FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

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Week-02
Lecture-05
Linear Operators - Part 02

Consider two orthonormal bases. One is $|\chi_n\rangle$ and one is $|u_n\rangle$, in the same vector space V. They are both orthonormal bases, it means we can write $|\chi_n\rangle$ as $\sum_m W_{mn}|u_{\mathrm{m}}\rangle$. We can write the vectors of one orthonormal basis as a superposition of the other orthonormal basis. Now, since this is an orthonormal basis, then $\langle\chi_k|\chi_n\rangle$ should be δ_{kn}. That is the definition of orthonormal basis. If we substitute this expression for $|\chi_n\rangle$, we get $\sum_{m_1,m_2} W^*{}_{m_1k}\, W_{m_2n}\, |u_{\mathrm{m}}\rangle\langle \mathrm{u}_{m_1}|\mathrm{u}_{m_2}\rangle$. Since $\{|u_{\mathrm{m}}\rangle\}$ is also an orthonormal basis. So, this is $\delta m_1 m_2$. So, we can replace all m_1 with m_2 when we sum over m_2 and we just call it m. We get $\sum_m W^*{}_{mk}\, W_{mn}$. So, this has to be equal to δ_{kn}.

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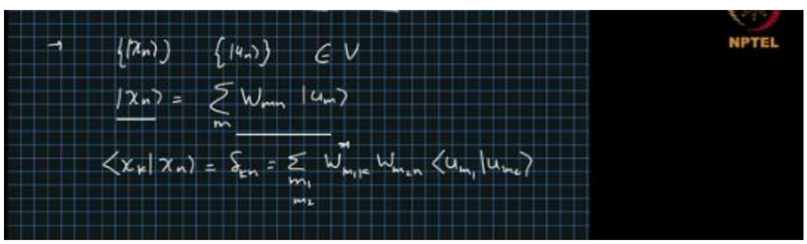

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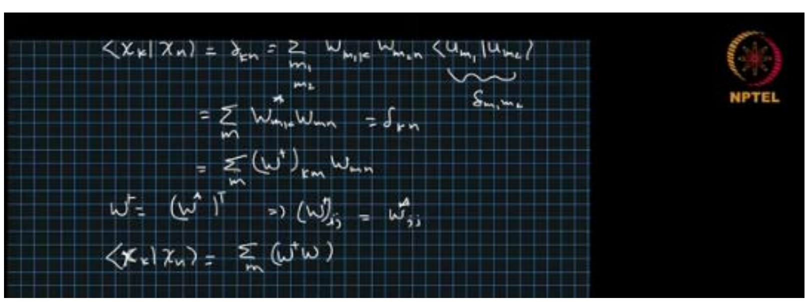

Now let us see what it looks like, $\sum_m W^\dagger{}_{km}\, W_{mn}$. Now, you can see that $W^\dagger$ is actually the $(W^*)^T$ if we have matrix W. And so, it means W_{ij} element of this matrix W, the W dagger's ij element will be W_{ji}^*. So, this is what we have done here. W_{mk}^*. becomes $W_{km}^\dagger$ element of $W^\dagger$ matrix. So, it means $\langle\chi_k|\chi_n\rangle$ becomes $\sum_m W^\dagger\, W$.

You can check that this is actually the matrix multiplication of $W^{\dagger}$ and W and the kn element of that. And this is equal to δ_{kn}. This implies that $W^{\dagger}W$ is identity. Similarly, we could have written u in terms of chi and we would have gotten $WW^{\dagger}$ equals identity. This implies that W is unitary.

From here, we can conclude that a unitary operator causes a basis transformation. And when we say basis, we mean orthonormal basis. Unitary transformation, a unitary operator takes one orthonormal basis and map it to another orthonormal basis. So, this is what we showed just now. We can do something else also.

