Quantum Physics

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Lecture No. # 29

Perturbation Theory

Today, let's look at a very important aspect of quantum mechanics which goes by the name of "Perturbation Theory". The idea is the following.

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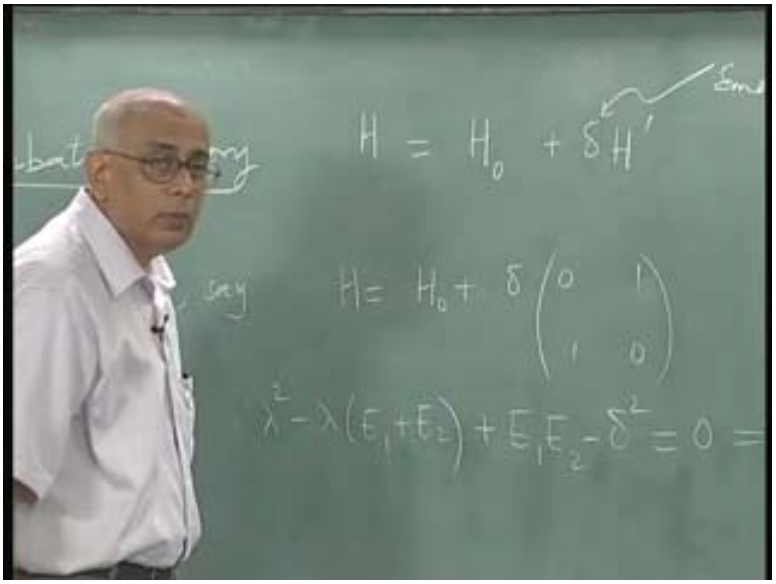

Generally, the class of problems or the class of Hamilton's for which you can find the eigenvalues and the eigenfunctions explicitly is very small. Apart from a few well know examples like the hydrogen atom or the harmonic oscillator and any number of dimensions, the number of exactly solvable problems is very small. Just as in classical mechanics too, you realize that the number of exactly integrable problems is also very small. Most problems are not integrable. In exactly the same sense, most Hamiltonians in quantum mechanics cannot be analytically solved. In the sense that, you can't write down eigenvalues and eigenfunctions explicitly for them. So several approximation methods have been evolved ever sense quantum mechanics began, as a matter fact with varying degrees of rigor and success and today Perturbation theory is a well-established part of quantum mechanics. What we are going to do here is to look at its rudiments, the very basic elements of certain kind of Perturbation theory. Now what I have in mind is a system whose Hamiltonian H can be written as a sum of 2 parts. The first part is supposed to be the free or solvable Hamiltonian, H_0 which we are going to assume is something for which you can find the eigenvalues and eigenstates explicitly plus a small correction to it.

Now of course, one has to make some sense out of this word "correction" classically. If I wrote down the correction as some H prime, then one could say if H prime is numerically always small compared to H_0, this is a small correction to it. To keep track of how big this correction is, one introduces generally a parameter, lambda which is taken to be small. This is sufficiently small that lambda H prime serves as a correction to H_0. Now, quantum mechanically H_0 and H primer operators. So the question of what do you mean by "small" is not very clear immediately. We can do it in 2 ways, either i say that lambda is a parameter very close to 0, some real number which is very close to 0 and H_0 and H prime are comparable to each other. That's one of the possibilities. or I set lambda = 1 and i say H prime is such that all its matrix elements are very small compared to H_0 in some given basis.

Now we are going to take the attitude that lambda is a small parameter. we will put it in explicitly because we would like to keep track of terms of first order, second order, third order and so on and they would refer to powers of lambda. In this course, we have restricted our attention to Hermitian Hamiltonians. So H_0 and H prime are Hermitian operators and lambda is a real number. So the eigenvalues of H would continue to be real which is what we want. What I mean by smallness of this term lambda H prime will become clear as we go along. Now of course you could also say, in general the Perturbation that you apply to an unperturbed system with Hamiltonian H_0 could be time dependent.

You could actually apply an electric field on a charged particle which has got some time dependence. So in general this is the time dependent Hamiltonian. If H_0 has energy levels of some kind, then the moment you switch on H prime, it would cause transitions between these stationary states. And the question of physical interest is given the system initially in some given eigen state of H_0, what's the probability that it's going to jump to some other state under this Perturbation. What's the probability per unit time? These are called transition rates or transition probability and they will become relevant. On the other hand, you could also have situations where H prime is not dependent explicitly on time. It's just a Hermition operator. We would like to ask: given the eigenvalues and eigenfunction of H_0, can you find the eigenvalues and eigenfunction of H_0 + lambda H prime. Now you appreciate the problem is totally trivial if H prime commutes with H_0. Then if you can diagonalize, you can simultaneously diagonalize 2 mutually commuting matrices and find a common set of eigenstates. Therefore there is no fun in it at all. On the other hand, if H prime doesn't commute with H_0, then nontrivial things can happen. Just to set this stage and show you what can happen, let's take a very simple example where H_0 is a 2 by 2 matrix.

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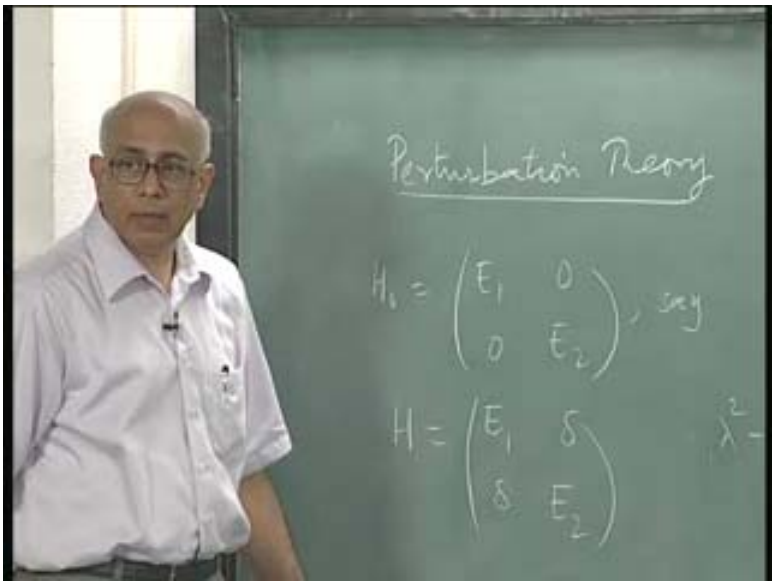

Suppose H_0 has 2 energy levels, let me call them E1 and E 2. i have already diagonalized H_0 and written it in its eigen basis so that you have 2 eigenvalues and the off diagonal elements are 0. Now it's easy to see that if H prime is another diagonal 2 by 2 matrix, then the eigenvalues are obvious. You write them down immediately. On the other hand, if H prime is not the diagonal matrix and doesn't commute with H_0, then you have to do a little bit of work. Suppose H = H_0 + lambda times (0 1 1 0). This is the simplest you could have. Then the question is: what are the new eigenvalues. Well, this is not hard to do because H now is E1 lambda lambda E 2 and the task is to find the eigenvalues of this 2 by 2 matrix which is not very hard to do. But they clearly will not remain E1 E 2. They will have certain function of lambda here in addition to the original eigenvalue. You have to solve the following secular equation. So lambda1, 2 = lambda squared - lambda times E1 + E 2 - + E1 E 2 - delta squared = 0. That's the secular equation which is going to give me the eigenvalues of H. and what are the roots here?

