions of position and time, and these wave packets are classical-like, localized objects that move following the Newton's equations of motion with the center of the wave packet.

And again, there are a whole bunch of integrals you're going to need in order to do these things. And so right now, we're starting with the best problem for these integrals, because a harmonic oscillator has some special properties. And the lecture notes are incredibly tedious, and they're mostly proofs. And I'm going to try to go fast over the tedious stuff, and give you the important ideas, but since there is some important logic, you should really look at these notes.

So what we're going to be doing today is we start with the coordinate momentum operators, we're going to get these operators in dimensionless form, and then we're going to get these a and a-dagger guys. So this step is reminiscent of what I did at the beginning of the previous lecture, and then this is magic because this magic enables you to just look at integrals and say, I know that integral is zero, or I know that area is not zero. And with a little bit more effort-- maybe something that you'd put on the back of a postage stamp-- you can evaluate that integral, not by knowing integral tables, but by knowing the properties of these simple little a and a-dagger.

And that's a fantastic thing. And it's so fantastic that this is one of the reasons why almost all problems in quantum mechanics start with a harmonic oscillator approximation, because there is so much you can do with this a and a-dagger formalism. Now, at the beginning I also told you that in quantum mechanics, the important thing that contains everything we're allowed to know about a system is the wave function.

But I also told you we can never measure the wave function. We can never experimentally determine it, and so we need to be able to calculate what this wave function does as far as what we can observe, and these a's and a-daggers are really important in being able to do that. So I'm going to start with covering what I did in the notes, but I'm going to jump to final results at some point-- governed by the clock.

And so the first thing we're going to do is these. And so what we do is we define the

relationship between the ordinary position coordinate. And this little twiddle means it's dimensionless, and so we can write the inverse of that. And that's the one we are going to want to-- well, actually, we go both ways.

And we do the same thing for the momentum-- p is equal to h-bar mu omega square root, p twiddle and the inverse which I don't need to write. And finally, we get the Hamiltonian, which is p squared over 2 mu plus 1/2 kx squared. And we'll put that into these new units.

So we have h-bar mu omega over 2 mu, p twiddle squared plus k over 2. This is all very tedious, but the payoff is very soon. k over 2 times hr mu omega, x twiddle squared. Oh, isn't that interesting? We can combine-- we can absorb a k over mu in omega, and so we get, actually, a big simplification.

We get h bar omega over 2 times p twiddle squared plus x twiddle squared. Well, that looks simpler. And so the next thing we do is-- it looks like a simple problem from algebra, let's factor this. Now, it's a little tricky because you know you can factor something in real terms if this is a minus sign. But we are allowed to talk about complex quantities, so we can factor that.

And so this term, p twiddle squared plus x twiddle squared is equal to ip twiddle, plus x twiddle times minus ip twiddle, plus x. And you can work that out-- that ip times minus ip is p squared, and x times x is x squared. And then we have these cross-terms, ip times x and x times minus ip.

Whoops, they don't commute. If this were algebra-- well, they would go away, but they don't. And so what you end up getting is p twiddle squared plus x twiddle squared, plus i times p-- I'm going to stop writing the twiddles. So we have this.

I want to make sure that I haven't sabotaged myself-- that's going to be-- yeah, that's right. So we have something here that isn't zero. And it looks like i times the commutator of p twiddle with x twiddle. But we can work that out because we know the commutator of p ordinary with x ordinary.

And so I did that. And so we have this commutator, p twiddle, x twiddle. After some algebra, we get plus 1. A number-- pure number-- no? I want you to check my algebra.

So you just substitute in what this is in terms of ordinary p and the ordinary x. Use a commutator for ordinary xp, which is ih-bar, and magically, you get plus 1. So this very strange and boring derivation says, OK-- well, let's now give these two things names.

This guy, we're going to call as the square root of 2 times a, and this one is going to be the square root of 2 times a-dagger. So H is going to be h-bar omega over 2, times square root of 2a-hat times the square root of 2a-dagger-hat minus 1. Remember, when we factored it, we got this extra term which was 1.

And in order to make it correct, we have to subtract it away. And so this becomes h-bar omega, a-dagger-hat minus 1/2. Well, isn't that nice? Now, we have the Hamiltonian expressed as a constant, which we know is important because it's related to the energy levels, and times these two little things, which turn out to be the gift from God. It's an incredible thing, what these do.