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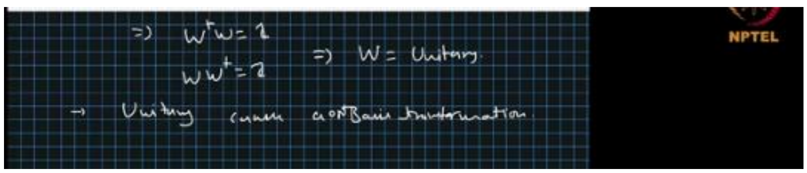

Let us say we have Z, which is $|\chi_n\rangle\langle u_n|$ and sum over n. Now, if Z acts on $|u_m\rangle$, it will give us $|\chi_m\rangle$. This is also a transformation from one basis to another. So, we can see what is $ZZ^{\dagger}$, that will be $\sum_n|\chi_n\rangle\langle u_n|\sum_m|u_m\rangle\langle\chi_m|$. And when we multiply, $\langle u_n|u_m\rangle$ will give us δ_{nm}, $\sum_{nm}|\chi_n\rangle\langle\chi_m|\,\delta_{nm}$, which is equal to $\sum_n|\chi_n\rangle\langle\chi_n|$, which is identity. Similarly, $Z^{\dagger}Z$ is also identity so this is also a unitary so now this is another example of unitary which is taking one orthonormal basis to another. So, can we find a relation between the two unitary ? So, this can be one assignment problem. This will be a fun problem, not very complicated, but not really straightforward.

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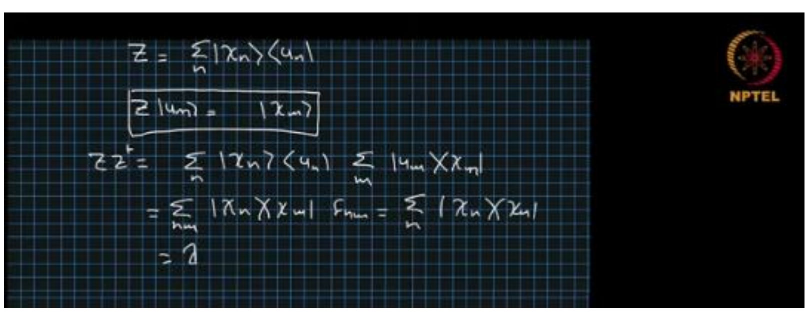

So, I will recommend everyone to try this thing and try to figure out what is the relation between Z and W. So, with this, we have covered all the important classes of operators, but there are some operators which we will encounter eventually and which are, which will come at a little later stage of our course, positive definite and positive semi-definite operators. So, if an operator A, if we take the inner product of $|\psi\rangle$ with $A|\psi\rangle$ and this sometimes is called expectation value also. So, if the expectation value of an operator A is always positive, then it is called positive definite operator. This should be true for all $|\psi\rangle$ in the vector space V. If this is true, then it's called positive definite. If it can be zero and positive, then it's called positive semi-definite.

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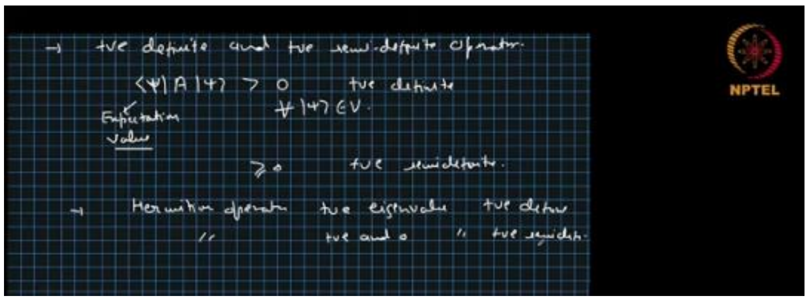

And any Hermitian operator with positive eigenvalues are positive definite operators. And Hermitian operator with positive and zero eigenvalues are positive semi-definite operators. So, this was the one class which we will be using time and again when we talk about the states and density matrices. Now, there is some interesting expressions and representations of operators, the various operators we just discussed. So, we will be discussing that.