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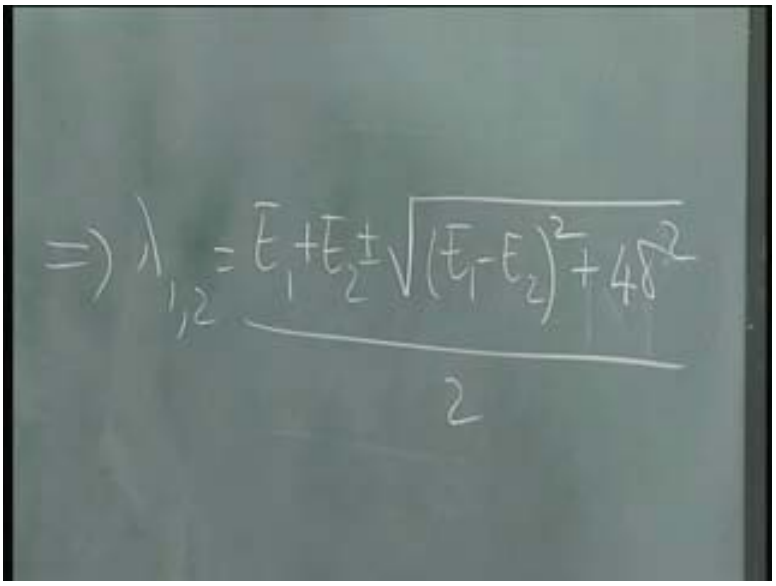

This implies that the roots lambda1, 2 are E1 + E 2 + or - square root of E1 + E 2 whole squared -4 times E1 E 2 - delta squared. So E1 + E 2 whole squared -4 E1 E 2 is E1 - E 2 whole squared. So this is root (E1-E2) whole squared +4 delta squared divided by 2. Now of course to simplify it further you have to tell me whether E1 is bigger than E 2 or E1 is less than E 2.

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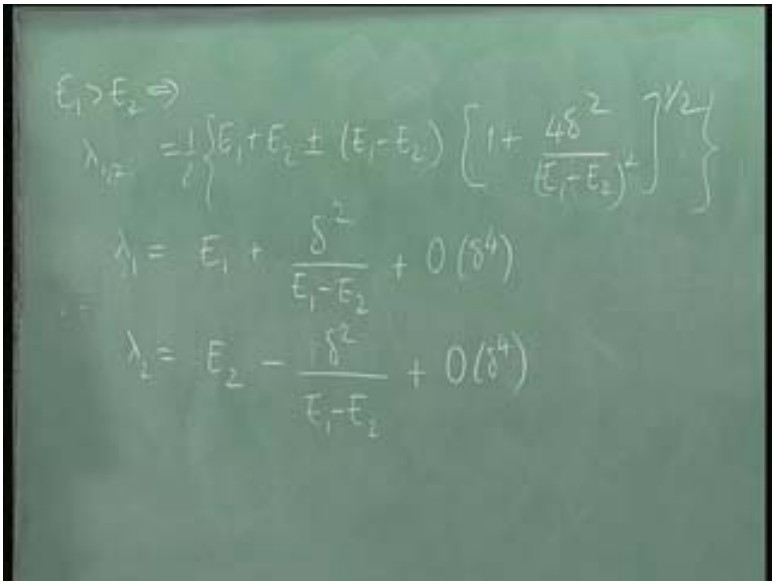

Let's without loss of generality take E1 to be bigger than E 2. Then this implies that lambda1 is E1 + E 2 + i pull this out and it becomes E1 and - E 2. so it's E1 + E 2 + E1 - E 2 times1 +4 delta squared over E1 - E 2 whole square to the power half and this whole thing raised to one half. So what does lambda1 become? lambda1 = E1 + delta squared over E1 - E 2 + order delta to the power 4. It goes on to all powers. So the important lesson is that even though the parameter was linear in the Hamiltonian, this had just first order term in delta. When you compute the eigenvalues, you have all powers of delta in general.

Similarly lambda 2 is E 2 - delta squared over E1 - E 2 + terms of order higher order of delta 4 and so on. So what's the important lesson we learn? Even if the Hamiltonian has a parameter like lambda or delta and it's linear in delta, when you actually compute the eigenvalues in general you expect an infinite series. There will be corrections to the eigenvalues of order delta, delta squared, delta cubed and so on. In this particular problem, the way it appeared since the same delta appeared in both places, only delta squared appears and therefore all the odd powers vanish. Only the even powers of delta remain. But that's not true in general. It's clear that depending on the form of the Hamiltonian, you would have an infinite series in delta. Now in the 2 by 2 case, the problem is completely trivial because you give me a 2 by matrix and I can diagonalize it provided certain conditions are satisfied. I can find the eigenvalues always. There is no difficult at all. We would like to address this problem in general. This perturbation which in this case was just delta is not sufficient that this delta is small compared to the 2 original eigenvalues E1 and E 2. So if you look at this matrix and say the unperturbed is just these and these are the perturbations, perhaps the perturbation can be the corrections can be found in a power series as long as the off diagonal elements are small compared to the diagonal elements. What's the actual criterion here? It must be small compared to the energy differences. So it's not sufficient to say that it is small compare to the original eigenvalues but it should be small compared to the differences in energy.

Then it looks like we are in business and we can do perturbation in a power series. The reason I emphasize this is because in general, you are not going to be able to get an analytic formula like this. You see once I have an explicitly formula, I don't need the perturbation theory. But in general, for more complicated problems, you will only be able to find things to a certain order in this Perturbation. Therefore we must be careful to find out when this series converge. So with this a little toy model, let's look at the general problem. The other important lesson is what happens if E1 = E 2? Then you have something totally different happening. This kind of expansion is not permitted at all. Then you have to do what's called degenerate perturbation theory. You have to now do the problem all over again. You can't do this kind of little trick here. So we are going to assume, to start with that this perturbation theory is time independent and non-degenerate. Slowly we relax all these conditions. By that I mean, the levels of H_0 are taken to be non-degenerate. If 2 of the eigenvalues were equal then you have to be very careful by the way. In this particular case, it will be totally trivial but look at what happens. We had the correction with the infinite series and so on. But look at what happens if you set E1 = E 2. So let's do that and ask what are the new eigenvalues.

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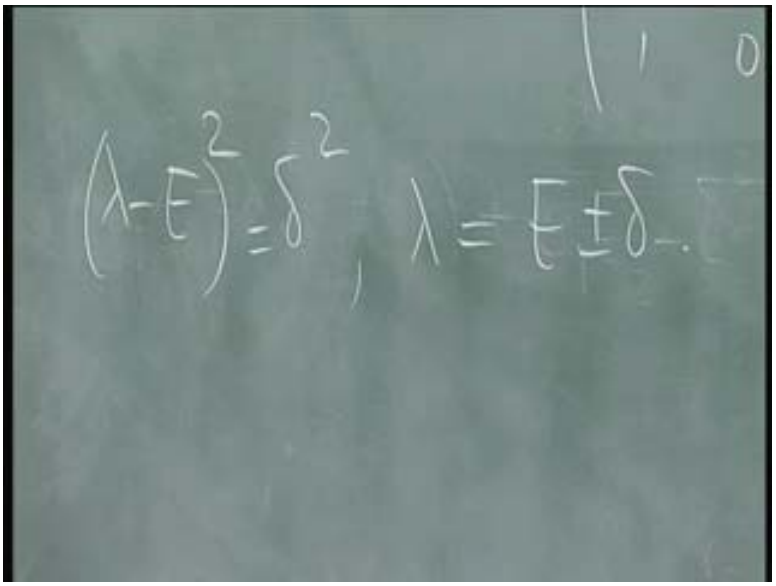

The character of the eigenvalues is going to be change completely because now its lambda - E whole squared = delta squared. So lambda = E + or – delta. It's correct to all orders in delta. So this big infinite series just collapsed and you just got a + and a -. Now incidentally that again illustrate a general principle.