So we have gone through some algebra, and we know the relationship between a, and the x and p twiddles, and similarly for a-dagger. And we can go in the other direction, and we know the commutator, and now we're going to start doing some really great stuff. Well, one thing we're going to want to know about is a-hat. a-hat, a-dagger, that commutator-hat. And that turns out to be-- well, I already derived it-- it turns out to be plus 1.

And as a result, we can say things like this-- a a-dagger-- So using this trick, we can show we can always replace something like a, a-dagger by a-dagger a plus this commutator, which is 1. And so we have this really neat way of reversing the order of the a's and a-daggers.

So with this, we're going to soon discover the a operating on the eigenfunction gives square root of v times psi v minus 1. And a-dagger operating on this wave function gives v plus 1 square root of psi v plus 1. Which is the reason these things are valuable, because if you have any eigenfunction, you can get all the others.

So suppose you have the lowest eigenfunction-- you apply a-dagger on it as many times as you need to get to, say vth function. So you don't actually-- you're not going to be evaluating integrals, you're going to be counting a's and a-daggers, and permuting them around, and getting 1's, and stuff like that. Yes?

AUDIENCE: In this line with the commutator, you didn't move the dagger.

ROBERT FIELD: I didn't what?

AUDIENCE: For a, a times the square root of a a-dagger plus a-dagger a, it should be a a-dagger. And on the right-hand side, you need to move the dagger.

ROBERT FIELD: OK, so this is to switch the order, and I've done that. And that then is-- no, I think-- wait a second. So we have a a-dagger-- so that's a a-dagger minus a-dagger a, and that's-- oh, yeah. Thank you.

It's very, very easy to get lost, and once you're lost, you can never be found because you've made a mistake that's built into your logic, and you're never going to see it. You see it took me a couple of minutes to even accept-- that the insight from my TA who's sitting there calmly thinking, and I'm trying to do several things in addition to the thinking. So we can do things like this. Suppose we have psi-- I can't use this notation yet.

So suppose we have psi-star v, and we have a-dagger, a-dagger, a-dagger, psi, v prime, dx. These are raising operators, so this is going to take v prime to v prime plus 3. That's the only integral that's not 0. And we get v prime plus 1, v prime plus 2, v prime plus 3, square what? It has the constants.

And this would be v prime plus 3. So instead of evaluating an integral, looking at what the x's and p's are, we just have a little game we play. So now, we have to prove some of the things I've said. So we have h, and we're going to operate on a-dagger psi v.

So what does the Hamiltonian do to this thing? So what we're going to want to do is to show that this thing is an eigenvalue-- eigenfunction of v plus 1, and that's what we are going to get. So let's just go through this. So we have h-bar omega, a-dagger a plus 1/2, times psi v.

So what I did is-- where did I-- yeah, I showed that the Hamiltonian-- or did I not do that yet? Oh, yeah-- I did it right here. The Hamiltonian is h-bar omega, a a-dagger minus 1/2, or if we reverse these, it's equal to h-bar omega, a-dagger, a plus 1/2.

So we can use either one, so I'm using that one-- except I wanted an a-dagger here, because we want to show what the Hamiltonian does to this. Now, we can pull in a-dagger out to the right, because this-- if it's 1/2 times a-dagger, well, that doesn't matter.

This a-dagger, a, a-dagger-- well, we can pull this a-dagger out. So we have h-bar omega, a-dagger is equal to a a-dagger plus 1/2-- so iv. Now, we use our magic commutator trick to replace this by a-dagger a plus 1. So now, we have h-bar omega, a-dagger, and we have a-dagger a plus three halves is iv.

Well, this is Ev plus h-bar omega. We've increased the number that started here. Here is Ev--

that was Ev plus 1. And so now, we have no operators in here, and we can stick the a-dagger back here. And so we have h-bar omega, Ev plus 1, a-dagger

Well, what do we have here? We have an operator, we have this function, we have some constant times the same function. So what we've shown is that this thing is an eigenfunction of the Hamiltonian that belongs to the eigenvalue Ev plus 1. We've increased the energy by 1.