So, consider an operator A acting on, so the eigenvalue equation, the characteristic equation of an operator and for a Hermitian operator, like A is a Hermitian operator. Let us define a matrix S which is made by using the eigenvectors of the operator A in the following way. We put first column as the first vector, second vector, second column as the second eigenvector and nth column as the nth eigenvector. In that way, we are assuming the matrix A was n by n. So, the vector psi n will be also n-dimensional vector and there is n of them. So, S is a n by n matrix. Let me repeat, we stack the eigenvectors of operator A, Hermitian operator A, the columns of matrix S and hence we get a n by n matrix.

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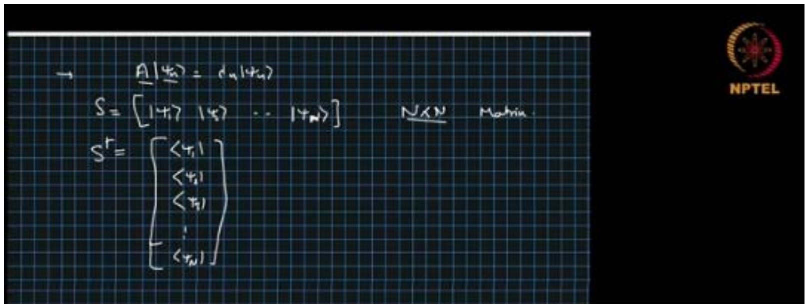

Now, interesting thing about S is, first of all, let us see what is $S^\dagger$. $S^\dagger$ will be $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ and $|\psi_n\rangle$. Now what is $SS^\dagger$, that will be $[|\psi_1\rangle, |\psi_2\rangle,.. |\psi_n\rangle]$ times $[\langle\psi_1|, \langle\psi_2|,.. \langle\psi_n|]$ $(column\ of\ vectors)$. There is no trick I am using here. You can put the vectors. You can take the explicit form of vector. You can put them and you will see this is a valid matrix multiplication. Then when we multiply, it will be the first element of the vector. We can treat this thing as the vector of vectors.

And this is a column of vectors. This is a row of vectors. This is a column of vectors. So, the first element here and first element here, we multiply second, second and we add all of the elements. So, it becomes $\sum_n|\psi_n\rangle\langle\psi_n|$. So, $SS^\dagger$ is $\sum_n|\psi_n\rangle\langle\psi_n|$. Since $\{|\psi_n\rangle\}$ are the eigenvectors of a Hermitian operator, so they form an orthonormal basis and they form a complete basis, it means $\sum_n|\psi_n\rangle\langle\psi_n|$, this must be identity.

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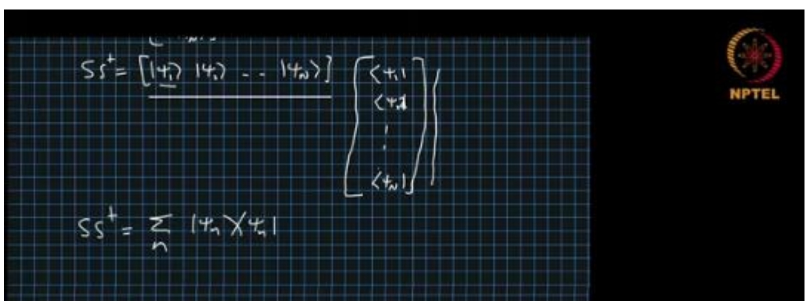

Now let us try $S^\dagger S$, that will be $[\langle\psi_1|, \langle\psi_2|,.. \langle\psi_n|](column\ of\ vectors)$, $[|\psi_1\rangle, |\psi_2\rangle,.. |\psi_n\rangle]$. This is the matrix. The first element here will be $\langle\psi_1|\psi_1\rangle$, $\langle\psi_1|\psi_2\rangle$ and so on, $\langle\psi_2|\psi_1\rangle$ and so on up to $\langle\psi_n|\psi_n\rangle$. Now, $|\psi\rangle$ are orthonormal. So, only the diagonal element will be 1. Everything else will be 0. So, matrix will be 1, 1, 1, 1 and so on and 0 everywhere else, which means identity. So, from here we can see that $SS^\dagger$ equals $S^\dagger S$ equals identity.