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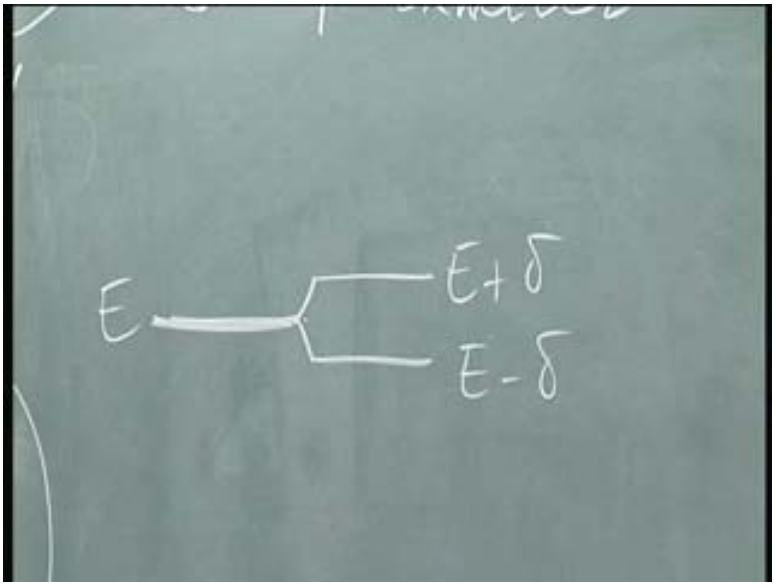

We had a degenerate level at E. i switched on this off diagonal perturbation and it split into 2.There was an E + delta and an E – delta, taking delta to be positive. So it's as if this degeneracy got lifted by the perturbation and one of them went up and the other went down. That too will turn out to be a general feature. But appreciate the fact that the moment these levels became degenerate, the nature of solution became very different. There wasn't this infinite series in delta at all. It simply collapsed. That may not happen all the time but it's immediately evident that you have to redo perturbation theory. By the way, this problem also gives us a hint as to how to solve a general problem in which you have pair of degenerate levels or more than a level with some finite degeneracy. In the subspace of that degenerate level, you have to redo the problem in this fashion. So that's what is going to happen. Now let's put all this down in a formal way. So what are we going to assume? We are going to assume, to start for simplicity, that this H_0 is solvable and that it has a discrete spectrum. Later we must generalize this to a continuous spectrum. That's not very hard to do. And also these levels are all non-degenerate from each other. When you have a continuous spectrum, you have to be careful because the levels are actually sitting on top of each other in a continuous band. So you have to go back and do it carefully.

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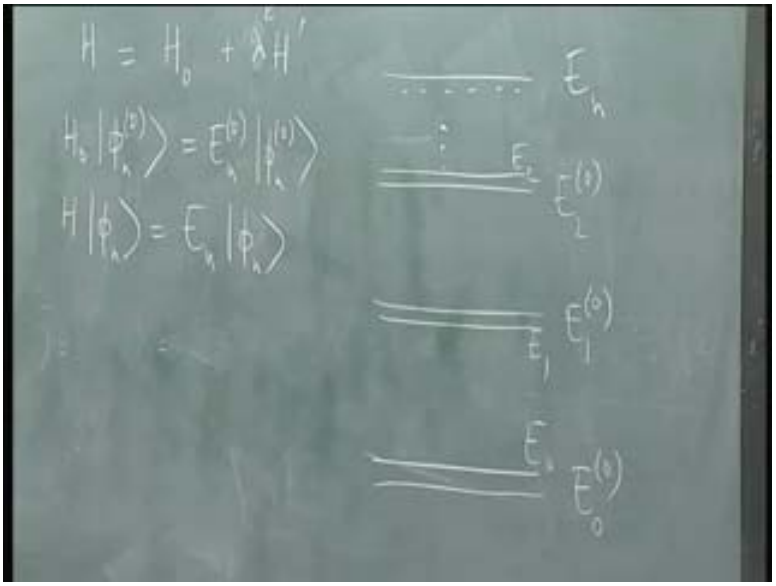

But to start with, let's assume it's a discrete spectrum and H_0 has a spectrum which is not equally spaced. I assume that H_0 has eigenfunctions phi $_n^0$. I am going to put superscript 0 to denote the unperturbed portion of problem. This is equal to E_n^0 phi $_n^0$ and this quantum number n labels these levels. Now I switch on the perturbation and ask what happens to these energy levels. If the Perturbation is sufficiently small, in a sense which will become apparent as we go along, then i physically expect that this energy level will shift a little bit, up or down. We are going to assume that the perturbation is such that the matrix elements of lambda H prime are going to be small in some definite sense compared to these energy splitting.

So that if this jiggles around a bit, you can still identify the n th level. If E_1^0 came down and E_0^0 went up there, then of course you have a very different problem altogether and you can't handle it with perturbation theory. But otherwise we have got a very modest aim which is to say these levels are still distinguishable and they get shifted a little bit. The question is: what's the shift. And these states would also get shifted. There is no reason why phi and superscript 0 should be the Eigenstate. So we assume that corresponding to these is H on phi $_n$ = En phi $_n$. so we assume the same labeling is possible except that En is not quite En 0 but En 0 + some corrections and phi n is not phi n 0 in the state space but its the vector + some corrections. The task is to find out what are these corrections. Now we are going to impose normalization. So I am going to assume that this forms a complete set of state in this space. So this original Eigen functions form a complete set of states and form an orthonormal basis.

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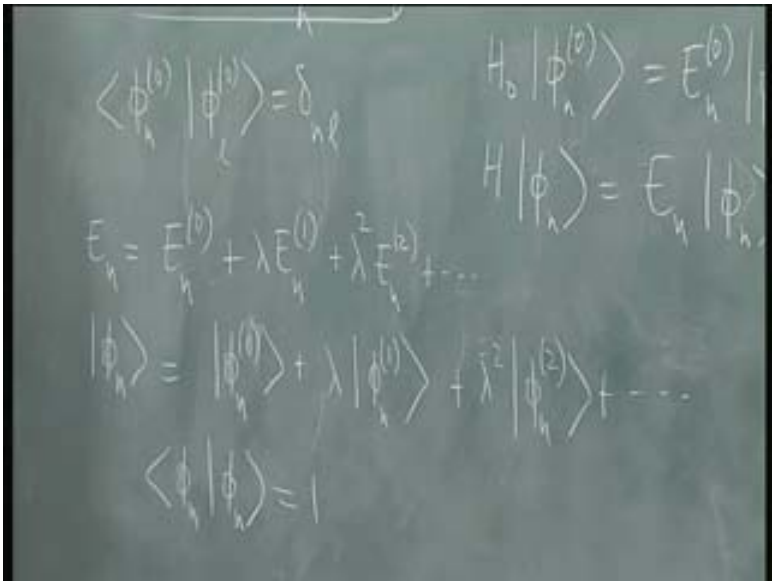

So certainly I am going to assume that phi n 0 phi $_l$ 0 =delta $_{nl}$. They are orthonormalized now I try to find out what's phi n going to be. So what would be the general form for phi n? It's clear that if i focus on one particular state. So this is n th energy level. This was the original state. Maybe the new state is here, E $_0$. Maybe the next state is here, E1and E 2 etc. En is the unperturbed state. Now I would like to find out what it is in general? So, the starting point is to say that based on our experience with this 2 by 2 problem, in general if i fix a particular n, then i can certainly write En = En ^{0} ,the unperturbed energy level + corrections to it which would depend on lambda. I am going to assume that these corrections can be written in powers of lambda. We are going to question that assumption later but we will make this assumption to start with. Then I call the first order correction En1. So what is the meaning of this assumption? it says that this perturbation is such that it's analytic at lambda = 0, in the sense that, the actual perturbed energy level is a power series in the small parameter lambda which converges inside some radius of convergence. That's the assumption and therefore it starts lambda, lambda squared and so on.

If you discovered the correction, the first correction was proportional to square root of lambda, and then this assumption is wrong. Similarly I am going to assume that phi n = phi n ^{0} + first order correction which is lambda times phi n^{1} + lambda squared phi 2 + … In general, it's an infinite series. So the idea is to use this normalization. We have to find normalized eigenfunctions. So we are also going to say phi n phi n equal to1. Actually we would have phi n phi l = delta nl. But right now, i am focusing on just 1 of these states. Phi n is a normalized eigen function with this input now, we have to consistently solve the problem. We have assumed that everything is a power series in lambda and is absolutely convergent which means if 2 powers series are equated, you know you can equate term by term if they are absolutely convergent. And that's the whole point of successive approximations. You assume things are convergent in absolutely convergent power series. Put a small parameter there and equate coefficients of like powers. That's all that's going to be done. Now you could ask: what's the rational for it? How do we know this is going to happen? That you don't know in general. If these operators are crazy operators, you don't know it. for example, if H prime is a differential operator and you write everything in the position basis for example then there are theorems which tell you that if you have differential operators in which a parameter appears in an analytic fashion, then the eigen function and eigenvalues are also analytic around lambda = 0. Based on that, we are going to now use it and try to generalize it of course there would be notable spectacular exceptions and i will let you point them out as we go along. But right now let's assume things are not pathological and ask what happens here.

