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**PROFESSOR:** Very good. So today, we'll begin with a study of one dimensional potentials and the energy eigenstates or properties. And we'll discuss this for about half of the lecture. And then go into the variational principle. So let me go back then to our discussion of last time, where we were talking about energy eigenstates and the Schrodinger equation in one dimension.

So there's a term that we use all the time. This term is called the bound state. And bound state seems something sort of very non-trivial. But mathematically, we can say quite clearly what it is. A bound state is something that is not spread all over space, basically. And the way we therefore use the terminology for bound state it that we only speak of bound states when there are energy eigenstates. So an energy eigenstate may or may not be a bound state, but any bound state is an energy eigenstate.

So an energy eigenstate is a bound state if the wave function goes to zero when you go sufficiently far away. So it's a simple definition, but it helps us understand that the basic idea is at the state is just not spread all over the world. Now remember we're trying to find energy eigenstates, and that is to find wave functions, time independent wave functions, that solve the time independent Schrodinger equation. Which I have written there for convenience. This is the same equation we wrote last time.

For a time independent potential, so that the full wave function can be written as a phase that contains the information of the energy times a function of  $x$ , sine of  $x$ . That still may be complex, but it doesn't have to be complex. As you can see, this is a real equation.

Now in order to clean up some of the constants in this equation, it's-- yes?

**AUDIENCE:** Why is it not  $V \times$  minus  $e$ ?

**PROFESSOR:** Well you have to look back at the Schrodinger equation, and bring the things to the other side, and take care of the signs. It is correct as stated. Check it. Now we have, in order to do this and just to write things with a little more clarity, we scale the energy. So we define a calligraphic energy, which is  $2m$  over  $h$  squared times energy  $E$ . And a calligraphic  $V$  with the same scaling factor.

So that the Schrodinger equation then takes the form-- this same equation-- sine. And I'll use the double prime notation for two derivatives. Plus now  $E$  minus call of  $x$  sine equals zero. So this is how our equation looks. It's relatively simple. And can be treated without carrying constants all over the place.

Now we're going to discuss a few results that are extremely important that you keep in mind for the future. It helps you think clearly. So these results are little theorems that I'm going to state. And the proofs are given in the notes. I will skip some of the proofs, although I will tell you what the strategy is for the proofs and then show how the theorem implies, as a corollary, interesting things that could easily be misconstrued.

So let me give you the first theorem. Theorem one. This is just the statement that if you are talking about bound states in one dimensional potentials, there are no degeneracies. So let's write it. There is no degeneracy for bound states of one dimensional potentials. So it's a fundamental result. We'll see some way to understand it a little later. And you have seen this in 804, I believe.

So what is a strategy to a proof? So we want a rigorous proof. So what is a strategy? I will not go through the proof. The strategy is to assume there is a degeneracy. So strategy, assume a degeneracy. So sine 1 and sine 2 different with the same energy. And then you write this equation for sine 1 and sine 2, and they have the same energy.

Then you take the two equations, and you multiply the first by something, the

second by another thing. Subtract it. Do a bit of algebra. And you suddenly can prove that one solution is equal to a constant times the other solution.

So you do the work, and that's what comes out. Once you've shown that one is proportional to the other, we've declared in quantum mechanics that two wave functions that differ by a constant have exactly the same physics. You can normalize it, and normalize them. And the constant can be just a phase, but the phase doesn't matter. So those two wave functions are really the same.

So you get a contradiction. You thought they were different. But the difference is just too trivial, and therefore they are really the same wave function. Because we've said that two wave functions that differ by a constant should be identified. So that's this theorem. And it's a key theorem.

Let's go to the next theorem that is also important. So theorem two. Energy eigenstates  $\psi(x)$  can be chosen to be real. So here it is. We mentioned that this differential equation allows for real solutions. There's no contradiction, because there's no  $i$  in there. But now we say more. That even if you find a complex solution, you can work with real solutions.

So what is the strategy here? Again strategy. To have you get a complex solution.  $\psi(x)$ . And then you go about to prove that actually this complex solution implies the existence of two real solutions. So this complex solution implies existence of two real solutions. And moreover, two real-- I should say it better here-- degenerate solutions. How could you prove that?

Well, it probably would occur to you that you would take a solution and say, oh, this solves it. Then you would show that  $\psi^*$  also solves this equation. And then by linearity of the Schrodinger equation, you could form what we would call the real solution formed by taking  $\psi + \psi^*$  and adding them. Or the real solution that comes from the imaginary part.

You see the real and imaginary parts of a complex number are real. So is the case here as well. That they can take  $\psi$  and  $\psi^*$  that are different. And the sum is

real by construction. You put the star, and recalling that star of star gives nothing, you see that this function is equal to its star. So it's real. So is this one.

This function, which is the imaginary part of the solution that you had, is also real. So you get two real solutions. Moreover, you can show that sine and sine star have the same energy. Therefore sine  $r$  and sine  $m$  have the same energy. So I'm really skipping very little. But I don't want to clutter the blackboard with the whole derivation at this moment.