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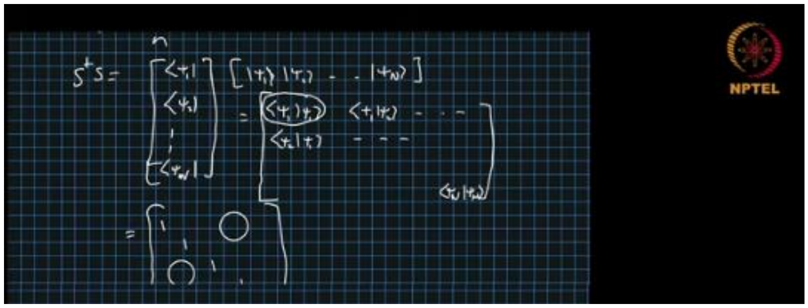

So, somehow the matrix S turned out to be unitary. What we have done is we have taken a Hermitian operator A. A is Hermitian, and we have eigenvectors of it, and we have eigenvalues of it. We make a matrix S out of the eigenvectors of A and we see that this matrix S turns out to be a unitary matrix. So, now let us simplify the equation. We get A S, which is A acting on $[|\psi_1\rangle, |\psi_2\rangle, .. |\psi_\mathrm{n}\rangle]$, which is, if we do the calculation, it will be $[A|\psi_1\rangle, A|\psi_2\rangle, .. A|\psi_\mathrm{n}\rangle]$, which will be $[\lambda 1|\psi_1\rangle, \lambda 2|\psi_2\rangle, .. \lambda 3|\psi_\mathrm{n}\rangle]$, which will be $[|\psi_1\rangle, |\psi_2\rangle, .. |\psi_\mathrm{n}\rangle]$, times diagonal matrix with elements λ_1, λ_2,.. λ_n, where everywhere else it is 0.

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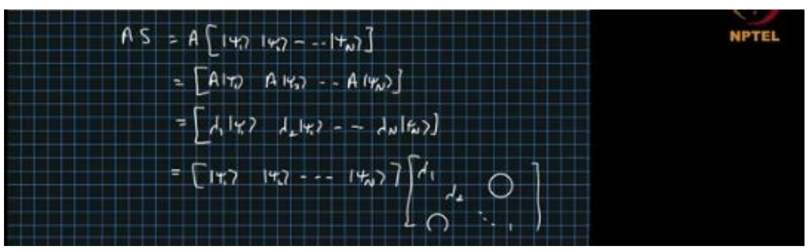

So, we have seen that and this we can write as the same matrix S and this diagonal matrix D. So, we have seen that AS equals SD. So, we have written the whole eigenvalue equation in this matrix equation. Now, since S is unitary, we can multiply with $S^\dagger$. $SS^\dagger$ is identity. So, we get $A=SDS^\dagger$.

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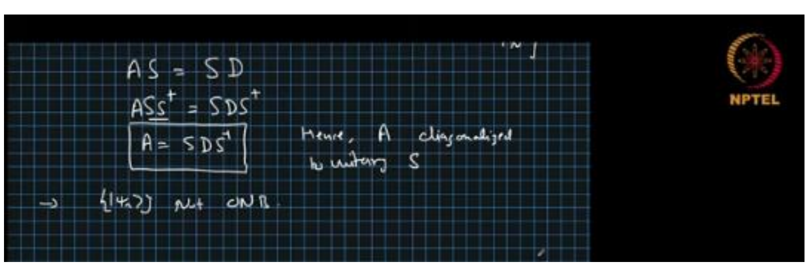