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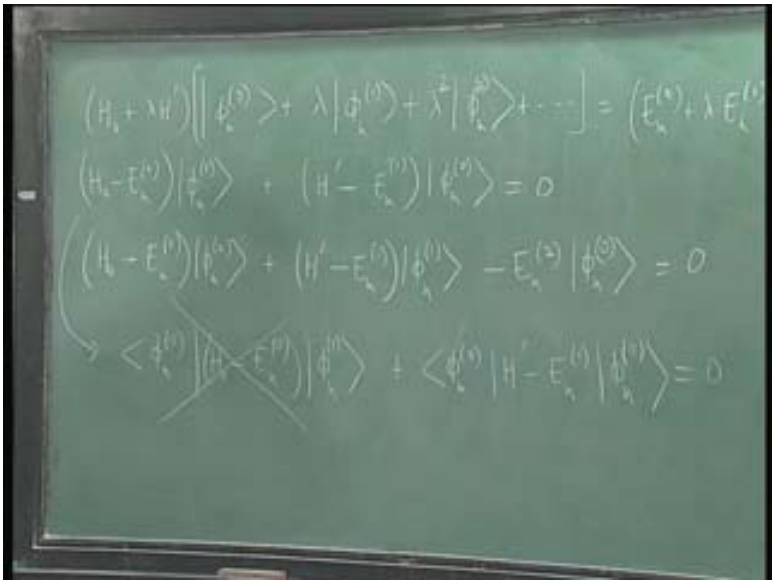

So I plug this expression and this expression into that and what we get is H $_{0}$ + lambda H prime acting on phi n ^{0} + lambda phi n^{1}. We will work up to lambda squared. So let's work correction to order lambda squared just to see what happens and we could if you had enough energy to write down lambda cubed, lambda 4 and so on. But we will see a pattern emerging.

This is En but En is En ^{0} + lambda En^{1} + lambda squared En ^{2} + etc acting on the same thing. Now we equate powers. Well, H $_{0}$ on phi n ^{0} by definition is En ^{0} on phi n ^{0}. So the order lambda terms already match. Then we ask: what are the first order terms? We equate coefficients of lambda. So what we get is H $_{0}$ acting on phi n1 and then there is a contribution which is H prime on phi n ^{0}. Those are the only order lambda terms on the left hand side. Look at the lambda squared terms. There is again an H $_{0}$ it acts on phi n ^{2} that's got to be matched by an En 0 acting on phi n 2 and i bring it to the left. So it's H $_{0}$ - En 0 acting on phi n ^{2} and the other terms. Now you begin to see the pattern. H $_{0}$ - En 0 appears here all the time acts on the highest correction phi n1, p hi n 2 here and so on. Then H prime on the first order correction acts on the immediately lower correction phi n1 and then finally En 2. So as the correction in the energy level goes to higher order, what it acts on is of a lower order obviously so that the powers of lambda match. You write the entire series down in this fashion. If this series converge, then you have an infinite set of equations to find all the coefficients. So what's the task?

The task is to find phi's and the E's. Please remember that these are vectors in Hilbert space. So there is no guarantee that one vector is parallel to the other vector. It has other vectors in this Hilbert space pointing in other directions. This is the set of equations that we have to solve. Now it's very easy to see how to do this systematically, order by order. From this equation, I can find phi n1 and En1 and they act as inputs into this. The first obvious thing that comes to our mind is take the scalar product of both sides with respect to phi n 0. Well, you don't know what this does when it acts on phi n1, but you know what this does when it acts on this (Refer Slide Time: 37:04) and that's just En 0 because it's just this equation and it's a real number. So if i take the adjoint, you get phi n 0 bra with H $_{0}$ acting on the right which is En 0 bra phi n 0. So this term cancels out. This is 0 by definition. En1 is a number and therefore it comes out and phi n 0 phi n 0 is unity since it's normalized. So it gives us our first important result.

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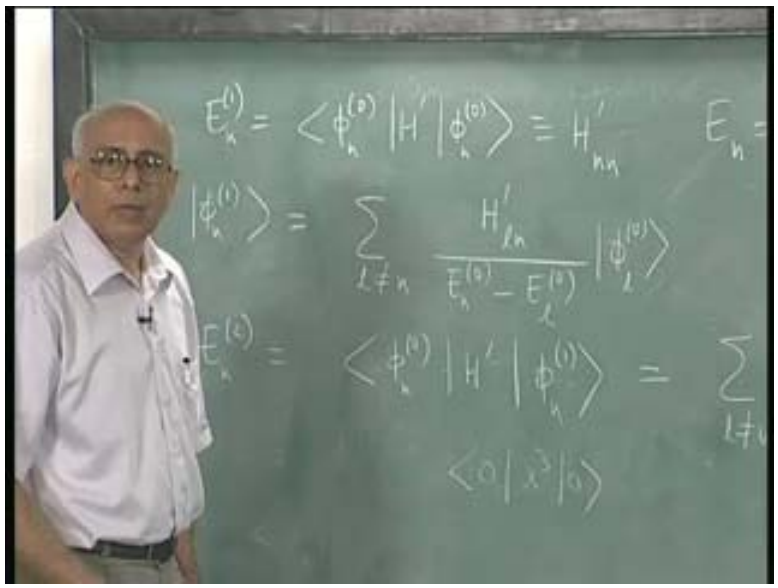

It says phi n E En1 = phi n 0 H prime. In other words, you give me the perturbation and i find the diagonal matrix element of this perturbation in the unperturbed basis and that's the first order correction. So by definition this = H prime $_{nn}$. It's the nn th matrix elements in the unperturbed basis. Remember, I assumed the Hamiltonian H_0 is diagonalizable. I find its eigenvalues and eigenfunctions. Then all these operators can be represented in this basis which is a set of eigenstates of H_0. So in that basis, this is the diagonal matrix element. The first order correction was just the diagonal matrix element. Recall that the other earlier problem we did with an E1, E2, and a delta delta, the first correction that came was a delta squared. There was no delta correction at all and the reason was the perturbation did not have any diagonal part. In the original basis, the matrix became E1 delta delta E 2 and there was no delta appearing in the diagonal elements. Therefore there were no diagonal elements and that perturbation did not give a first order correction. That's the reason it started with a delta squared. So now we have this crucial piece of information that you perturb a system and ask what's the perturbation of n th energy level. Then correct to first order, it's just the diagonal matrix element of the perturbation in this unperturbed basis. The question of what phi n1 is still remains.

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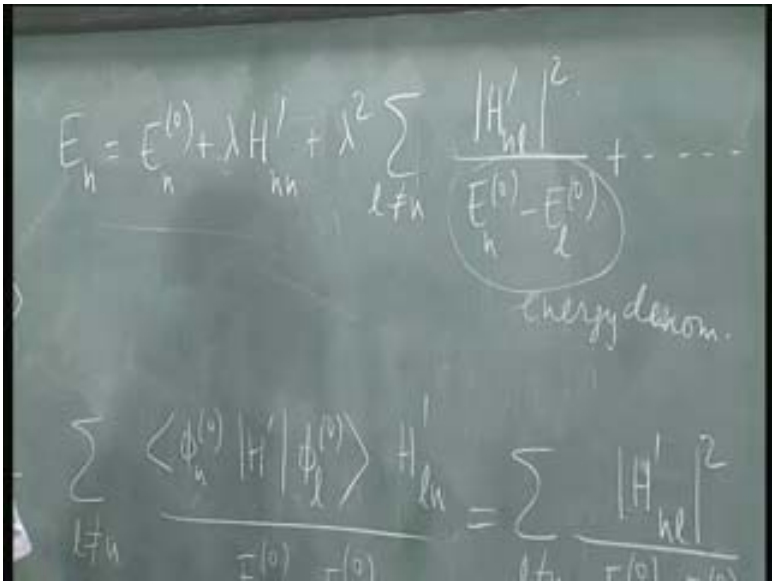

Phi n1 can be written as a superposition of states in this Hilbert space and the basis set we have chosen are the eigenstates of H_0. So I can certainly write this as a summation over l over all phi l 0s with some coefficients. These coefficients would depend on which energy level I am trying to correct. so that's going to depend on n and of course it would involve also the summation index l. if i do that, i need this equation but I will come back to it and write this down.