So here is the strategy. A complex solution implies two real solutions. And therefore, since you have real solutions, you can always choose them to be real. No loss of generality. You had a complex solution. You say, I like just real solutions. And you chose your two real solutions. You give them. You've given the whole thing.

But then there is a nice corollary for the case of one dimension bound states. So this is the part that is perhaps somewhat interesting. And the corollary is that if you're talking bound states of one dimension, any solution is equal to a real solution up to a constant. You may say, well what's the difference? Let's write it down and look at it.

Corollary for bound states of one dimensional potentials. Any solution is, up to a phase, equal to a real solution. So how does that go? Maybe we can use more of this blackboard.

Why would any solution be, up to a phase, equal to a real solution? OK. Suppose you have these two solutions here. Well this is real, so that's trivially true. And this is real. But what if I put a linear combination of them? Or take the original complex solution? Why would it be, up to a phase, equal to a real solution? The answer is the following. Because of theorem and, that there's no degeneracy, you've got two solutions that claim to be different and degenerate. But that can't be.

So by theorem one, you must have that-- in the notations, I have here-- sine imaginary of  $x$  must be equal to a constant times sine real of  $x$ . Now if these function's anyway are real, the constant here must be real. Therefore, even if you

form the original complex solution,  $\psi$ , which is  $\psi_{\text{real}} + i \psi_{\text{imaginary}}$ . You can check that. It's clear by definition that that's the way it should be.

If you think this, this is equal to  $1 + i c \sin \theta$ . Therefore this is equal to a constant times the phase of-- this is a complex number. So this is yet another constant that we could say, the norm of  $1 + i c \sin \theta$  times  $\sin \theta$ . So you see that any solution, any linear combination, in fact, with any numbers of  $\psi_{\text{real}}$  and  $\psi_{\text{imaginary}}$ , will be a constant times a phase times this thing. So it is really just real anyway.

So you can just have one solution. And any solution that you may write, that represents a bound state, is, up to a phase, equal to a real solution. OK. So that's our theorem two. Theorem three. It's also very famous. If the potential  $V$  of  $x$  is even-- that is,  $V(-x) = V(x)$ -- the eigenstate can be chosen to be even or odd under  $x \rightarrow -x$ .

OK. So here is another claim. So the potential is even. There's no theorem for all the potentials. No clear theorems, no simple theorems for all the-- but if the potential is even, the claim is that you can choose eigenstates to be even or odd. The word chosen is very important here. Otherwise, this would not be a precise statement. You cannot say the eigenstates are even or odd. You can choose them to be.

So how does the proof go? Strategy begin with a wave function,  $\psi(x)$ , that is neither even nor odd. And then you do a little work with the Schrodinger equation. Take the Schrodinger equation, change all  $x$ 's to  $-x$ 's and show that, in fact, not only is  $\psi(x)$  a solution, but  $\psi(-x)$  is also a solution. With the same energy.

So prove that  $\psi(-x)$  is a solution with the same energy. And in this case, of course, we can already have shown that we can choose these wave functions to be real. So we can choose all of these wave functions to be real. And what do we do next?

If we have these two solutions with the same energy, then you can build of sine  $s$ , which is  $1/2$  of sine of  $x$  plus sine of minus  $x$ . And of sine  $a$ .  $s$  for symmetric, and  $a$  for anti-symmetric. And of sine  $a$ , that is  $1/2$  of sine of  $x$  minus sine of minus  $x$ . And this tool would be this even, under the exchange of  $x$  for minus  $x$ . This one odd, under the exchange of  $x$  for minus  $x$ .

And both would be solutions by superposition. And both would have the same energy. So that's the end of the theorem because then these things are even or odd and have the same energy. So the solutions can be chosen to be even or odd under  $x$ . So if you've proven this, you've got it already. But now we get the corollary.

For bound states in one dimension, the solutions not anymore the word chosen. We can delete the word chosen. The solutions are either odd or even. So it's a lot stronger. It's not anymore, you can choose them to be, but a general one is neither odd nor even. No. You try to find the solution that is neither odd nor even, and you can't find it. So it's very strong. Yes?

**AUDIENCE:** Is this for even potentials?

**PROFESSOR:** Even potentials. Yes. For bound states in one dimension with even potentials.  $V$  of  $x$ .  $V$  of minus  $x$  equal  $V$  of  $x$ . Yes. So how do we show that? Well, again, you've got two solutions here that are degenerate that have the same energy. Sine of  $x$  and sine of minus  $x$ . So given that there's no degeneracy in one dimensional problems, this thing that they have the same energy, the only thing that can be happening is that sine of minus  $x$  is equal to a constant times sine of  $x$ . Where this constant is real.

Why real? Because we said already by the previously theorem, wave functions can be chosen to be real. So you've got this thing already that this is true. Sine of minus  $x$  is equal to  $c$  times sine of  $x$ . Which, if you use this property again by saying, oh, but sine of  $x$  is equal to  $c$  times sine of minus  $x$ . Basically, what this says is that you can change the sign of the argument by putting an extra  $c$ . So you do it again, sine of  $x$  is equal to this.

