**Symmetry and Group Theory**
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**Lecture -37**
**Direct Product Applications**

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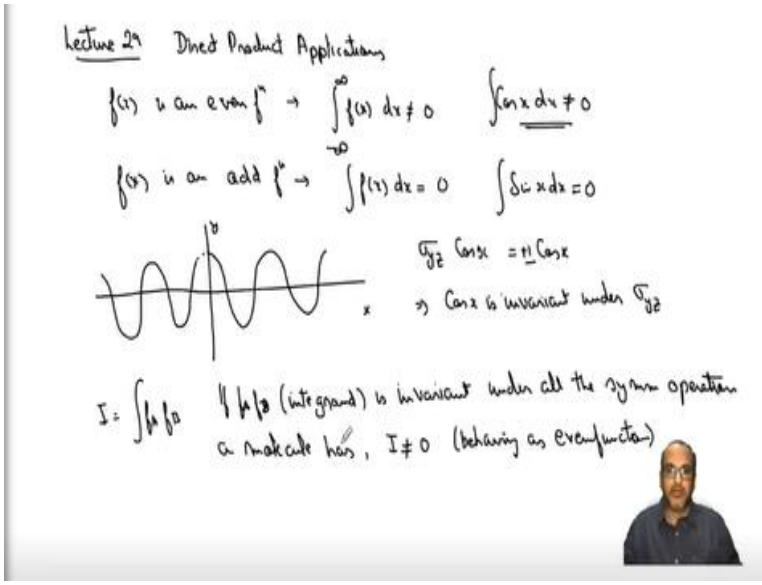


So, in the previous lecture we have seen what is the direct product. And we calculated the direct product of various irreducible representations. So, in this lecture we will be looking at how direct product is used to solve quantum mechanical problems, problems of quantum mechanics. So, Direct Product Applications. So, let us start with what we know? So, we know what is an even function and what is an odd function. So, let us suppose that fx is in even function. And if it is so then assuming that it is continuous over all range.

The integration of fx will not be equal to 0, because it is an even function. Whereas if fx is an odd function, then the integration of fx dx will be equal to 0. So, we can see this example as cos x, so cos x dx over all space will not be equal to 0 whereas sin x dx over all space will be equal to 0. So, why is it so? Because let us draw this function to understand it more clearly. So, if we draw the cosine function it goes like this and then on the other side it goes like this. Assuming this is my x axis and this is my y axis.

So, that means if I am putting a plane which is yz plane. So, sigma yz if I am putting then if I operate sigma yz on to the cos x, I will get cos x. That means the character under this is plus 1. So, this would imply that cos x is invariant under sigma yz. So, this tells us that invariant because our character is plus 1 when we apply sigma yz on to cos x. So, now we understood when we how we apply cos various symmetry operations we can on to different molecules.

So, similarly we can apply this symmetry function symmetry operation on to a mathematical function as well. So, whereas if you apply sigma yz on to sin x you will not get plus 1 as a character. So, now let us think that you have integration to solve where you have two functions f A f B. You do not know whether it is even and odd or the product of that is even or odd. It is sometimes not easy or straightforward to calculate.

But we can see how in context of symmetry and group theory we can solve this integration. Or we can at least tell whether it is going to be 0 or non-zero. So, let us say if this integrand f A f B, let us call this integrand the product of f A and f B is invariant under all the symmetry operations a molecule has. So, we are talking about a molecule and the corresponding symmetry operations. So, whenever we are considering the molecule then it has certain symmetry operations.

And then it falls under a particular point group. So, in that context if two functions which form basis of certain representations. So, they are invariant under all the symmetry operations a molecule has, then let us call this as I then the integration will not be equal to 0. That means it is behaving as even function just like we saw the case of cosine x. So, just like we saw the case here.

Cos x dx so because it is invariant under sigma yz. We saw that it is not equal to 0. Similarly, the integrand is invariant under all the symmetry operations. Here the symmetry operation was we chose was only sigma yz. But here we are saying that if the integrand is invariant under all the symmetry operations, then I will not be equal to 0. Otherwise, if it is variant that means if it changes by application of a symmetry operation.

Then the integration will straight away go to 0. So, it is a very useful thing in quantum mechanical problems whether a integration will be equal to 0 will vanish or will not vanish. So, we will see that let us see that.

