Group Theory Methods in Physics
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Lecture – 27
Selection Rules

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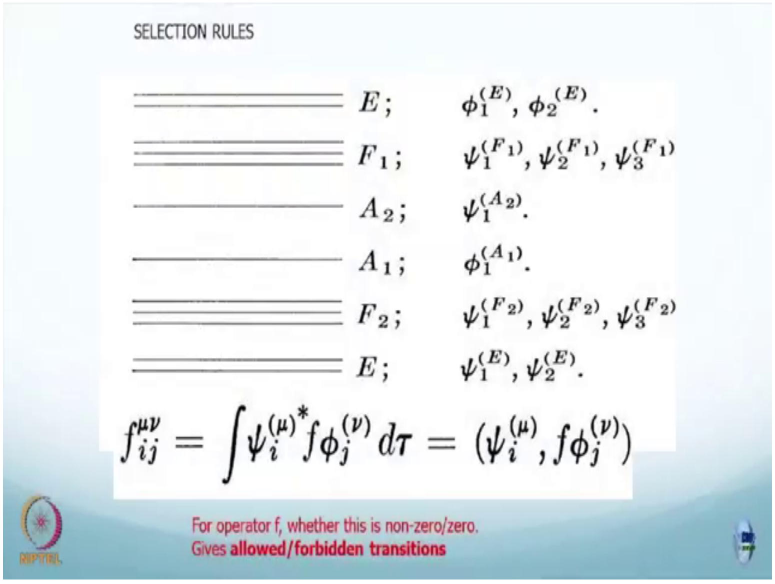

Ok. So, now, I am going to get to the Selection Rule where the operator F can be any of those physical observables operators of the physical observables F could be an electric dipole moment, or F could be a magnetic dipole moment or F could be a quadrupole moment tensor. So, these are some examples of the F which I have written formally can be any of these observables not just three, but any of you can have more observables.

Essentially, what you have to remember is that the observables which I am going to look at should have some leg in one of the irreps, if it does not have we cannot talk say anything about it. If it has a leg then what we want to do is we want to do suppose I want to do a transition from one ground state level to another level, ok. Just recall your harmonic oscillator a 1d harmonic oscillator and also the two-dimensional particle in a box, just for the sake you can recall those two examples.

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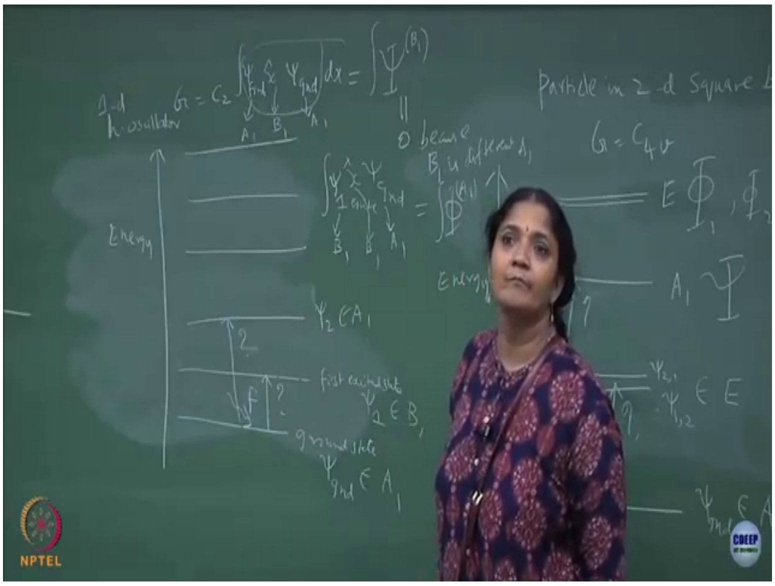

So, this is the energy line you have a ground state and it belongs to so, let me call it a psi ground, and it belongs to which irrep, A 1 irrep, right and then you can have a first excited state. Let me call it as one here to remember it is the first excited state and that will belong to it is an odd function, this is an even function, right. So, this will belong to B 1, it belongs to the irrep B 1.