So this is  $c^2 \sin(-x)$ . So  $c^2$  must be equal to 1. And therefore  $c$  is equal to either plus or minus 1. No other option. So the functions are either even or odd, but they can't be arbitrary. This point is sufficiently settled that part two general exam at MIT 10 years ago had a question like that. And the person that invented the problem claimed that there would be a solution that could be neither even nor odd. So even faculty members at MIT sometimes get this wrong.

It's not as weak as this, that can be chosen. But it's really either or other in the case you have one dimension. OK. So these are our main theorems. And we're going to proceed now by clarifying a little more the nature of the spectrum. So are there questions? Yes?

**AUDIENCE:** Can you give an example of state that's not bound?

**PROFESSOR:** OK. The question is can I give an example of a state that is not bound? Yes. We can give such state. You have a potential like this. And you have an energy like that. And then the wave function could look like this. Then do something like that. And then look like that. It just doesn't vanish when you go to infinity.

**AUDIENCE:** So that can't be normalized?

**PROFESSOR:** Can't be normalized. That's right. If it's not bound, it can't be normalized. Other questions? Yes?

**AUDIENCE:** So you can't really represent-- it's doesn't really represent single particles, more like a stream of particles?

**PROFESSOR:** Yes. So it doesn't represent a single particle. Now trying to interpret it as a stream of particles is a little delicate. So what we usually do is we build superpositions of those states that can represent a localized thing. But it's true that, morally speaking, it seems to represent more than one particle. OK.

So now we talk a little about the nature of the spectrum. So what do we want to say here? We want to go back to the Schrodinger equation here. And just move one term to the right hand side. And just see what can happen in terms of singularities

and discontinuities.

So first of all, we always begin with the idea that sine must be continuous. And the reason sine must be continuous is that we don't want singularities worse than delta functions in potentials. If a function is continuous, the derivative might be discontinuous, and the second derivative would have a delta function. So the second derivative would have a delta function.

But if the function is not even continuous, the second derivative would have derivatives of delta functions. So somehow the potential would have to have that. And we don't want it. So to simplify our life, we say that sine must be continuous. Now if sine is continuous, we will consider several possibilities, possibilities for  $V$ , possibilities for  $V$  of  $x$ . So first possibility-- one,  $V$  is continuous. So  $\psi$  is continuous, and  $V$  is continuous. If  $\psi$  is continuous and  $V$  is continuous, this product is continuous.  $\psi''$  is continuous. And  $\psi'$  is continuous.

Two,  $V$  has finite jumps. Well, if  $V$  has finite jumps, and  $\psi$  is continuous, this product has finite jumps. So  $\psi''$  has finite jumps. If  $\psi'$  has finite jumps, the worst is that  $\psi'$  still must be continuous.

But it changes.  $\psi'$  could look like that, could have a corner. But it cannot be worse than that. Because if  $V$  has finite jumps, if  $\psi''$  has finite jumps, and if  $\psi'$  is not continuous, it would have delta functions.

So for these two conditions, continuous or even finite jumps,  $\psi'$  is still continuous. Things change qualitatively if three,  $V$  has delta functions. If  $V$  has a delta function, then  $\psi''$  has a delta function. And  $\psi'$  therefore jumps.  $\psi'$  is not continuous.  $\psi'$  jumps.

This may be reminiscent to you whenever you had to solve the problem of a bound state of a delta function, you got a wave function that looked like this in which  $\psi'$  jumps. And it has to jump. Because  $\psi''$  has a delta function. Another case in which  $\psi'$  jumps is for if  $V$  has a hard wall. That is, the potential suddenly at one point becomes infinite, and it prevents the particle from

moving across. A hard wall is a place, as you remember in the infinite square well, in which the wave function vanishes, but the derivative doesn't vanish.

So you could say that  $\psi$  is 0 here outside.  $\psi'$ , then, jumps in that it's non-0 here and it's 0 afterwards. So now, you could object to what I'm saying by explaining that, well, we shouldn't talk about the wave function beyond the hard wall. And in some sense, you're right. But suppose we do and we say the wave function is just 0 everywhere, we see that  $\psi'$  jumps. So really,  $\psi'$  jumps.

So this is as bad as things can get. So we can summarize this in just one sentence. And the sentence reads,  $\psi$  and  $\psi'$  are continuous unless  $V$  has delta functions or hard walls, in which case  $\psi'$  can have finite jumps.

So basically,  $\psi$  and  $\psi'$ , continuous. Exceptions-- delta functions and hard walls, and  $\psi'$  can change. So questions. There was a question before. Maybe it's still there. Yes.

**AUDIENCE:** Do you absolutely need that function [INAUDIBLE]? Or do we just assume that [INAUDIBLE]?

**PROFESSOR:** We assume it-- so the question is, do I need that in absolute generality to do quantum mechanics? I don't think so. I presume you could discuss some potentials that lead to  $\psi$  that are not continuous and still make sense. But we will not discuss them. And actually, I don't think I've encountered any of those. Yes.