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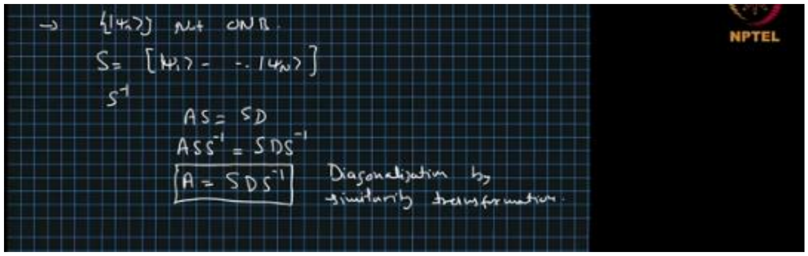

Any Hermitian operator A can be diagonalized using a unitary operator S. This is very simple and intuitive proof that any Hermitian operator can be diagonalized using a Hermitian operator S. Not just that, anti-Hermitian can also be done there because anti-Hermitian is just i times Hermitian. So, the proof goes in a similar way. And for other operators also, we can do whatever is related to Hermitian operator. Now, what will happen if A was not a Hermitian operator?

If A is not a Hermitian operator, then $|\psi_n\rangle$ are not orthonormal. But let us assume that A, but we have n number of linearly independent vector $|\psi\rangle$. Then S, which is $[|\psi_1\rangle,\ldots |\psi_n\rangle]$. This is the matrix of n linearly independent columns. If you remember our linear algebra from our 12th standard, if we have matrix with n linearly independent vectors, then the S inverse, the inverse of the matrix exists.

So, it means AS equals SD, that did not require any information about the unitary of S. So, here if we multiply with S^{-1}, we get SDS^{-1} and we get A equals SDS^{-1}. This is the diagonalization by similarity transformation. It's called diagonalization by similarity transformation. The previous one with unitary that is also similarity transformation, but of a very specific type that we are using the unitary matrix instead of invertible matrix, instead of just invertible matrix. So, there are two problems, two assignment problems we can think of right now that if you have two Hermitian operators, self-adjoint operator A and B such that they have same eigenvectors.

Then they commute. That is, [A, B] = 0, okay prove this thing, this is an assignment problem. If A and B have the same eigenvalues, then they are related by a unitary transformation. So, these are the two assignment problems one should try and they will be very intuitive, very interesting to understand. Now we will discuss functions of operators. We will be mostly concerned with either Hermitian or anti-Hermitian or unitary operators.

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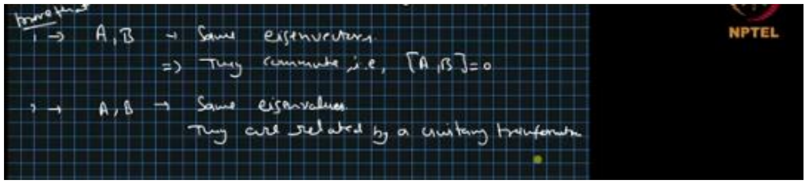

But if we have operator A, which is SDS†, like we have seen, then A^2 will be (SDS†)(SDS†), which is SD^{2}S†. If we extend this thing, if we have a function of A, any function of A, then it will be S, the same function of D, S†. So, this we can see by like one example we can consider, which is the exponential of A. The exponential of A will be written as identity plus A plus A square over 2 factorial and so on. And we can write A, S D S† plus S D^2 over 2 factorial, S dagger plus and so on. And this identity is also SS†. This is S, identity plus D plus D^2 over 2 factorial and so on, S†.