So, what is the group symmetry here? Group symmetry is C 2, 1-d harmonic oscillator harmonic oscillator, group symmetry is C 2 and I can start and you know every level is non-degenerate because it is an abelian group. Each element is a class by itself and you can show that if it is a 1-d basis, there is no way you can get degeneracy. So, this is going to keep going and so on.

Question can be asked, suppose I am in the ground state and I put in an interaction given by some electric dipole moment operator line. Can the particle which is in the ground state? Can it go to let us say this one; question mark, can it go to let us say this one, ok. Are both possible, something is possible, something is not possible is the questions we are asking.

You understand the question, is there a transition allowed going from a initial state to a final state due to interaction by some operator associated with it also you have an irrep, ok. This observable also has a it is also associated with the irreps, is that clear. So, this is the question can we find a transition happen, ok.

For example, if I take the initial state to be ground state and if I put the operator as x operator, let us look at only the x component of your electric dipole moment is non-zero and if I want to look at psi final dx. You all know how to do this right, all of you know how to do this which one will be nonzero, which one will be 0 is the question, right. If this was an even function and if this 1 is also an even function will this be zero or no?

Student: Zero.

Zero, right. So, you know that. So, if this belongs to A 1, if this also belongs to A 1 ok, x operator belongs to B 1, clear. So, operator belongs to B 1, you can show that product of A 1 with B 1 will be what, A 1 is unit; A 1 with B 1 is again B 1 and B 1 with A 1 is also A 1, B 1 sorry.

So, ultimately this object can be treated as if there is some I do not care about the numbers it is something which depends on B 1. You all agree this is what I get out of this in group theory using tensor products states also belong to irreducible representations, operators also belong to irreducible representation.

If you take the x component of the electric dipole moment operator, it belongs to the B 1 irrep of C 2 and if I blindly treat it like a tensor products of irreps. I end up getting something which will give me some object which belongs to B 1 could be a tertiary bases. And, by odd even argument you have already argued this is odd, sorry this is even this is odd this is even that integral has to be zero is what you argued.

Now, we want to see how to argue it is 0 from group theory ok. So, that is what is the theme now and then the great orthogonality theorem again comes into our rescue to say that it is going to be 0.

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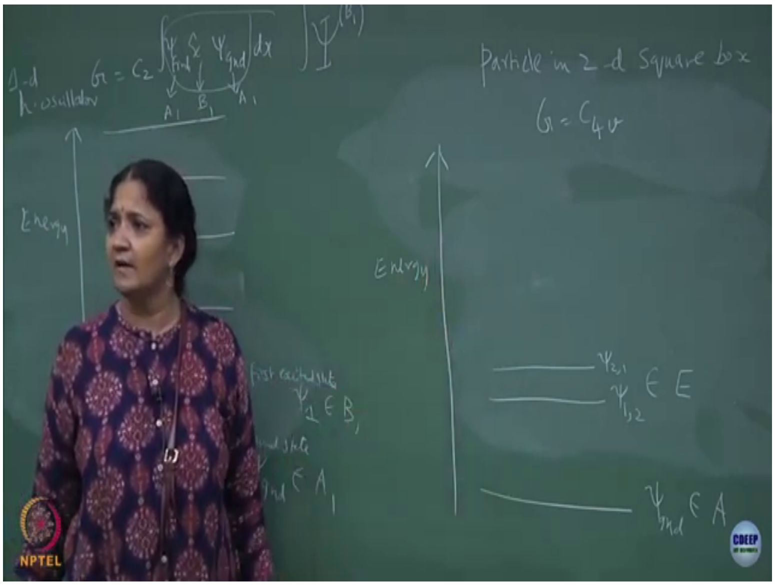

If you go to other examples like particle in a two-dimensional box, the group symmetry is C 4 v, ok. Again, you can plot as an energy, ground state will be the lowest energy which should be a belonging to A 1, ok. Then you can start looking at psi 1 comma 2, psi 2 comma 1 because you can start giving degeneracy, because C 4 v allows for two-dimensionally irreps you can have a elements of E, ok.