**AUDIENCE:** Can you give an example of a physical system whose potential is well approximated by a delta function [INAUDIBLE]?

**PROFESSOR:** Yes, there are systems like that. For example, this one that is somewhat well approximated by a delta function. For example, a nucleus sometimes is considered to be like a spherical cavity in which particles are bound by a deep potential and don't escape.

So the nuclei are moving like that and don't escape. In that case, it would be a three dimensional delta function that vanishes at the origin. I presume there are many

examples. Any potential that sort of begins like a finite square well that is sufficiently deep will start to look like a delta function after awhile.

**AUDIENCE:** [INAUDIBLE]

**PROFESSOR:** Well, it's again neither-- yeah, I guess so. But it depends how big is this  $\psi$ . So yeah, probably you're right. This looks a little more like an analog of a hard wall. But if a hard wall is very narrow and very deep, it looks like a delta function. So it's idealizations for sure. But I'm sure we could get a better example. And I'll try to find one.

Now, the next thing we want to do is give you intuition for this incredible result that there's no degeneratives in one dimensional potentials. That is not to say that the proof is not good enough. It is just to say that we can illustrate that without going into a mathematical proof that is more complicated. So how do we do that?

We'll consider the following case, a simple case, an example of a potential of this form.  $V$  of  $x$ -- this is  $x$ . And here is  $V$  of  $x$ . And we will try to find a solution with some energy that is like that, an energy that is right there below the barrier.

So this would be a bound state. Why? Because solutions here are exponentials that decay, exponentials that decay. And here, the wave function would be oscillating presumably. So the wave functions go to 0 and infinity. You could get a bound state.

So let's see how we get a bound state. Now, the argument I'm going to follow is just an elaboration of something you can read in Shankar. And it's a nice and simple argument. So we want to understand why we would get here no degeneracies. Or even more-- in fact not just no degeneracies, but the spectrum is quantized. That is, you find one energy, and then another energy maybe, and another energy.

So how do we see that? Well, you look at the way you can write solutions and count the parameters of the solutions and try to see how many conditions you have to satisfy. So here, the wave function would be a decay in exponential. A decay in exponential is of the form  $\alpha e^{-\kappa x}$ . Because  $x$  here is negative. So this decays as  $x$  goes to minus infinity if  $\kappa$  is positive. And that's how a solution

looks.

You need one coefficient here to determine this solutions. So I'll put a 1 here. Now, in here, the solution is oscillatory. So it's a sine plus cosine. So you need two coefficients. In here, the solution must again be decaying. And therefore, you just need one coefficient. Again, this time it would be a  $\beta e^{-\beta x}$ . The fact that this potential looks symmetric-- I'm not assuming it is. Yes.

**AUDIENCE:** Won't one of the coefficients be unconstrained by normalization? Isn't one just the normalization factor?

**PROFESSOR:** OK, how about normalization? Indeed, we have one, two, and two and one, so a total of four coefficients, four parameters. But indeed, suppose you wrote your whole solution. You could say, look, let me divide this solution by 3. That's an equivalent solution. I'm just checking if it solves the Schrodinger equation. That's all I have to check. I don't have to check normalization.

Normalization, in fact, is sort of irrelevant here. You just need to know if a bound state exists. So indeed, even though you have these four parameters, given that you can multiply the solution by a constant, there's just three constants to fix. Four parameters via normalization or the multiplication by any constant-- just three constants to fix.

But this potential is nice enough that  $\psi$  and  $\psi'$  must be continuous. So you get two conditions here and two conditions here. So four conditions-- continuity of  $\psi$  and  $\psi'$ , continuity of  $\psi$  and  $\psi'$ , four conditions. So what did we get? We got in trouble. We've shown that this is unsolvable in general. Because there are more conditions than parameters. Now, this equation could to be a little peculiar. Maybe this is not completely general. But you seem to have more conditions than parameters.

But here comes the catch. The solution really is determined. Like  $\kappa$ -- do you know  $\kappa$ ? Well, you know  $\kappa$  if you know the energy of the solution.  $\kappa$  is determined by the energy of the solution. So some parameters in the solution

depend on the energy. So the way we have to think of this is that in fact three constants to fix, but four conditions. So we really need four constants to fix. And the fourth constant is the energy.

So the energy is the fourth constant to fix. And with four conditions, these three constants that we had there and the energy, they can just be fixed. So the solution should fix the energy and should fix this coefficient.

So the solution exists for some energy, or possibly some values of the energies, but not all values of the energy. So this shows, or at least very clearly illustrates, that you are going to find sets of energies for which you have solutions depending on how the equations look, and one solution each time. So you get what is called a discrete non-degenerate spectrum.

Now, there are more cases to discuss, the case in which you have just the step, or the case in which you have three bound states. And I will not do them but state the results. Again, all that I don't do explicitly can be found in the notes. So you would look at them later.