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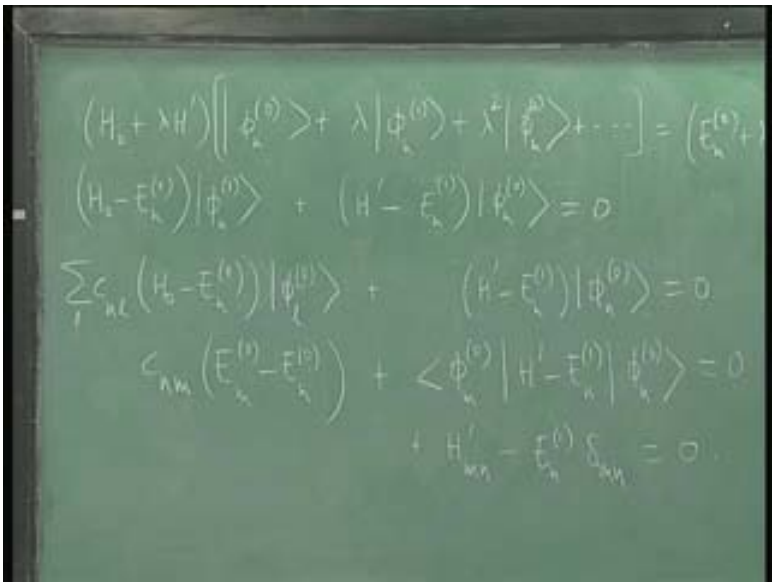

So let me substitute for phi n1, the first order correction to this vector which is an infinite series in the original basis. I plug that n there. then i get a summation over l C_{nl} H_0 - En 0 on phi l 0 + H prime - En1 phi nl. By the way, i am going to treat En1 as a known number. So we may just leave it here. The task is to find Cnl's. I take the scalar product on both sides with some member of the unperturbed basis, phi m for example. So I do phi m 0 on both sides. Phi m 0 is going to act on H_0 and it will produce Em 0. This is just a number. It's going to remain as it is. So this term will become summation over l C_{nl} Em 0 - En 0 phi m 0 and then it's going to be phi m 0 acting with phi l 0, scalar product which is a delta lm.

Because it's a delta lm, this entire thing collapses and you are left with just C_{nm}. so this term is Cnm Em 0 - En 0. because it's orthonormal, phi m 0 phi l 0 gives you Kronecker delta along with + phi m 0 H prime - En1 phi n 0 = 0. Now what is this going to give us? Well, the matrix element between m and n is just H prime mn. So this term here is + H prime mn. Nothing more than that (En1), which we already know. phi m 0 phi n 0 is delta mn = 0. So we are in business. There are 2 things here. First is what happens if n = m and the second is what happens if n is not equal to m. so it gives us a solution which says if n is not equal to m, then this term (Refer Slide Time: 45:40) is 0.

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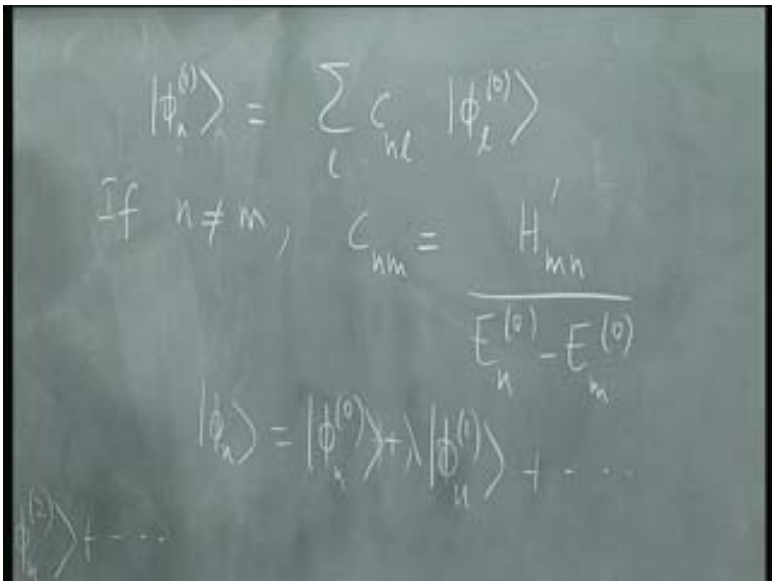

So you immediately get Cnm = H prime mn over En 0 - En 0. What is it if m = n? What's the diagonal portion? What's the physical meaning of the diagonal portion? you are trying to find the first order correction to phi n. we already know that phi n is already phi n 0 + lambda times phi n1 + higher order terms. We are writing an expression for this first order correction and the coefficient are what we are trying to find out. Now this state has to be normalized too. It's easy to see that this equation is not enough to determine Cnm because you put n = m, this vanishes. But you now take recourse to normalization. I would like phi n phi n to be normalized order by order. so what's going to be happen if there is a first order correction here and this was a 0 here (Refer Slide Time: 47:29)? You can, without loss of consistency take that over lap to be 0. in other words, if you insist on normalization and put some arbitrary Cnn, you will discover that to correct to first order when you normalize, it suffices to set Cnn = 0. That's the consistent way to normalize the state.

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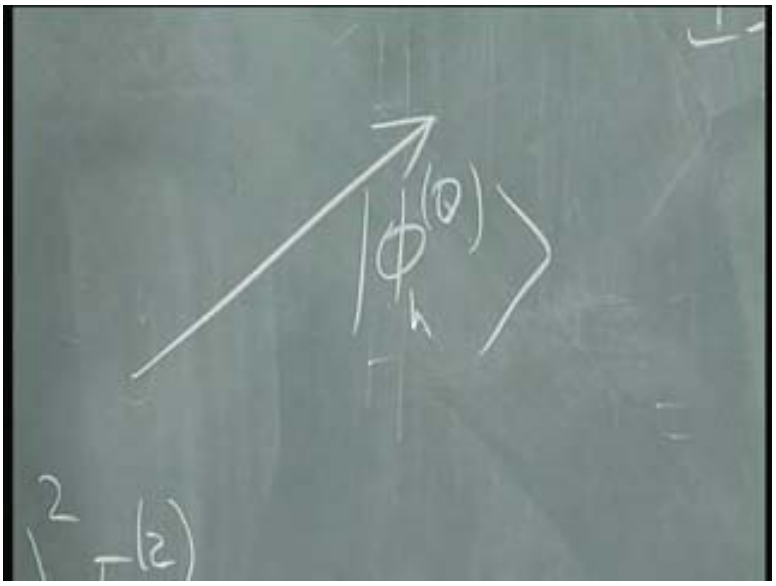

That's not surprising because you see this is the original phi n 0. It's some vector in the Hilbert space. Now my statement is: the correction to it might have a component along this to first order and in general, in all transverse directions. The statement I am making is that the first order term, if you want it to be normalized; there is no change along this direction at all but only orthonormal to it.

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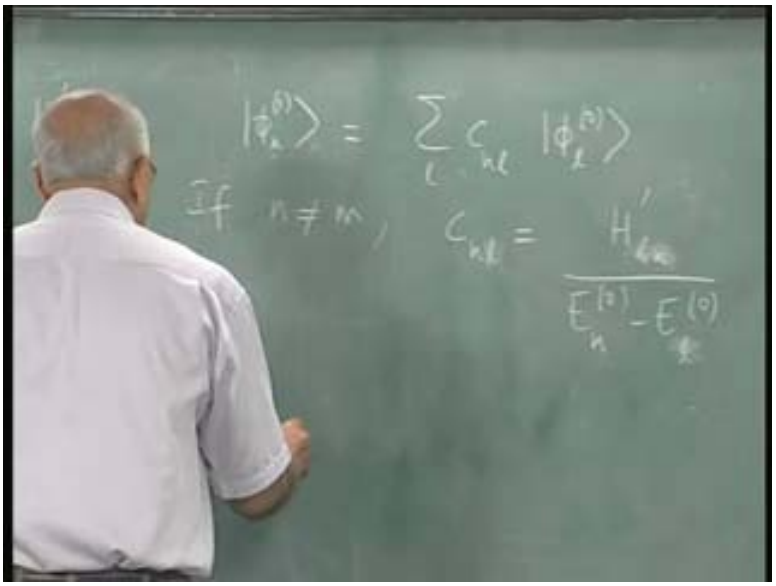

So with that proviso, we can write this term down explicitly. C_{nl} is just ln.