Similarly, other irreps I am not really writing what the other irreps are, but each thing will repeat this has happening for the ground state does not mean A 1 should not happen some other like here, you know the second excited state psi 2 belongs to A 1, ok. So, the repetition is allowed; so, this belongs to this, the energy scale decides for you whether it is a lower energy or higher energy.

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So, there could be repetition another one with A 1 belonging to A 1, but a different wave function, and then another two-fold degenerate; the two-fold degenerate you should draw it close. So, that you know that both have the same energy that is the meaning of drawing those lines very close. So, if this will belong to E some other wave function and so, on there will be phi 1 and phi 2 because it is two-fold degenerate and so on.

Now, our claim is that we again want to see that if there is a triggering by an external operator F which corresponds to some measurable observable, whether the particle will undergo a transition to this or a transition to this and so on, clear. So, this is the theme of selection rules, I cannot get you a number, I can always say whether it is zero or nonzero.

So, I can say whether this transition is allowed or forbidden, this transition is allowed or forbidden, clearly you know which one is allowed, which one is not allowed now in this example, right. If you go from let us say ground state to the first excited state it is allowed for the excite operator; to go from ground state to the second excited state, it is forbidden from odd or even you can argue. Now, we are going to argue from group theory and see that this is exactly what is going to happen.

So, selection rule will not give me an number for the nonzero answer, it will only tell you whether the transition triggered by an observable operator F is going to happen or not happen; not happen means it is 0, happening means I cannot give you the exact value for it, but I can say if this will be C, is that clear.

Student: What will be (Refer Time: 11:43) for group theory (Refer Time: 11:45)?

I am going to do that; right now I have not done that, but what I will said here is that just the odd or even you can argue to zero when you have to do an integration, but now I am going to do the group theory. Before you do the group theory, I am warming you up what to expect from the algebra that is why I am trying to give you this examples, ok. So, that you are all alert to see how the great orthogonality theorem gives you the answer, I want you to appreciate it, ok.

Student: Here (Refer Time: 12:15) it is the function of E 1 therefore, which is the (Refer Time: 12:18).

No, no, no; so, this turns out to be this, I am going to argue that this is zero.

Student: Ma'am, one there could the (Refer Time: 12:28) return the extensible (Refer Time: 12:30), who?

No, no, one particular example I am taking can do magnetic dipole transitions, if you do a perturbation by an external electric field you can have the speed or t kind of term in the Hamiltonian. You can start doing these kinds of transitions, you understand what I am saying. So, these are the matrix elements which you will compute and explicitly you can do the computation, but from group theory and group symmetry you can at least without even doing the computation you can say it is zero or non-zero that is the power of group theory. You do not need to compute the matrix element between an initial state and a final state due to this operator, ok.

You can do it elaborate quantum mechanics like the way this one you can write the explicit wave function, do the integral and show it to be 0. This simple thing you know odd even and all you have learnt, but in a complex situation you may not have these information without even doing can you say it 0, it cannot be 0, it can be 0, is itself a powerful tool and that is what I want you to appreciate from group theory, yeah.

Student: (Refer Time: 13:50).

Because this is a dx integration which is going from minus infinity to plus infinity, if you do any change of that x to minus x, this answer will become minus of itself.

Student: (Refer Time: 14:06).

Is it that is I am trying to say, but this is odd even argument, but I am also trying to tell you how to see from group theory here, I have still not proved to you that this is 0 which I will prove now, yeah. Any, is it clear what we are going to now look for. So, essentially I am saying in any complex system with some group symmetry there could be three-dimensionally irrep, two-dimensional irrep; the close lines means, they are degenerate there will be so many wave functions. I am just calling it as psi 1, psi 2, psi 3 and you can have for F, A 1 you know all these possibilities. So, this I am calling it as a different function phi 1 and so on.

So, I am just trying to say a hypothetical situation where you have the energy levels and you want to look at the matrix or this left hand side due to the initial state phi j in an irreped mu, due to the operator f, going to a final state phi j in the irrep nu.