And so here is the second case, a potential like this and an energy like that, energy level. And what you get here is that in fact, doing the counting and analyzing the boundary conditions, you should do it by yourselves. But you will see the answers in the notes. You get here continuous spectrum, non-degenerate. So you will get a solution for every value of the energy-- that's to mean, continuous spectrum-- and one solution each time. Finally, this case-- if you have an energy like this,  $e$ , you get continuous spectrum and doubly degenerate, so two solutions.

Now, after this, there's one more result that qualifies as a theorem. And it's hard to prove rigorously. I will not attempt to prove it here nor even in the notes. It's hard enough. So this theorem has to do with nodes. Theorem-- so if you have the discrete bound state spectrum of a one dimensional potential, and you list the energies  $E_1$  less than  $E_2$  less than  $E_3$  like that,  $E_1$  is the ground state energy. Remember, this spectrum is discrete. So this is less than  $E_2$ , less than  $E_3$ , and it goes on like that, the ground state energy. Then, you have associated wave

functions, energy eigenstates  $\psi_1$  of  $x$ ,  $\psi_2$  of  $x$ ,  $\psi_3$  of  $x$ .

Here is the theorem. The theorem tells you something about the vanishing of the wave function. It says that  $\psi_1$  has no nodes.  $\psi_2$  has one node.  $\psi_3$  has two nodes. And so it goes so that  $\psi_n$  has  $n$  minus one node. So  $\psi_n$  is greater than-- well, it's correct. Any  $n$  greater or equal to 1 has  $n$  minus 1 nodes.

Now, there are several ways people show this. Mathematicians show it in a rather delicate analysis. Physicists have an argument as well for this, which is based on approximating any potential by infinite square wells to begin with. So suppose you have a potential like that. Well, think of it as first being a little potential like that, an infinite square well. And you start making the window of the square well bigger.

The argument-- it's a neat argument. Maybe you can discuss it in recitation. I would suggest that. It's a good argument. But it's not rigorous.

But still, one can do something like that. You make it grow. And what you know is that the infinite square well, the first wave function has no node. And as you change the screen to make the potential really what it's supposed to be and not just that of a square well, the wave function cannot gain a node.

On the other hand, what you will show in the homework is something that is a partial result which says that the solution with  $n + 1$  has at least one more node than the solution with  $n$ . So it's part of what you can show. And it doesn't take too much effort. And you can prove it rigorously. So we will assign that eventually for a homework to do.

In the homework that you have for the first homework, you also have a problem with delta functions. And I suggest that you read the notes that will be posted today. Because there's an example there with delta functions. If you study that example, you'll find the problem quite easy to solve. You may have solved already. Some of you are very eager to get going with the homework. So it's something you can study first, and then make your life a little easier.

So what we're going to do now for the rest of the lecture is consider the variational

problem, which is something you probably haven't seen before, the variational problem. This problem has to do with calculus of variations. Now, calculus of variations is something considered fairly advanced. And therefore, as you will see, we will avoid some of the major difficulties of calculus of variations in our discussion of the variational principle.

But I wanted to mention a little story about this problem. So this calculus of variations is a more complicated version of maxima and minima in which in maxima and minima of functions you look at the function. And if you could plot it, you could say, here's a maximum, here's a minimum. If you want to figure out where they are, you know. You take a derivative, set it equal to 0, you find the maxima and minima.

So the typical calculus problem is one in which you have a function, and you want the maxima and minima. The variational problem is a problem in which you want to maximize or minimize something. But what you don't know is not where the maximum or minimum occurs, but which kind of function will give you this maximum or minimum. So your unknown is not a point where there's a maximum or a minimum but a function where there is a maximum and a minimum.

So it's slightly more complicated. So this is the calculus of variations. And people wonder when did it start. It actually seems to have first been discussed by Newton. And it's quite an interesting story. Newton was trying to understand apparently the following problem. If you would have a cross sectional area like this, he asked the question, how should you make a solid out of this by tapering it and ending with this, tapering it, in such a way that as it moves in a viscous fluid, the resistance is the minimum possible-- very complicated problem.

And as you can imagine, this is a complicated problem because you're trying to find a shape-- not just a maximum or a minimum of a function but what shape maximizes or minimizes this. So apparently, he solved the problem and wrote it in *Principia* but didn't explain his solution. And people for years were trying to figure it out. And nobody could figure out how he did it.

Then, the story goes that this mathematician Johann Bernoulli in 1696 came up with

a challenge to all mathematicians. At that time, people would announce a problem and challenge to see who's smart, who can solve this problem. So Johann Bernoulli in around 1696 poses a problem of, you're given two points in the plane, in the vertical plane like this blackboard, point this, A, and point B in here. You must design the curve of shortest time for fall, so some curve here. If you put an object and let it fall, it will get the fastest to that point, so maybe something that looks like this.

It's a complicated curve, or at least not all that simple. And he asked all the people to solve it, gave them one year to solve it. So who was around at that time? Well, one person that got the letter was Leibniz. He got it on the 9th of June of that year, 1696. And he answered it, sent an email back, by the 16th of June with a letter with a complete solution.