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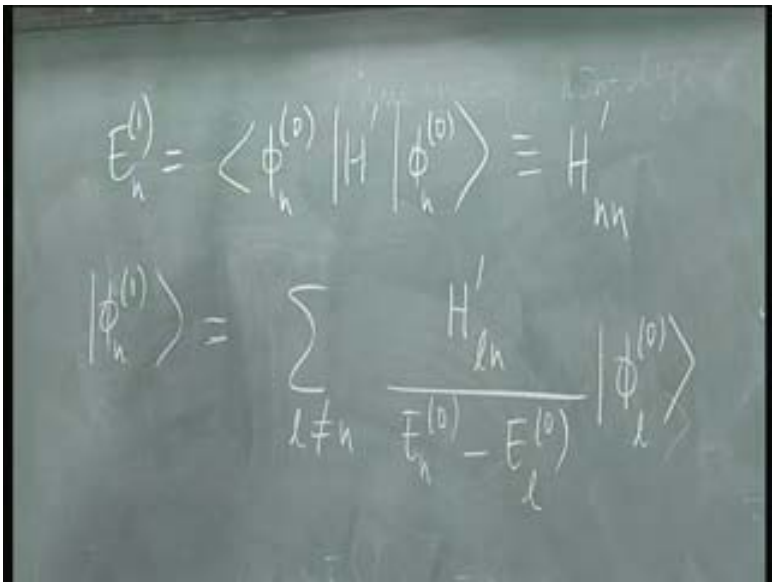

So I get a correction which says phi n1 = summation over l not equal to n H prime ln divided by En 0 - El ^{0} acting on phi l ^{0}. So that determines the first order correction. You can check that the function phi n 0 + lambda times phi n1 is also equal to1 to first order in lambda. Of course, if i take phi n1 phi n1, that's not equal to 0. There is a correction to order lambda squared but that's going to be compensated by the lambda squared correction to phi n. so the whole idea is to keep normalizing correct to some order and pushing the problem further and further away. then you get a consistent solution. So these are the first glimmerings and I want you to step back a little bit and appreciate what's involved here. So the first order correction to this level En 0 has shifted a little bit. It could have shifted upwards or downwards depending on this sign of the quantity En^1. Just the diagonal matrix element of the perturbation in the unperturbed basis. It's a very simple formula to remember. The first order correction to the state vector is phi n is phi n 0 + lambda times phi n1 and phi n1 has all these off diagonal elements because l is not equal to n and this divided by this quantity called the energy denominator. Now you began to see why this energy denominator cannot vanish. Then you have degenerate perturbation theory. The denominator is explicitly summed over all l not equal to n in this sign. What's the second order correction? One plugs in all this information into the second order equations and solves for En 2 and phi n 2 and so on. let me just write down the answer for En 2.

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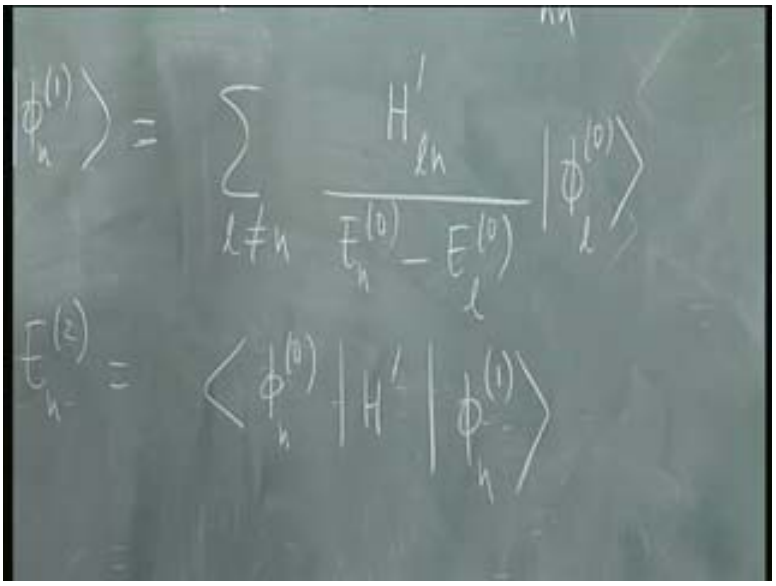

This turns out to be phi n 0 H prime phi n1. it turns out to be the overlap of the matrix element between the unperturbed and the first order correction and that is l not equal to n, phi n 0 H prime H prime ln divided by En 0 - El 0.

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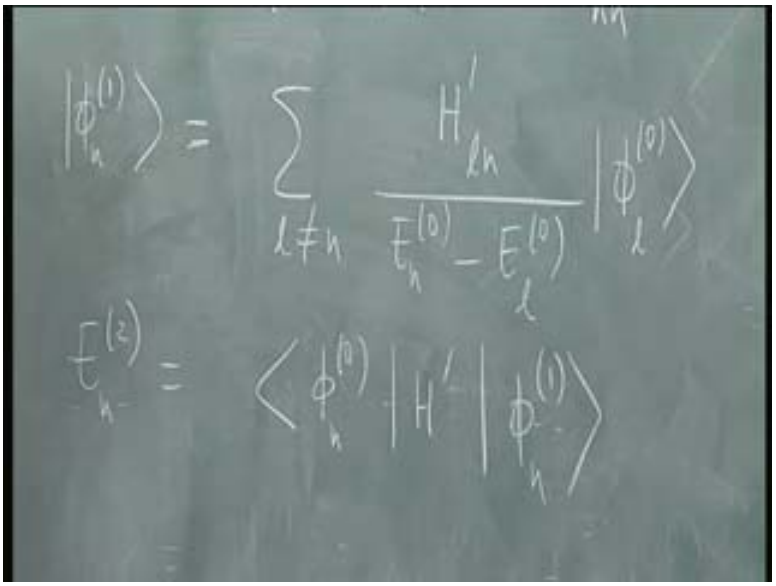

Remember these are numbers and not operators. This is the matrix element of H prime in the unperturbed basis between n and l. Therefore its H prime nl and nothing more than that.

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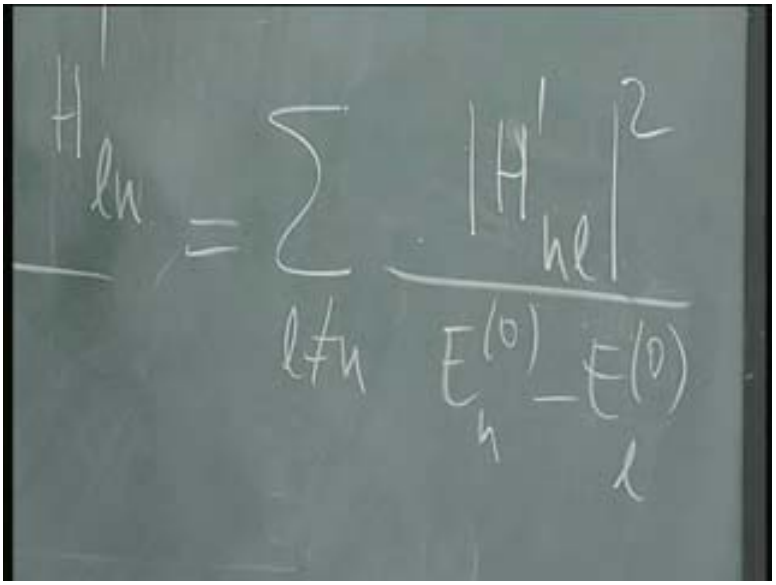

So this is summation l not equal to n H prime nl H prime ln divided by En 0 - El 0. Similarly, a longer expression for phi n 2 which I leave you to work out. But you can simply this a little bit. These are both complex numbers and this is Hermitian (Refer Slide Time: 54:11). So if I took the complex conjugate of this, you get phi l on the side phi n on that side and H prime remains itself because it's equal to its Hermitian conjugate.