And this matrix element is it zero or nonzero clear, if it is zero you say that going from the state phi j in the irrep mu to this one triggered by this operator or this interaction is not possible that is the elaborate meaning of this expression. So, for operator F whether this is non-zero or zero gives allowed or forbidden transitions ok.

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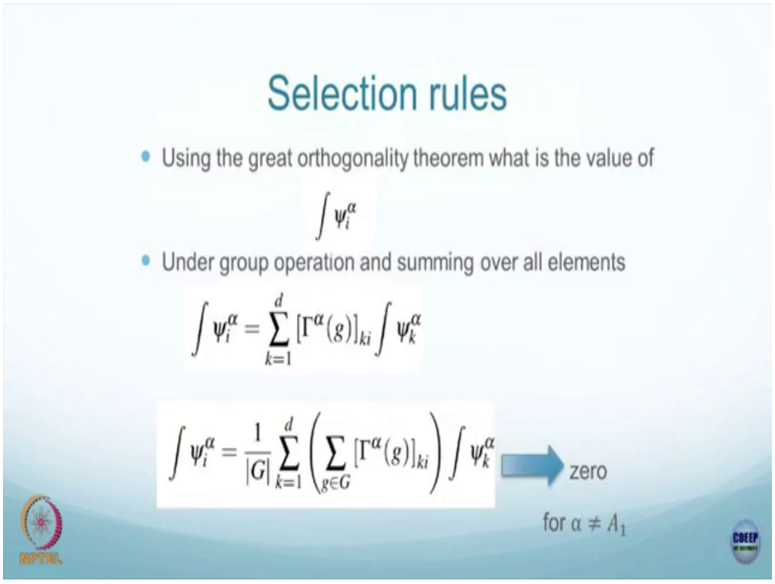

So, now I am coming to the proof. So, suppose I want to work out what this is ok, I want to work this out, clear. So, to work it out that integral regions and all I do not need to mention. Let us keep it as formal integration it could be in dx, it could be dx, dy, if it has other internal quantum numbers you may have to sum up over those quantum numbers also, but as of now let us keep the integral as formally an integral let us not worry about it.

It belongs to an irrep which is given by alpha in this particular example, it belongs to B 1, ok. But, I also taught you that whenever it has a group symmetry like C 3 v or any group symmetry C 2. You are allowed to do a group operation on a state belong to an irrep, Ii it is one-dimensional irrep, it will be constant times itself; if it is two-dimensionally irrep, it will become a linear combination of the basis which in that irrep which is that degenerate lines which I have drawn, right.

If it is let us take this two-dimensional irrep, if I do a if I take phi 1 from that, if I do a group operation on phi 1 it can in principle give you a linear combination of phi 1 and phi 2; you all agree, right. So, it will always be a linear combinations of them, that linear combination coefficient depends on what is your group operation. If you do a identity operation it will be phi 1, if you do let us say a C 2 operation then something else can happen and so on, C 3 v if you are doing you can have a linear combinations of mixing between phi 1 and phi 2, is that clear.

So, that is what I am doing now, apply a group operation and sum over all the group elements, ok. So, group operation psi i alpha for a particular group element, there is a matrix for each of the irreps. If it is a E dimensional irrep, it will be a 2 cross 2 matrix; if it is one-dimensional irrep, it will just be the character depending on which you are looking at it will be in general a matrix, ok.

And you get a linear combinations within the same alpha irrep, it does not move from alpha to some other irrep if it belongs to the E-dimensional irrep. The rotation operation given by the matrices 2 cross 2 matrices will only mix these two, it would not give you anything from here is that clear and then I am summing up over all the elements also.

Now, tell me if I just look at this thing this one, you can use this great orthogonality theorem taking the other irrep to be your unit representation then you will get delta alpha A 1. Why, because the unit representation matrix elements, are all 1 right, are you all fine with that you remember. So, you can take this gamma alpha of g then gamma A 1 of g, it is same as that summation over g, ok.