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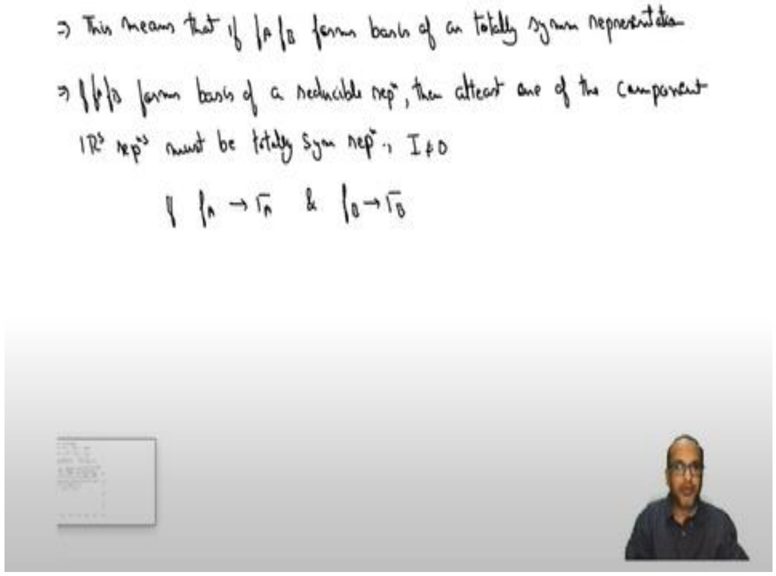


So, what does it imply? This means that if this product f A f B forms the basis of a totally symmetric representation. So, we know what a totally symmetric representation is? It carries one under all the symmetry operations. So, if f A f B the product of this or the integrant here forms the basis of a totally symmetrical representation, that would mean that it is invariant under all the symmetry operations.

And then the integrant or I will not be equal to 0. So, let us say if f A f B forms basis of a reducible representation. It is possible that it can form basis for a irreducible or a reducible representation, we do not know. So, let us say if it forms the basis of a reducible representation then at least one of the components IRs or IR representations must be totally symmetric representation and in that case, I will not equal to 0.

So, either it should form the basis for a totally symmetric representation or it should form the basis of a reducible representation which in turn should contain at least one IR representation. So, when would that be? So, let us say if f A forms the basis of tau A. And f B forms the basis of tau B.

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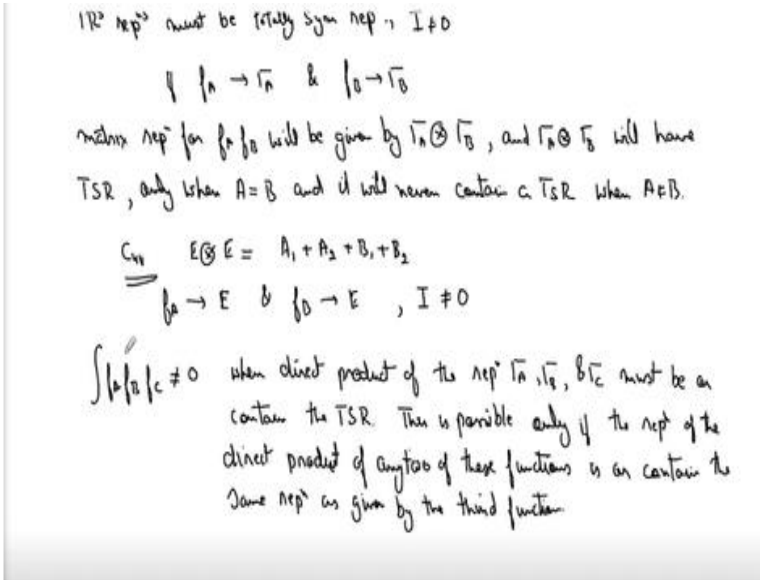


So, in that case the matrix representation for f A f B will be given by tau A direct product tau B and tau A tau B direct product will have totally symmetric representation TSR, only when A = B and will never contain a TSR when A is not equal to B. So, that means direct product of a IR representation with itself will contain totally symmetric representation. So, that means f A and f B should form or must form the basis for same IR representation then only the integration will survive. Otherwise, the integration will go to 0.

So, for example in the case of C4v, when we calculated our direct product of E cross E, we saw that it can be reduced to A1 + A2 + B1 + B2. So, that would mean that if f A forms the basis of E and f B forms the basis for E in this particular case. Then I will not equal to 0. Otherwise, if f A and f B are forming basis for two different representations, then I will be equal to 0. So, the problem is now very simplified. All we have to do is given a function we have to find out what is the irreducible representation to which that particular function is forming the basis of.