It's a funny thing that actually apparently Newton was very busy and didn't receive this letter. Or something happened, and he got it one day, and he actually solved the problem in one night. It took him one full night to solve it. Now, you say, well, how brilliant. And true, but given that he had solved this problem, he was criticized as being really slow and-- how come you took 12 hours to solve this problem?

So it's quite amazing. There's a lot of Bernoullis. And apparently, this question by Jacob Bernoulli, the main purpose of this question was to demonstrate to everybody that his older brother, Jacob Bernoulli, who had invented the Bernoulli numbers, was actually an incompetent person that could not solve this problem. So that was apparently what he wanted to do.

It's a rather famous family. But they obviously didn't get along. But apparently, Jacob did manage to solve the problem. So Jacob Bernoulli, Leibniz, and Newton all solved the problem. Johann Bernoulli, the one that started this problem-- and I think it's maybe with a double N, I'm sorry-- his son is Daniel Bernoulli. And engineers know him, because that's the Bernoulli of the Bernoulli fluid dynamics stuff.

So the problem is not all that easy. And calculus of variations determines this shape. So the calculus of variation applied to quantum mechanics asks, here, this function

is determined by the principle that it minimizes time. So you have the Schrodinger Equation. And you could ask, you have all these Eigenfunctions. What do they minimize? Is there something they're minimize? And the answer is yes. And this is what you'll understand in the next few minutes.

So what is the problem we want to solve? We want to solve the problem  $H\psi = E\psi$ . So some Hamiltonian. Now my notation will be such that it applies to three dimensions as well. So I'll put just arrows on top of it, and you would have to write the proper Hamiltonian. It will not be necessary for you to know the Hamiltonian. So I'll put  $\psi$  of  $x$  here, meaning that this is equally valid for more than one dimension.

Now we want to find solutions of this equation. And you can say, what do they maximize or minimize? Well we won't get to it until 15 minutes. First let's try something simpler. How about, can we learn something about the ground state energy of the system? So let's try to think about the ground state energy. State energy. Now consider ground state energy and we'll consider an arbitrary-- arbitrary is the most important word here--  $\psi$  of  $x$  that is normalized. Is normalized. So  $\int \psi^2 dx = 1$ .

And here comes the claim. The first claim that we can make. You see, this wave function doesn't solve the Schrodinger equation. That's what we mean by arbitrary. It's just any function of space that is normalizable. Doesn't solve the Schrodinger equation. Never the less, you are commanded to compute the following quantity.

This quantity is also by definition what we call the expectation value of the Hamiltonian in the state  $\psi$ . I love the fact, the remarkable fact that we're going to show now, is that this thing provides an upper bound for the ground state energy for all  $\psi$ .

So let me try to make sure we understand what's happening here. Here it says you don't know the ground state energy but you're going to learn something about it. Something that's interesting is if you know that it has an upper bound, so the ground state energy is definitely not higher than this one, so you learn something. Would be ideal if you had also lower bound so you knew it's in this range. But an upper bound

is a nice thing to have. And the claim here is that each time you try an arbitrary function, you put anything here, you ever write, you've got an upper bound.

So how is this used? You try arbitrary functions that you think look possibly like the wave function of a bound state. And you get numbers and you already know that the ground state energy smaller than some number. So it's a rather nice way of getting some information about the ground state energy. So this  $\psi$  effects is called a trial wave function. Is a trial wave function.

So is the statement of this theorem clear? Not the proof, but the statement. Do we have questions? Yes.

**AUDIENCE:** Is there any statement about how using the wave function will give us how accurate an estimate [INAUDIBLE]

**PROFESSOR:** No. We're going to become good and figure out some nice way of choosing wave functions, but no. Once you tried you got some information. And you may not know so easily whether you could go much lower. You can try a little, but there's no clear way to know. This is just some partial information. OK.

So let me first prove this. We'll prove it and then explain a little more what it all means. So the proof. Now it's a proof under quotation marks. I will make a few assumptions. Basically, that I don't have a continuous spectrum. Now that assumption is done for me to write a simpler proof, not because the result doesn't hold. So the proof is good, but I will just consider for notational purposes no continuous spectrum.

So we'll have a ground state energy which is  $e_1$  that is maybe less than or equal to  $e_2$  less than or equal  $e_3$  like that. So you even may consider the [? genorisies. ?] And we have  $\hat{H} \psi_n$  is equal to  $e_n \psi_n$ . So what do we have? We have a trial wave function. So your trial wave function since it's an arbitrary function of  $x$  should be expandable by completeness as a serious or a superb position of the energy eigenstates.

Let me clarify this point. This is a trial wave function. Doesn't solve the Schrodinger equation. So this Doesn't solve this energy eigenstate equation. So in fact, it doesn't solve it because this is a superb position of many in here. So that's consistent with this, and the fact that this wave function as given in here just can be represented using the energy eigenstates. But being a superb position, it's not an energy eigenstate which is true because a trial wave function is something that you invent out of your head. It's not a solution. If you had a solution, you wouldn't need this. So you don't have a solution. You invent the trial wave function, and you have this.