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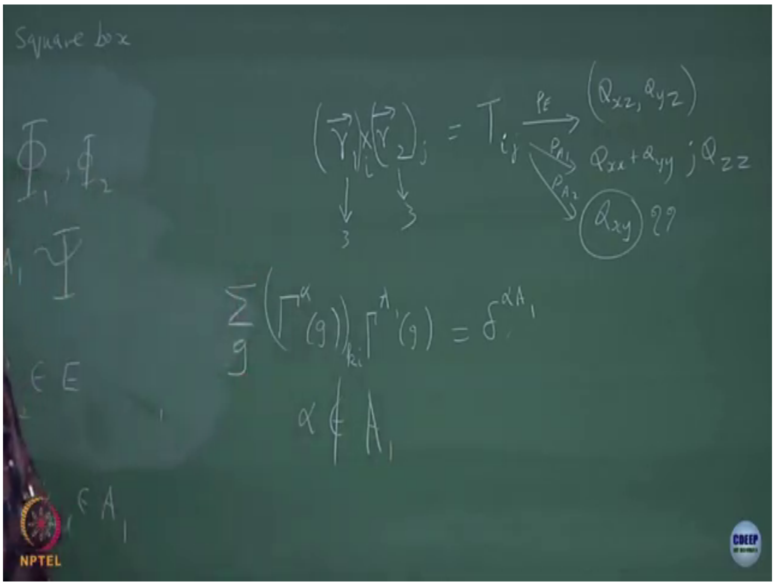

So, it is exactly same as that this is anyway 1 by 1 matrix you can show that this is going to be delta alpha A 1, right. So, which means alpha if it is not belonging to A 1, it is always zero; is that clear. So, that is what is the last line that this bracketed one piece this piece by great orthogonality theorem will be nonzero only for A 1, it will be zero otherwise, clear.

Here we got B 1 which is not A 1 by doing this tensor product I said it belongs to B 1 go to that top step here psi i alpha when alpha is not equal to A 1 is 0, is that clear. So, what have I proved, I wanted to find what is psi i alpha and I proved using great orthogonality theorem, it is 0 if alpha is not equal to A 1, clear.

So, that is why this combination when I do, I get a B 1 and invoking that line I will say that this will be 0, because B 1 is different from A 1, right. Let us do for the sake of doing this, instead of doing this we did this for ground state to this excited state that is 0. What about this one to this one, can you check what happens there?

Suppose, I take first excited state x operator psi ground, this one belongs to B 1, this one also belongs to B 1, this one belongs to A 1. A 1 times B 1 is B 1; B 1 times B 1, what is it you just have to multiply the characters right, the characters multiplied will give you that is A 1.

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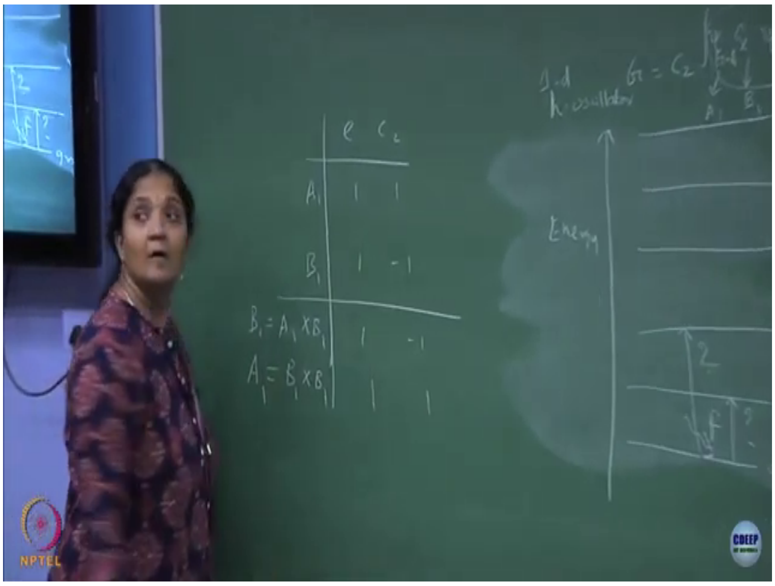

So, this multiplication of B 1 times B 1 is A 1, A 1 times A 1 is A 1. So, essentially it will give you a piece which is A 1 and by this argument it will be nonzero. So, what I have tried to prove for you that there is a transition allowed to go from ground state to first excited state triggered by the x component of the dipole moment operator, but there is no transition possible to go from ground state to second excited state for example, triggered by the dipole moment operator.