If the two functions are forming basis for a same representation, I will not be equal to 0. If the two functions are forming basis for two different representations, I will be equal to 0. So, very simple know. So, now let us also look at in the same way let us also look at integration of triple product whether it will be equal to 0 or not. So, this will not be equal to 0 when direct product of the representation tau A, tau B, and tau C assuming that f A is corresponding to tau A f is corresponding to tau B, and f C is corresponding to tau C, must be or contain the totally symmetric representation. So, either they form a totally symmetric representation or they must contain totally symmetrical representation once and when is this possible? This is possible only if the representation of the direct product of any two of these functions or as contain the same representation as given by the third function.

So, let us try to digest this. So, what we are saying is that if there are three IR representations corresponding to these three functions, then the direct product of all three must contain totally symmetric representation. So, this is possible if two of this if the representation of the direct product of any two of these functions let us say tau A into tau B must contain tau C or tau B into tau C must contain tau A and so on. Let us see how it works.

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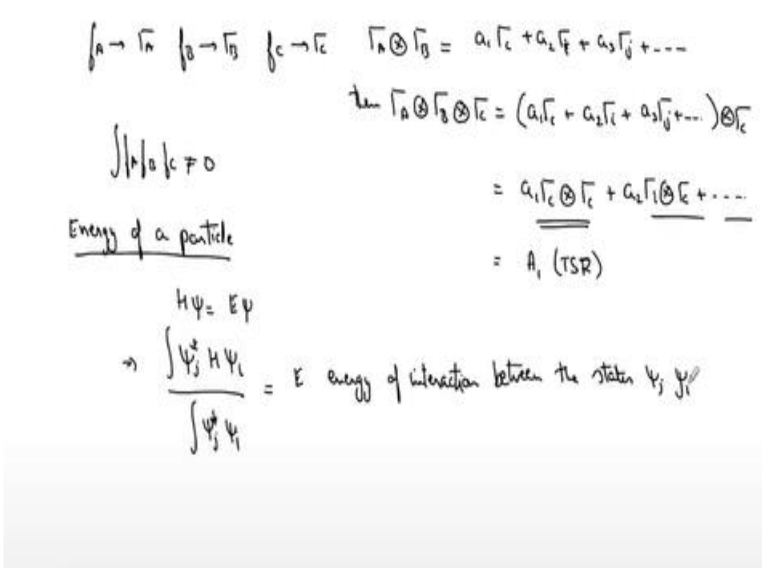


So, let us say if we have f A is the basis for tau A, f B is the basis for tau B, and f C is the basis for tau C. And we have what we are trying to calculate is direct product of tau A and tau B that may contain a1 times tau c + a 2 times tau i + a 3 times tau j and so on. So, now then if we calculate the triple direct product now tau B, tau C then this will be a1 tau C + a 2 tau i + a 3 tau j direct product tau C.

Now if you see a 1 tau C direct product tau C + a 2 tau i tau C and so on. So, this is the only one which will give you A1 or let us call it as TSR, Total Symmetric Representation. None of the other direct products because they are direct products between two different IR representations, they will never give A1, that is the Total Symmetrical Representation. So, you will get totally symmetric representation only from direct product of tau C into tau C.

So, that means tau A into tau B must contain tau C. So, only if tau A into tau B contains tau C then we have A1 present in the system. And if we have A1 present in the system, we can say that the integration of f A, f B, f C is invariant under all symmetry operations. If it is invariant it behaves like even function and the integration is not equal to 0. So, that is the point what we are trying to make.

So, let us say now let us try to see where this particular integration is useful. In the energy of a particle, in calculating energy of a particle, energy between those states and so on. Let us say in quantum mechanics, we often come across with integral where we have to calculate energy of a particle like. How do we do that? So, we know this equation H psi= E psi and what we can do is? We can multiply we can write this thing equation write it like this.

Let us say this is star and psi j star psi i this will be equal to E. So, now this is the energy of the interaction between the states psi j and psi i. So, now how to solve this integration now?