A couple of things. The psi squared integral being one. You can do that integral, that condition, is the sum of their  $b_n^2$  is equal to 1. This I use the orthonormality. You can elevate this. It's sort of the kinds of things we're doing last time. Please make sure you know how to do that.

Then there's the other computation that we also have sketched last time, which is that the integral of  $\psi^* H \psi$  which is what we want to compute,  $\hat{H} \psi$  is actually  $b_n^2 E_n$ . So that was something we're doing towards the end of last lecture. And this computation takes a few lines, but it was there. It's in the notes.

And now comes the kind of thing we want to say. Look at this sum. It has  $b_1^2 E_1, b_2^2 E_2, b_3^2 E_3$ , but  $E_2, E_3, E_4$ , all those are bigger, or at most, equal to  $E_1$ . So if I did, here, the following bad joke of substituting  $E_n$  for  $E_1$ , which is not the same, if I put here  $b_n^2 E_n$  equals 1 to infinity. I put here  $E_1$ , well this is bigger than that because  $E_2$  is possibly bigger than  $E_1$ ,  $E_3$  is bigger than  $E_1$ . But it may be equal. But at this moment,  $E_1$  can go out of the sum. So this is  $E_1$  times this sum which is 1 because  $b_n^2$  is equal to 1. And  $E_1$  is the ground state energy by definition. So the ground state energy is less than this which is the expectation value of the Hamiltonian. Pretty simple, in fact, the proof is really a little too simple.

Where do we go from now? Well let's make a more general statement of the variational principal. Again, sometimes it's not all that convenient to have normalized wave functions. So recall that if  $\psi$  of  $x$  is not normalized,  $\psi$  of  $x$  over the square root of integral of  $\psi^2 dx$  is.

Therefore if you hand me an arbitrary  $\psi$  of  $x$  that is really arbitrary. You don't even bother to normalize it. Then when I plug here in this formula it is supposed to be normalized. So I plug the second expression there. So therefore I get that less than or equal to the integral of  $\psi^* h \psi$  over  $\int \psi^* \psi dx$ .

This is actually nicer in one way because you don't have to work with normalized wave functions. And that result must be true still. Yes?

**AUDIENCE:** [INAUDIBLE]

**PROFESSOR:** Sure. It cannot be completely arbitrary, the function should be normalizable. Doesn't have to be normalized but normalizable. So here you got. And here let me introduce just a little name.  $f$  of  $\psi$ .  $f$  of  $\psi$  is what is called a functional.  $f$  of  $\psi$  is a functional. What is a functional? A functional is a machine or an expression whose input is a function and whose output is a number. So here  $f$  of  $\psi$  is a functional. And maybe I should use brackets. Many times people with brackets denote that, watch out, this is not a function, it's a functional. And here it is. No dash there.

You give me a  $\psi$  of  $x$ , which is a function, and then this is a number because you've done the integrals. So that is like the Brachistochrone problem, that a funny name for it. Here it is. There is a function now which is the time that it takes to go here. You give me a path, a function, and I can calculate the time it will take the mass to get here. So this was the issue of finding a critical point of a functional. So actually we start to see, it seems that the ground state energy is the minimum of this functional.

And what this interesting as well is that when you get the minimum you will have gotten a ground state wave function. So the ground state wave function actually is the thing that minimizes this functional and gives you some value, the ground state energy. A little more in a couple of minutes. Let's do an example.

How do we use this so now if you think about this carefully it's kind of dizzying because what is a functional, really? It's, in some sense, a function in an infinite dimensional space because a function itself is specified by infinitely many numbers

that you can change. So how many dimensions you have is how many ways you can move your hands, but they are linearly independent.

But if you have a function, and you can change it, you can change it here, you can change it there, or you can change it there, and those are all orthogonal directions. You're finding a critical point. When you find the critical point, you should imagine that you're plotting a function that is not one dimensional function or two dimensional function, but it's infinitely dimensional function. Direction one, direction two, infinitely many directions. And suddenly in this infinitely many directions you find the critical point. It's really incredible that one can do these things. So you're at that critical point, and you can deform the energy eigenstate by making it a little fatter here or thinner here or up there. And those are the infinite directions in any direction that you will the energy goes up because you're at the global minimum it's pretty amazing.

Something that you will prove in the homework is that actually it's even more. Every single eigenstate is a critical point of this functional. So you've got the lowest energy state and in that infinite dimensional space in every direction that you move you go up. The first excited state is another critical point. But it will not be an absolute minimum. It will be a [? saddle ?] an infinite dimensional [? saddle ?] which are infinitely many directions in which you go up. There's one direction in which you go down because you could flow towards the ground state. So the first excited state is the [? saddle ?] but these are all stationary points of this functional.

So we'll conclude by doing this example. Sorry, what is the question?

**AUDIENCE:** [INAUDIBLE]

**PROFESSOR:** I didn't assume it's non-degenerate. So if you have two things that have the same ground state, the functional will have, in fact, the degeneracy there will be two solutions that have the same energy. And any linear combination of them will have the same energy. The proof that I did here doesn't assume non-degeneracy, it's even true with degenerate things.