Explicitly you can do, but now I have invoked this argument to say that anything which is nonzero is happening when after you have done all the tensor product that alpha turns out to be A 1 it will be nonzero, the alpha turns out to be not A 1 you can blindly set it to 0. You do not need to do any computation, yeah.

Students: Ma'am, in this situation (Refer Time: 25:31) whether it comes with A 1 because we have to bring it down state here (Refer Time: 25:35).

No, no, nothing to A 1 is a trivial representation whose character is always 1, you can always insert it anytime.

Student: Why we have taken A 1, why not B 1 or (Refer Time: 25:45) a similar thing?

Yeah, if you take B 1 in that expression which I have written is same as this expression only when I put A 1 because these are just 1. I am just inserting, see this expression which I have it on the screen did not have that gamma A 1, I am saying that this expression is same as multiplying with gamma A 1 because gamma A 1 does not do anything to it. It is like inserting something just for the for convenience, but by inserting that I can do this argument of great orthogonality theorem to argue it is 0, is that clear.

So, also 1 of your problems which I gave it in your exam. No second which expression this is together say, I am just saying apply the group operation and after that you do a summation over all the elements and average it over it that is all, ok. So, I am not doing anything more than that.

Student: A 1 to B 1.

In a regular representation can be written as a direct sum of the.

Student: A (Refer Time: 27:00).

Yes, if it is regular representation, I am not doing any regular or anything I am just looking at a state which belongs to 1 irrep, I am just doing a group operation if it belongs to a degenerate irrep then that is the group operation will actually mix them and I am just trying to see what happens under this operation that is all. Yeah, any other question, see both sides you can put that summation, it is just that 1 over G will make it 1 because it is not really acting on that ok, is this clear um.

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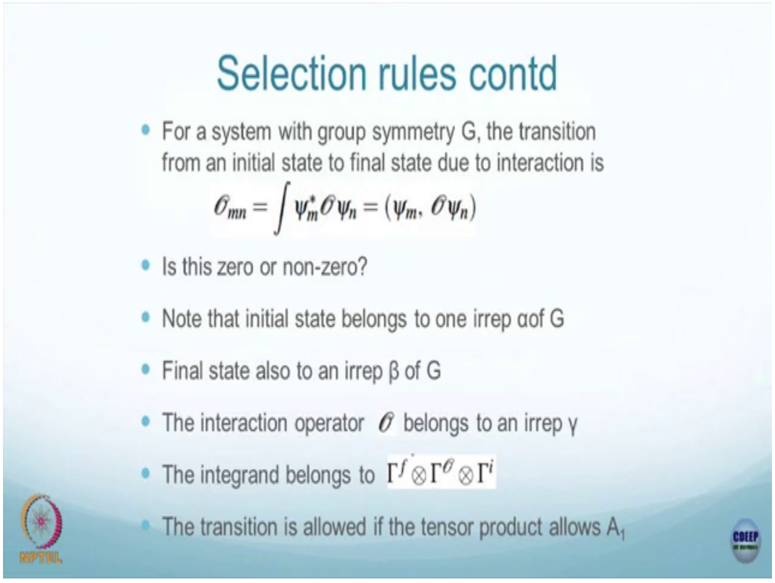

So, now I am just trying to add it to the system, I am just summarizing whatever I said now with these two examples.

Student: Whether it is fixed or produce to the group (Refer Time: 27:47) x belonged?

Yeah in this particular harmonic oscillator x belongs to the basis here will be z and this will be x because I am looking at x going to minus x, ok. The x 1 will change sign, I am doing a 1d harmonic oscillator. So, I am just I know that this belongs to the primary basis belongs like this ok, is that fine.