

Quantum Mechanics
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Lecture - 15
Basis for Operators and States in LVS - I

Okay so today let me just briefly summarize what we did in the last lecture. Make you recall all the notations again and in the process I will slowly take you to basis for operators. You have studied in your first course that momentum operator can be given a differential operator representation right. Momentum all the observables can be written as operators; we want to see just like we want to write a basis set in a linear vector space.

We would also like to see what is the basis for an operator okay. So that is the theme and I will just briefly summarize what we did in the last lecture.

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Dirac bra(ket) notation

- State of QM system is generally denoted by $|\psi(t)\rangle \in V$ (angular bracket called ket).
This state contains all the information about the system
- We talked about span and linear indep states belonging to linear vector space V giving basis set
Number of states in the basis set defines dimension of vector space V
- There is a dual vector space \tilde{V} whose states are denoted by $\langle\phi|, \langle\chi|$ (know as 'bra').
We can determine scalars by taking inner product $\langle\phi|\psi\rangle$

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State of a quantum mechanical system formally denoted as ψ , typically the ψ will have evolution in time, so we call $|\psi(t)\rangle$. Most of the time we suppress this t , this is the state of the system and this angular bracket is called as ket. So this state, once I give the state, this supposed to contain all the information about where this system is, what is the state of the system means.

It could tell me what is the energy of the particle, it could tell me where is the location, all kinds of informations are all stored in this bracket ket which is having a state ψ okay and we talked about span, can span the space and you could also make the span such that they are linearly

independent, if you have both spanning the space and linear independent states that connection is what you call it as a basis set for the vector space.

And the number of states in the basis set that defines the dimension of the vector space. Just an example we were looking at the three-dimensional space but you can do it in general an abstract space. Then, we talked about that there is a dual vector space which will denote it as V tilde, states in this V tilde they are given by a different angular bracket and they are called bra okay.

So this is the Dirac bracket notation which we are going to exclusively follow. And why do you need these dual vectors? If you have these dual vectors, you can determine scalars by taking in the conventional three-dimensional space you would have set dot product. Here we will say it as an inner product.

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The slide is titled "Finite dimensional vector space". It contains the following text:

- $|c\rangle$ can be represented by column vector with n components
- $\langle c|$ will be denoted by row vector with n components
 $= (x_1, x_2, \dots, x_n)$

Below the bullet points, there are two equations:

$$\langle c|c\rangle = \text{scalar}$$
$$|c\rangle\langle c| = \text{what is this}$$

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So we confine today with finite dimensional vector space, it could go to infinite dimensional so on, let us confine ourselves to finite dimensional vector space. If $|\psi\rangle$ so in this finite dimensional vector space, you can denote the ket, you can represent the ket by a column vector. So you can represent a ket by a column vector, let the column vector have n components so this $n=3$ is similar to what we saw in the three-dimensional space.

But you could have an abstract n -dimensional vector space where n is finite. Similarly, the dual of this ket which we call it as a bra some other state will be denoted by row vector that it is denoted by a row vector. Suppose the entries in the n components are x_1 to x_n some kind of an

n-tuple. These x_1 's to x_n could be real if it is a real vector space, it could be complex if it is a complex vector space.

So with these two states which I have given in the vector space and the dual vector space, you can find an inner product. What is inner product in this representation of a column vector and a row vector? It is multiplying a row with a column; you have done this in matrix mechanics right, theory of matrices. A row multiplying a column will give you a scale, so row multiplying a column is given by the inner product and that will be a scale.