So what we have-- so we can show that we apply a-dagger to any function-- we increase its energy, and we can do this forever. We could also do a similar thing if we apply a to psi v. We can go down, but at some point, we run out of steam because we've gone to the lowest energy, and if we go lower, we get 0. So a operating on psi min gives 0.

So we have this stack of energy levels and wave functions, and we have the same stack being repeated as we go down, but this one has an end. We bring back what a is, and so a psi min is 0-- that's the equation. We bring in what a is, and it's ip twiddle x plus x twiddle.

So we do some algebra, and what we end up with is a differential equation, psi min. dxx twiddle is equal to-- again, a little bit more algebra-- minus mu omega over h-bar times psi min. So what function gives-- there's an x in here too. So what function has a derivative, which is the function you had started with, times the variable, times a constant?

And so the answer to that is that psi min has to have the form-- some normalization factor times e to the minus m omega-- or mu omega-- sorry-- over 2 h-bar x squared-- a Gaussian. Well, it had to be a Gaussian, right? We know when we did the algebra that we're going to get some function times a Gaussian. But for the lowest function, the Hermite polynomial is 1, and all there is is the Gaussian.

And so we found the lowest level, and we can normalize it. So let's start over here. So what we have found is psi min of x is equal to mu omega over pi h-bar to the 1/4 power, e to the minus mu omega over 2 h-bar squared.

Well, that's useful. We knew that, but this time we got it out of a completely different path. And now, we can get all higher v by a-dagger, a-dagger, et cetera. So remember, we don't care anything about what the function is, we just know that we can bring it in and get rid of it at will, because what we want is the values of integrals involving that function and some operator.

So yeah, we can have all of those functions, and this is a way of generating all of the functions.

And so if we wanted psi v, we would do a-dagger to the vth power divided by v-dagger-- v-- what do you call this with an exclamation point? Factorial-- ha! So we apply this operator that raises us to whatever level we want starting from this Gaussian at the bottom, and we have this normalization factor which cancels out the fact the stuff that you get by applying av.

Now, there is some more logic in my notes, and I don't want to do that, but what we'd like to be able to show is that a-dagger on psi v gives some constant, and that this constant has some value-- we're going to evaluate what it is. And similarly, a psi v gives dv, and some constant v minus that. We can derive those things, and I'm not going to waste time deriving them-- I'm going to just give you the values.

But we already know that cv is square of v plus 1/2-- e plus 1 and dv-- and you can see the derivation in my notes. I don't think going through them is going to be instructive. And that's just going to be v and 1/2. So now, we have something that's wonderful, because everything you need to know about getting numbers concerning harmonic oscillator is obtained from these five equations. a-dagger on psi v is v plus 1 square root psi v plus 1. a on psi v is v square root psi, v minus 1.

I've said this before, but these are the most useful things you'll ever encounter. We have this thing called the number operator, and that number operator is a-dagger-hat, and the number operator operating on psi v gives v psi v. And so that's a kind of benign operator that can suck up all sorts of factors of a-dagger a, because it just gives a useful thing. And then we have a, a-dagger, and this is 1.

Well, you sort of know it's going to be 1, because a a-dagger gives an increase-- it gives v plus 1, and a gives v minus 1. So it's plus 1, not minus 1-- you know that it's hardwired. Well, I did it-- I got to the point where it starts to get interesting.

So we're going to be using this notation, a-dagger and a, for all sorts of stuff. And one sort of thing is transition intensities and selection rules. So you have a harmonic oscillator. A harmonic oscillator is, say a diatomic molecule which is heteronuclear.

And so as the molecule vibrates, you have a dipole moment which is oscillating. And so any oscillating electric field will grab a hold of that dipole moment and stretch or compress it, especially if that field is in resonance with h-bar omega. And I've got some beautiful animation showing this, but we can't do that until we have time dependent quantum mechanics.

So we have a time dependent radiation field, which is going to interact with the dipole associated with the vibrating molecule, and it's going to cause transitions. And so we can write the quantum mechanical operator that causes the transitions-- this is the electric dipole moment operator-- as a function of coordinate. And we can do a power series expansion of this, and we have-- so we have mu 0-- the constant term-- the first derivative of the dipole with respect to x, and the second derivative of the dipole with respect to x. And we have the x cofactor and the x squared cofactor.