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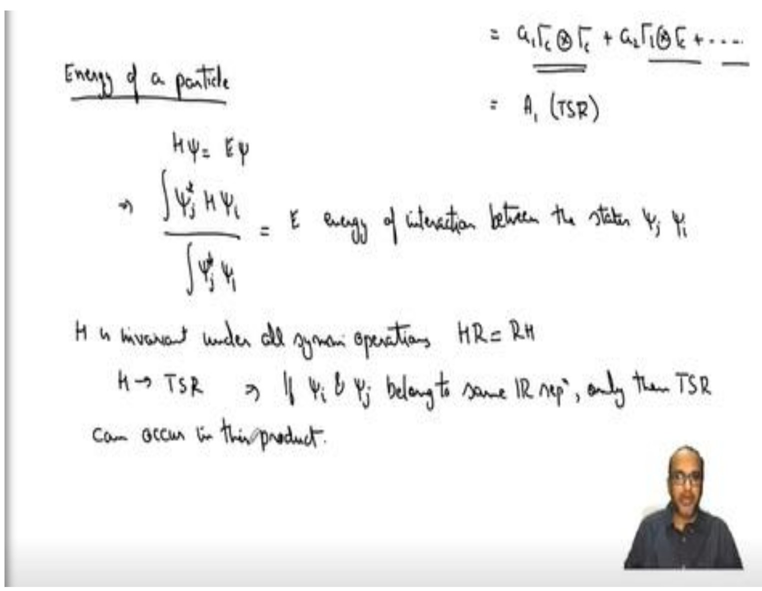


So, now we have to estimate or rather calculate what is the IR representation to which psi j, H and psi i are forming the basis. So, let us first talk about H. We know that H is Hamiltonian. We know that H is invariant under all symmetry operations, we have seen that earlier, all symmetry operations. So, we have seen that H and R commute with each other. That means it will not matter whether we are first operating the symmetry operation or first doing the energy estimation.

This would mean that H will remain invariant under all the symmetric operations, that means H will form the basis of Totally Symmetric Representation. So, that means now if we know tau j and tau i, then this does not actually matter because this is always tau A, A is the totally symmetric representation. So, this would imply that if psi i and psi j belong to same IR representation only then totally symmetric representation can occur in this product.

So, to know whether this integration will go to 0 or not, we need to identify whether these two will form basis of same IR representation or not. If they form basis of same IR representation then TSR will exist in this product, if TSR will exist the integration will be non-zero. So, that means there would be finite energy, otherwise integration will be equal to 0 if these two-form basis of two different IR representations.

And then we can say that the energy of interaction between the two states is 0. So, this whole if numerator goes to 0 the whole thing goes to 0. So, that is it. So, we can estimate the energy of a particle.

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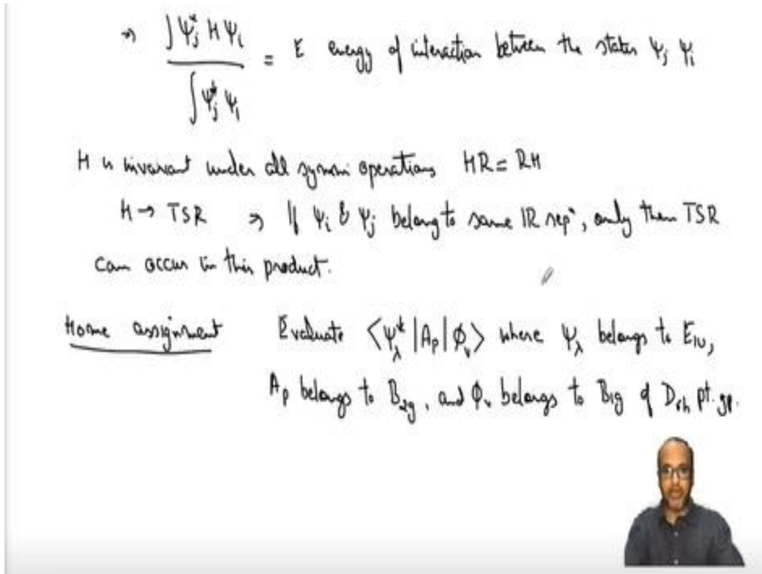


So, let us do a quick or let me give you a quick assignment. Let us do a home assignment to see if you can follow this. Otherwise, we can always discuss in the interaction session. So, let us say if I want to do evaluate psi lambda star lets say Ap and phi v. So, this is a bra-ket notation basically means the same thing the way it is, but it is not. This is another form you may get questions in different books.

So, that is why I am using this notation over here. So, where psi lambda belongs to E1u and Ap belongs to B2g and phi v belongs to B1g of D6h point. So, the three representations are given psi lambda is E1u A p is B2g and phi v is B1g. What you have to do is? Now you have to take the direct product of all three. And see whether and then try to use the reduction formula to see whether there is A1 present or not.

If A1 is present or A1g, whatever will be the totally symmetric representation. In this case, if it is present then it will not be equal to 0 otherwise it will be equal to 0. So, all you have to do is you have to tell whether this integration will survive. That means will not be equal to 0 or will be equal to 0. So, in next class we will see one more application of direct product. And then we will shift gears and we will look into symmetric adapted linear combinations.

So, we will see one more spend some more time on direct product for one more class go to next topic after that, thank you.