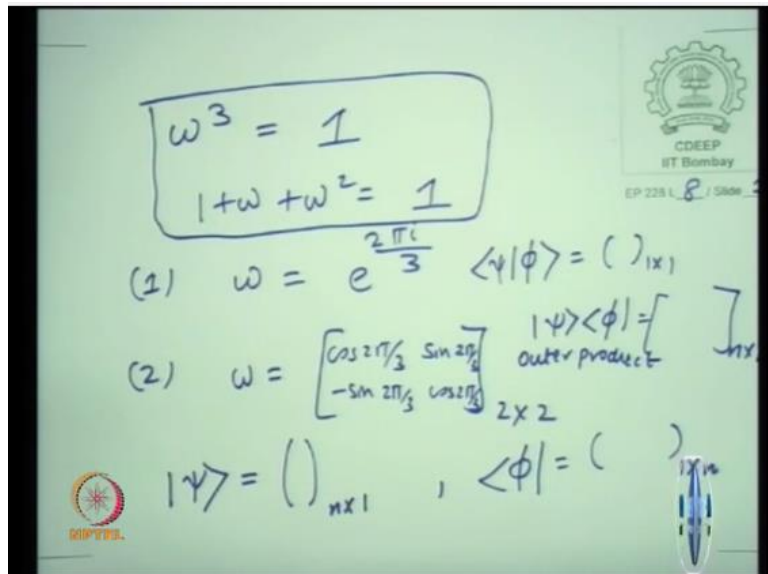
The next question you can ask us, if you write two states in this fashion the second line, what is this? That is the column multiplying a row. You have done column multiplying a row? What will that give you? It gives you an $n \times n$ matrices okay. So this is also an allowed operation but this does not give a scalar but it gives a matrix. If you represent the states by column vector and the dual vectors by a row vector, the inner product is a scalar.

This angular bracket is what we will call it is an outer product okay. So earlier we call the earlier one as an inner product, this angular bracket we will call it as an outer product. So outer product is going to be giving you not a scalar but it is a matrix. If the vector space is finite dimensional n -dimensional vector space, then it will be an $n \times n$ matrix. So in some sense in the Dirac notation, the outer product can be treated like an operator.

And which can be represented by $n \times n$ matrices okay. So representation means what? Suppose it is like giving a color to something okay. So it is some kind of I represent this by a blue color, I represent this by a green color, something like that, it is like different colors or different dresses. You can dress this operation, suppose I want to look at roots of unity right, you are all familiar with cube roots of unity right.

Omega is a cube root of unity because omega cube is identity and $1+\omega+\omega^2$ is 0. You can represent that ω by a 2×2 matrix. It can give a dress to that omega by writing a 2×2 matrix. What is a 2×2 matrix? It is just rotation about 120 degrees right, $\cos 2\pi/3$ $\sin 2\pi/3$ could do that. So this is what we call it as a representation.

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So $\omega^3=1$ and $1+\omega+\omega^2=1$. I can denote 1 representation as $e^{\frac{2\pi i}{3}}$. This is one representation. The second representation is omega could be written as a 2 x 2 matrix as $\cos 2\pi/3$ $\sin 2\pi/3$ $-\sin 2\pi/3$ $\cos 2\pi/3$, so these are called representations. Why representation? The one which are written here it satisfies both these equations.

Similarly, the 2 is a different representation or a different dress which satisfies both those equations. So given some equations you can try to write different representations and see whether it satisfies those conditions okay. Similarly, a formal abstract state ψ which I write I am giving a representation as a column vector with n rows and 1 column right. Similarly, a bra vector in the dual vector space will be denoted by a row vector, which is 1 column and n row, so this is what is happening.

So whenever you take an inner product, it becomes a number which is a 1 x 1 element. If you take an outer product, so inner product $\langle\psi|\phi\rangle$ is actually a number with 1 x 1, a $|\psi\rangle\langle\phi|$ will be a matrix which is n x n. It is very simple but if you start getting used to the left hand side notation, you can do many abstract calculations in a very neat and elegant fashion. Always recall with what you do in matrices and that will help you to remember this okay.

So this is what we call it as an outer product okay. So this is a representation if you want. You can represent the ket vector in a finite dimensional vector space by a column vector. You can represent the dual vector which is the bra as a row vector and this is what we conventionally going to follow. For a finite dimensional vector space, we can play around with matrices.

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So this is what I said column multiplying a row is the outer product and that will give you $n \times n$ matrix. In fact, we call this to be this outer product to be an operator in the Dirac bracket notation. By the way you remember that this inner product of the same state is called the norm and if you try to write it in this notation, you want the norm to be always ≥ 0 , when then it be 0, when ϕ is a null vector okay.