So the example is an example for illustration, not for solving something that you can't do otherwise. So it's a delta function potential.  $v$  of  $x$  is minus alpha delta of  $x$  with alpha positive. And the ground state energy is well known. It's minus  $m$  alpha squared over  $2\hbar^2$ . You've solved this problem many times in 804.

So trial wave function. Well you know how it should look, but let's assume you don't. And you say, it's some sort of [INAUDIBLE]. So trial. It would be  $\psi$  of  $x$  equals  $e$  to the minus  $x$  squared. While this would do, you're going to work hard and you're not going to reap all the benefits of this calculation. So what you should do at this moment is put a constant here. Minus beta squared  $x$  squared and I'll put the minus one half. This is our trial wave function.

You see, by this, you're going to get an expression. You calculate this number, and you're going to get the function of beta. Beta is not going to disappear. And therefore, you're going to know that the ground state energy is less than this function of beta. And then you can adjust beta to get the best bound. So beta is put as a parameter to begin with, and we hope to use it. So note that integral of  $\psi$  squared  $dx$  in this case is equal to square root of  $\pi$  over beta. So we have to calculate this whole functional. So this integral of  $\psi$  star-- well I don't have to bother with  $\psi$  star because it's real.  $\int \psi$  over  $\psi$ , and what do we get?

Well the denominator is easy. So we beta over square root of  $\pi$ , and let me write the whole thing here.  $\int dx$  the  $\psi$  would have  $e$  to the minus one half beta squared  $x$  squared minus  $\hbar^2$  over  $2m$   $d^2/dx^2$  minus alpha delta of  $x$ . And another wave function,  $e$  to the minus one half beta squared  $x^2$ . OK. So you have to evaluate that. And that's the part that is not so much fun.

For any integral that you have in 805, we believe that you can use Mathematica or Maple or MATLAB or whatever and do it. The only reason not to use any of these things is if you think you could not do the integral. But once you realize, oh, this is an integral, I know how to do, don't waste time. Use any of those programs. Now, this part of the integral is kind of easy because the delta function just picks the value of 0. So this part of the integral gives you minus beta alpha over square root of  $\pi$ .

The other part of the integral, however, is a little more complicated. Believe it or not, it makes a big difference whether you take the two derivatives of this function or you integrate by parts. If you integrate by parts, you save a lot of work. So let me integrate by parts. This becomes, plus beta over square root of h,  $h^{-2}$  over  $2m$ , integral dx of ddx of  $e^{-\frac{1}{2} \beta x^2}$ . So you integrate by parts one of the ddx and then you have the other ddx, so it's the thing squared. And that's an easier integral to do.

We don't want to bother with this, but this whole thing then becomes minus beta over square root of pi,  $\alpha + \beta h^2$  over  $4m$ . That's the whole answer. And that's the valuation of this whole thing. So look what you get. You got a function of beta indeed. So how does that function of beta look?

It's 0 for beta equals 0 is 0 for some other possible beta, it's going to look like this. So there's a point at which this function is going to have a minimum, and we should choose that point to get the best upper bound on the function. Our claim is that following from the variational theorem that we've proven is that the  $e$  ground state is less than or equal than the minimum value over beta of this  $\beta h^2$  over  $4m$  minus beta square root of pi  $\alpha$ .

So you minimize over beta, and yet still the ground state energy must be a little smaller than that. Well what do you get? You do this, this minimization gives beta equal  $2m \alpha$  over  $h^2$  square root of pi. It's a little messy but not terrible. And you substitute, and you get that  $e$  ground state is less than or equal than  $m \alpha^2$  over  $\pi h^2$ . And to better write it as  $2$  over pi times minus  $m \alpha^2$  over  $2h^2$  which is the true ground state energy.

So let's just make sure we understand what has happened. Here is the energy. Here is zero. Energy as just a vertical plot here is zero. The true ground state energy of this problem is this one, let's call it  $e_{gs}$ , is negative. And we go  $2$  over pi times that.  $2$  over pi is about 0.64. So the bound says that here is 0.64  $e_{gs}$ . So that's what the bound told you. The bound state energy must be lower than this quantity. We got close. Not impressively close, but the work functional was not all

that bad either. Question?

**AUDIENCE:** [INAUDIBLE] always going to be a constant times incorrect energy value or is it just the closest approximation?

**PROFESSOR:** Is it going to be what?

**AUDIENCE:** Is it always going to be a constant times the correct energy value or is it just--

**PROFESSOR:** Well it typically is like that because of dimensional units. You're looking for a constant because you're not looking for the function. So you will get a number times a correct value, yes, indeed. That's an illustration of the problem of wave functions. You know the variational principle tells you things about the ground state but allows you to find the first excited state as well if the potential is symmetric, will allow you to prove that any attractive potential has a bound state. And you will prove in the homework that stationary points of these things are the eigenfunctions. See you next Monday.