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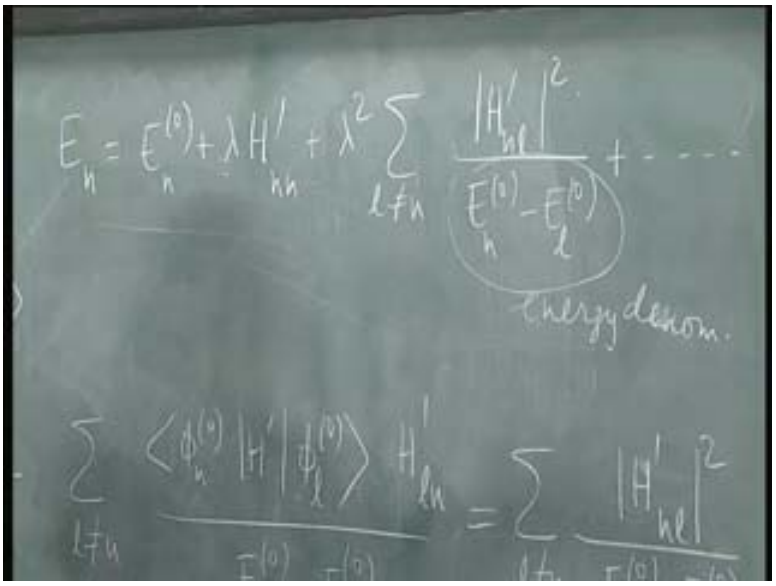

Therefore I can write this as H prime nl modulus squared. So we have En = En 0 + lambda H prime nn + lambda squared summation l not equal to n H prime nl whole squared En0 – El0. So we have a second order correction as well. It's clear for the energy denominator to converge. You are going to get more and more energy denominators and this is now a reflection of what we had already seen in the simple example where we got an E1 - E 2 and you got a delta squared. That's exactly what's happening here. So it's clear that the perturbation series has a chance of converging provided the matrix elements of this perturbation are small compared to the energy differences. That's the general rule under which you would have some hope of making this converge.

Now of course there could be special problems as we saw where this (Refer Slide Time: 56:10) vanishes and start with this and this could also vanish it could start with the x term and so on but1 has a systematic perturbation expansion. Notice something interesting. If I ask for the perturbation of the ground state of the system, then n is 0. Then in the ground state, E 0 0 is smaller than all the excited states and the summation is over all the excited states. This (Refer Slide Time: 56:35) number is never negative and the denominator is negative. So it means the second order correction to the ground state is always negative. Like I said there are many problems in which the first order correction could be 0. Then you are guaranteed that the first correction will be negative which means the ground state will go down rather than go up. That follows from this simple expression here. Let's try to apply this to a very simple problem. This problem is just the harmonic oscillator with a perturbation added to it.

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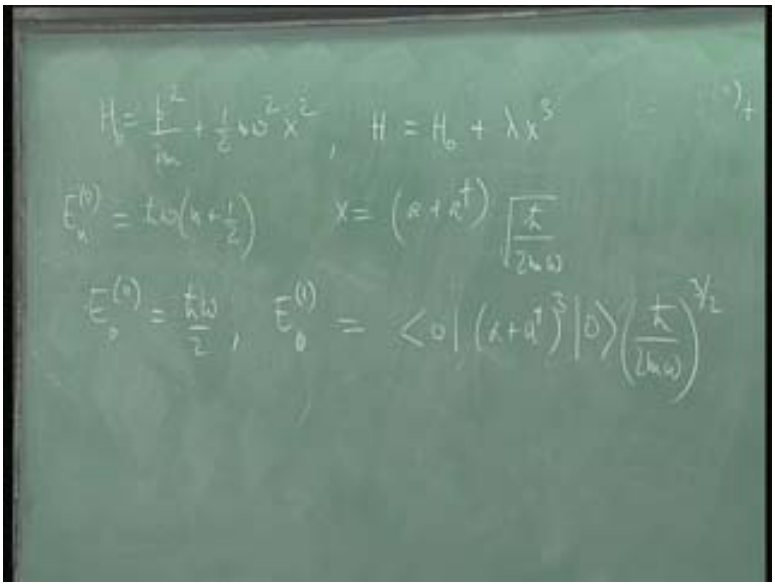

So I start with the harmonic oscillator which is p squared over 2 m + half m omega squared x squared. This problem is solved I know what the energy levels are. I am going to try to find to corrections to this under the perturbation. So this is my H_0 and $H = H_0$ + nonlinear terms. Let me add lambda x cubed in this case. Well, one could sit down and do this problem explicitly but you have to be a little careful. Let me ask if I add an x cube term, what do you think will happen to the ground state of the harmonic oscillator which had an energy half h cross omega? What do you think will happen if i had this with some positive number lambda? What do you think will be the first order correction? You have to find the matrix element of lambda x cubed in the ground state. That's all you have to do. Physically, what do you think will happen? You have this feeling, maybe this is going to become 0 because this potential was symmetric. Now you say you want to find the matrix element of odd functions. What's the matrix element? After all, this matrix element would correspond to calculating in our problem 0 x cubed 0. But if i wrote this in the position basis, then this stands for phi $_0$ of x which is a Gaussian e to the power - x squared over 2. That's a Gaussian and this is the complex conjugate of it. So you have product of 2 Gaussians e to the power - x squared and that's multiplied by x cubed and integrate it.

You expect it to be 0 (Refer Slide Time: 59:53). Indeed, that will happen because you see you can do this more easily as follows. x we know is a + a dagger square root of therefore I can write this as H prime nl modulus squared over 2m omega. h cross has dimensions ml squared t to the power -1 and the m and t inverse cancel with the m on the downstairs and so this is root of 2. So I have proper commutation relation between a and a dagger which should be 1. Therefore E 0 0 = h cross omega over 2. That's the ground state energy. I want to find first order in lambda. By our formula, it must be equal to 0 a + a dagger cubed 0 and then h cross over 2 m omega to the power 3 half's. Now if I expand this, we know a on 0 is 0. We know a dagger acting on the left of 0 is again 0. Now that expansion is going to either have 3 a cube

and a dagger cubed. All of which will give you 0 matrix elements. Or 2 a's and 1 a dagger which is going to vanish. So it's clear that the first order correction is 0 the second order will not be 0 in general. But this is a misleading problem because, if you draw the potential, classically what does it look like?

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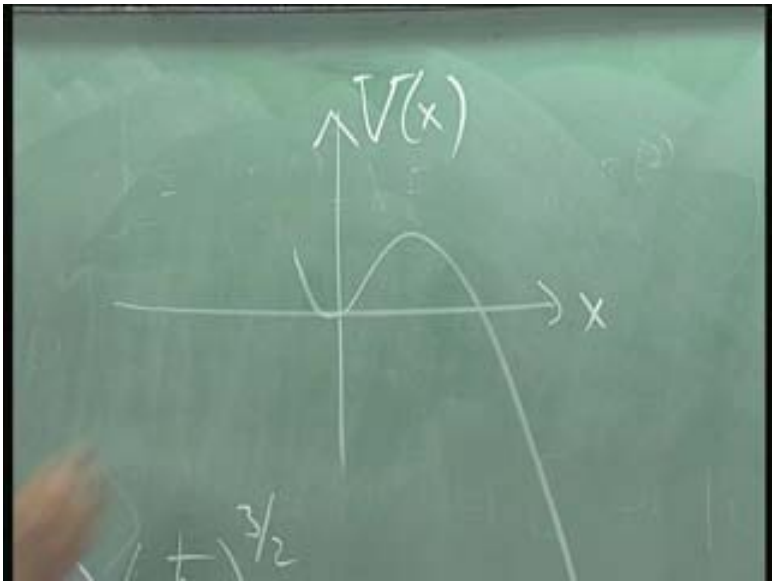

It's an x squared term + an x cubed. so it's clear that near the origin, V (x) near the origin is going to look like this but sooner or later, the x cubed term is going to take over. If lambda is positive, it's going to fall down and then of course this goes up. What's happening to the energy level here? It cannot be a stationary state because this will tunnel through out there and disappear if you wait long enough. So this is a symptom of that disease here. In this problem, although you can do this perturbation theory formally, the fact is our primary assumption that under perturbation, the set of bound states just shifted a little bit but remain bound states is no longer true. So in fact, this perturbation series cannot converge absolutely. You are going to write it down. It could be an asymptotic series or something like that. But if you work out all the terms it, cannot be an absolutely convergent series with any finite radius of curvature. However, it will give you the shift and energy because they form an order called metastable states. If the parameters are such that the tunneling time is very long, then the tunneling probability is small. It will give an approximation to the energy. So this was not so great an idea.