And so this guy doesn't have any x on it-- it's a constant. The only integrals involving-- the only integrals are delta v, v prime following the selection rule delta v v prime. So these integrals are 0 unless v and v prime are the same. And that says, well, an isolating field isn't going to do anything key to it, it's just going to leave it in the same vibration level. But it might have an electric Stark effect, but that's something else.

So this term does nothing as far as vibration is concerned. This guy, which is a plus a-dagger, has a selection rule, delta v of plus and minus 1, and this guy has a selection rule, delta v of plus and minus 2 and 0. So if we're interested in the intensities of vibrational transitions, it says, well, this is the important term and it causes transitions, changing the vibrational quantum number by one, which is called the fundamental. This gives rise to overtones.

So all of a sudden, we're in real problem land, where if we're looking at vibrational transitions in a molecule, that this enables us to calculate what's important, or to say these are the intensities I measure, and these are the first and second derivative of the dipole moment operator as a function of internuclear distance. Isn't that neat? I've gone so fast, I'm more or less at the end of my notes, but I can blather on for a while.

So suppose you have some integral involving an operator and a vibrational wave function. So we have psi v star, some operator, psi v prime dx. And we'd like to know how to focus our energies. We're very busy people-- we don't want any value integrals that come out to be 0, we'd like to just know.

So if this operator is some function of x or function of p, we'd have a power series expansion of the operator, and we then know what the selection rules are. So usually, you look at the operator and you find that it's a linear quadratic cubic function of x-- the leading term is usually linear. Bang-- you have a delta v of plus 1-- selection rule.

Or if someone has bothered to actually convert the operator to some form-- oh, it's the

operator-- this might have some form, a-dagger cubed times some constant. So if the operator looks like a-dagger cubed, we know that the selection rule is v to v plus 3, and we know that the matrix of the integral is v plus 1, times v plus 2, times v plus 3, square root of that, times the constant. So there is a huge number of problems that, instead of being pages and pages of algebra, are just reduced something that you can tell by inspection.

So one of the tricks is we have an operator like x squared or x cubed-- what we want to do is write this in terms of a squared, a-dagger squared, and maybe some combination of a-dagger a. So we want to take the a-dagger a's with the a a-daggers and combine them using the commutation rule. And then we have expressed this in this maximally simple form, and then you just apply a squared, apply a-dagger squared, and you apply this, then you've got the value of the integral.

So if you're a busy person and you want to actually calculate stuff, you want to know how to reduce operators-- usually expressed as some power of the coordinate or the momentum-- into a sum of terms involving these organized products of a's and a-daggers. And you're going to be absolutely shocked at how perturbation theory-- which leads to basically all of the formulas and spectroscopy-- it's an ugly theory, but it reduces everything to things that you can just write down at the speed of your pen or pencil, and that's a fantastic thing.

So you can't do this with the particle in a box, you can't do this with a hydrogen atom, you can't do this with the rigid-- well, you can do some of this with a rigid rotor. But the harmonic oscillator is so ubiquitous because every one-dimensional problem is harmonic at the bottom. And so you can use it and then you can put in the corrections. But also because you want to describe dynamics, you almost always use the harmonic oscillator, because not only do you know the integrals, but you know there's only a few.

Normally, you're going to be summing over an infinite number of quantum numbers, and that takes time, and it takes judgment to say, well, only certain of these are important. But for the harmonic oscillator, the sums are finite. All of these things are wonderful, and that's why whenever you look at a theory, you're going to discover that hidden in there is the harmonic oscillator approximation, because everything is doable in no effort.

And sometimes when you look at a paper like that, it doesn't show you the intermediate steps, because everybody knows what a harmonic oscillator does. And there's also a lot of insight because something like this-- this is an odd symmetry term, this is an even symmetry term,

and there are all sorts of things that have to do with, are you're conserving symmetry or changing symmetry?

And sometimes, the issue is how does the molecule spontaneously change symmetry by doing something interacting with a field, or interacting with some feature of the potential surface. So this is a place where it's labor saving and insight generating, and it's really amazing. So maybe I've bored you with this, but this is the beginning of almost every theory that you encounter just because of the simplicity of the a's and a-daggers. OK, I'm done. Thank you.