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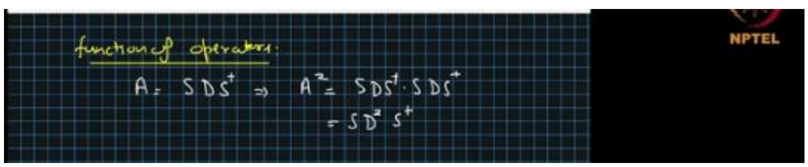

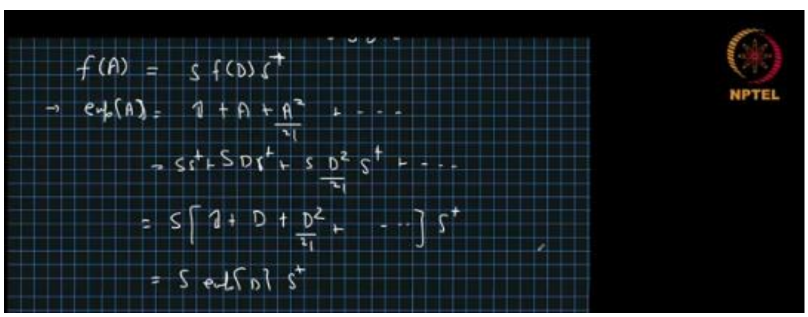

And this is S, exponential of D, S†. How is it useful? It's useful because calculating directly exponential of A is difficult. But exponential of a diagonal matrix, which is exponential of lambda 1, lambda 2, lambda n is nothing but exponential of lambda 1, exponential of lambda 2, exponential of lambda n. So, this part is trivial to calculate and then you have to just multiply it with the unitary matrix and we get the function of the operator.

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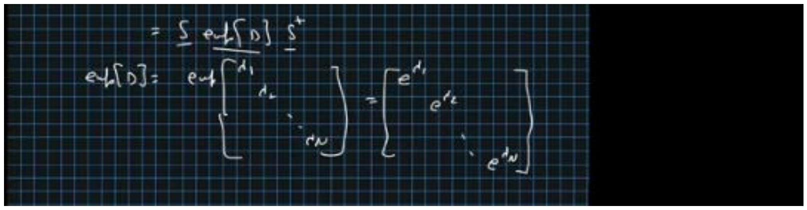

Now, let us say we have a matrix M which is exponential of A and let us say this is unitary. Then $M^\dagger$ equals M^{-1}. $M^\dagger$ can be written as exponential of $A^\dagger$ and M^{-1} is exponential of -A. This implies that $A^\dagger$ has to be -A and by definition $A^\dagger = -A$ implies that A is anti-Hermitian. Or, A can be written as iH where H is hermitian. This implies that any unitary operator M can be written as exponential of iH where H is hermitian and M is unitary.

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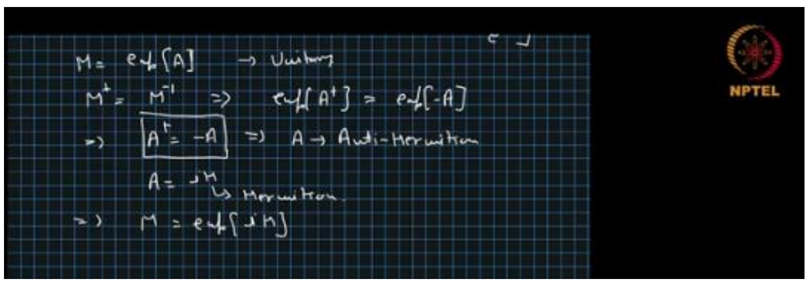

Now there can be an assignment problem which let's call 3. If we have a unitary operator M, the eigenvalues of M will be pure phases, that is exponential of i theta, that kind of form it will have okay and eigenvectors will be orthonormal basis, you have to prove this thing. And fourth assignment problem can be, let us say we have M_1, which is exponential of iH_1, M_2 which is exponential of iH_2, then M which is M_1M_2. You can see that if M_1, M_2 both are unitary then M, which is a product of M_1, M_2, this will also be unitary and this can also be written as exponential of iH. Find H.

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