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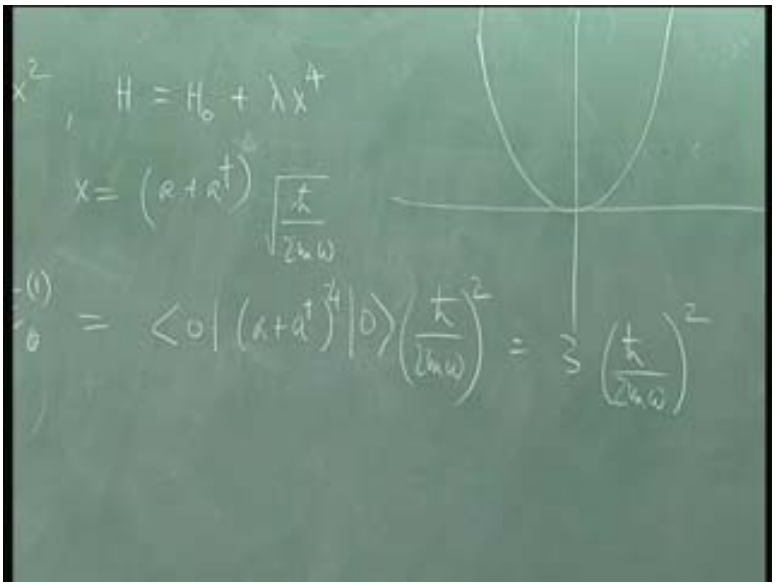

But what happens if I do this x4? Then you are in shape because now presumably, the potential looks still parabolic here but it becomes a little steeper. It is parabolic for sufficiently large x because the x4 takes over. Now you can see that classically, motion is always periodic orbits. quantum mechanically, it will be a discrete spectrum in this problem rigorously. Then, we could ask: what's the correction going to look like? How are you going to compute this number x4? What I have to do is to take this a + a dagger to the 4 and actually write it out. There is going to be a huge number of terms.

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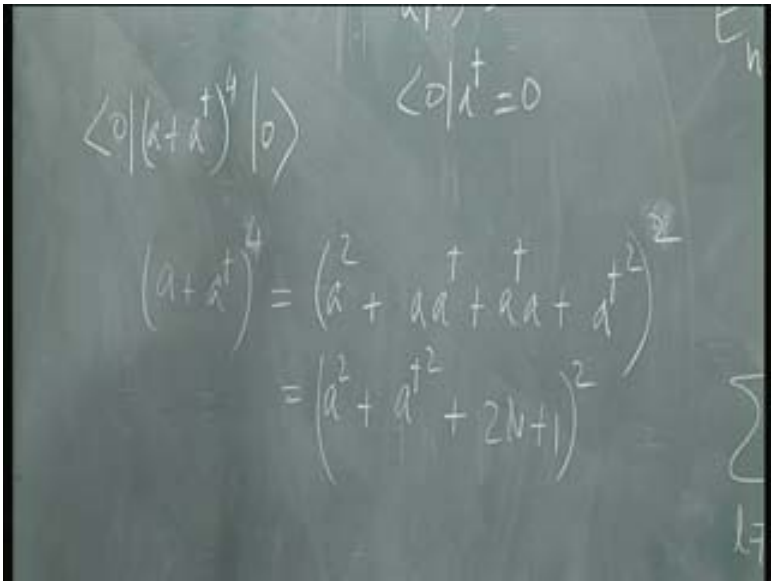

This is what I want to compute and please remember that a on 0 is 0 and 0 on a dagger is 0 because it's the ground state. If I expand this out, the a to the power4 term, the first term is obviously going to give me a 0. It's going to disappear. Similarly, the a dagger to the 4 is going to give me a 0. Then there are terms in which there are 3 a's and a single a dagger and that term is obviously going to be 0. Similarly 3 a daggers and a single a is also going to be 0. The only terms that will contribute are those in which you have a like number of powers of a and powers of a dagger and how do you compute this? Well, you have to sit down and write this thing out explicitly. But let's see if there is a cheaper way of doing this a + a dagger squared in this problem because this is a squared + aa dagger + a dagger a + a dagger squared. That's equal to a squared + a dagger squared. You should do what's called normal ordering. In other words, take all the a's to the right, take all the a daggers to left and then use the fact that a on the vacuum is 0 on both sides. So what are the terms that are going to contribute here? There is going to be a term which is a squared. So what I want is the 4th power of this term + aa dagger is a dagger a +1. But a dagger is a number operator. So this is 2 N +1 where N is the number operator. The number operator acting on the vacuum is 0.

So that's a cheap thing to do. So what is going to survive? It is a squared a dagger squared. The a's a dagger squared a squared term will vanish and then this squared is going to survive (Refer Slide Time: 01:08:35). When I do 0 here and 0 here on this side, this terminates in itself. This can be written as aa a dagger a dagger and you bring the a dagger to the left once again and write it in terms of number operators. You are going to get a contribution 2 from here and a 1 from here. So the whole answer is going to be just a 3. All other terms vanish. So this is a trick tried to normal order such products. Put all the a's to the right all the a daggers to the left and then when acting on the ground state, it gives you 0. Whatever numbers survive will be the only contributing factors. So in this problem, it will turn out that this is 3 times h cross omega whole squared. This is the first order corrections.

This goes up. The second order correction is guaranteed to go down. But if lambda is sufficiently small that will be negligible compared to the lambda correction. One final point, just to deflate the whole thing. Do you think that this perturbation series is absolutely convergent with a lambda x4? This is a very tricky issue. It's not simple at all. The answer is it cannot be an absolutely convergent series and the reason is very interesting. If this is true and the series converges absolutely, then it means that the power series that you get have a finite radius of convergence about lambda = 0. So everything is supposed to be analytic about lambda = 0. in other words the problem should be unchanged in a sense, even if a lambda is negative, the Hamiltonian should be Hermitian, so I can't make lambda complex, I can make it positive or negative, but if make lambda negative, what happens to that potential?

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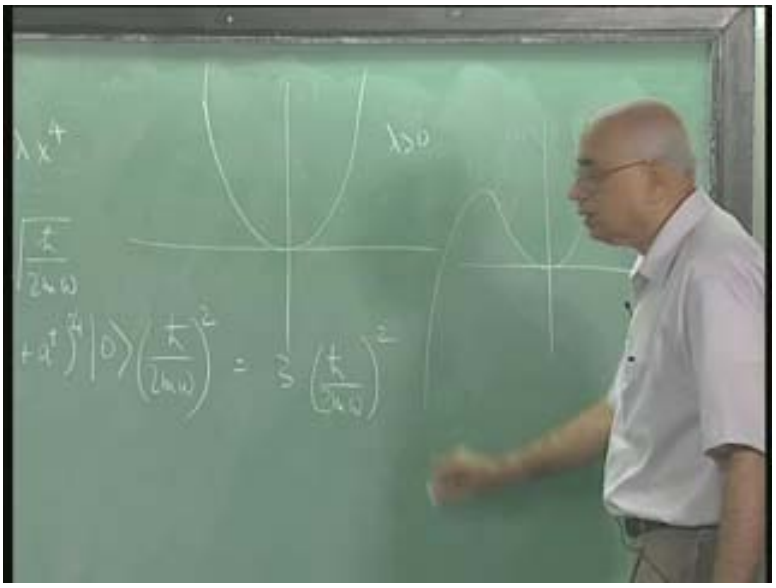

If lambda is negative, lambda greater than 0 or less than 0, it is still parabolic. But sooner or later, the negative lambda will take over and the potential will go down. So the ground state that you get here or any of these excited states would also be metastable states. That problem technically does not have only bound states for negative lambda. Yet that's the assumption that the perturbation is analytic in lambda and therefore makes sense as long as the Hamiltonians remains Hermitian. So this is a technical point and much work has been done on time to make sense out of this perturbation series. But it doesn't diminish from the fact that this perturbation series will give you a very good numerical value. This is very typical of what happens in asymptotic series. Numerical values would be very accurate but technically, the series itself may be formally divergent and so things of that kind start happening.

Here, I don't want to get into that but this tells you a little bit about how non-degenerate time independent perturbation theory functions. The crucial results for our purposes are that the first order correction is the diagonal matrix element of the perturbation. The second order correction is the off diagonal elements mod squared divided by the energy denominator with the corresponding expression for the wave function. Notice that even in the first order correction in the wave function in the state vector, these energy denominators appear. So in the second order correction, you would expect a product of 2. So this is the way the perturbation series is developed. The next task which I am going to do next is ask what happens if you have degeneracy. Finally, we will look at what happens if you have a time dependent perturbation and then look at its simple applications. So let me stop here today.