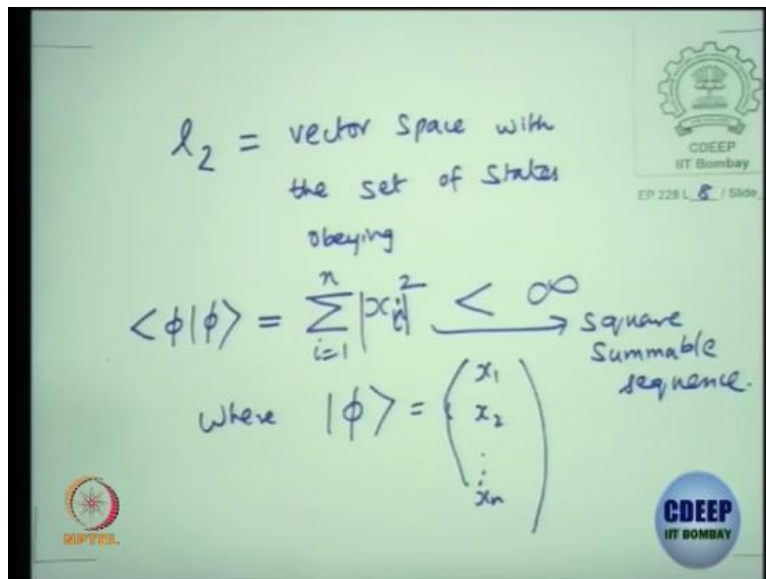
Otherwise, this is going to be in general positive and if you try to rewrite in the representations as a row vector with x_1 to x_n and the column vector with x_1 to x_n , then this is the condition you will get further in the product of these two vectors right, the square of the norm right and because this is positive definite, this will also be each one is the square, I have written x_n^2 , technically this is not correct.

When is it correct? When it is a real vector space. It is a complex vector space, I have to take conjugate and transpose of a column vector, complex conjugate. So you have to put x_1^* , x_2^* up to x_n^2 and this condition for a real vector space if suppose I take n to be very large even though I started with a finite dimensional vector space, n becomes very large, the squares which I add may become may blow up okay.

They become infinity, so you need the condition that the summed up quantity. For a finite dimensional vector space, you can always make it finite but if n becomes very large, there are chances that this would not be finite but you have to impose this condition, take the states in the vector space such that the norm is always finite. You did this in the wave functions; I said that those wave functions are all square integrable wave functions right.

I said this in a week or two weeks ago I said this. Similarly, this condition on a vector space which is on a finite n -dimensional vector space is supposed to be the sequence is supposed to be a square summable sequence if it satisfies this condition and this collection of such square summable sequence which are a set of ϕ_1 ϕ_2 , a set of states which belongs to this n -dimensional vector space, that vector space if it has these kinds of square summable sequence, then you call that vector space, you denote that vector spaces as l^2 .

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So l_2 is a vector space with set of states obeying summation over x_n squared to be $<\infty$, the states is $\langle \phi | \phi \rangle$. Technically, I should put $|x_n|^2$ because I am not specified whether it is a real vector space or a complex vector space. So the square summable sequence, so this condition which I have maybe I should put an i , i from 1 to n , so this condition is what we call it is a square summable sequence.

That it sums up and it is finite, so you can slowly see that when you go to in your course on integration, what exactly you do? Initially if the lattices spaced, you start doing discrete summations but suppose I make n to be very large and make it to be a continuum, then it could become a square integrable situation okay. So you can see that I am trying to make it as a finite vector space.

But at some point I will start making it as a continuum and look at square integrable functions and states so it is just to give you a feel of what exactly is happening in a finite dimensional vector space. This finite dimensional vector space is something which is not you know it happens in the systems right. How many of you have seen Stern-Gerlach experiment? Actually two beams and those two states are linearly independent and you can have a two-dimensional vector space.

So it is not that whatever I am saying here is not happening, it happens, so you do have two linearly independent physical finite dimensional vector space okay. So let me just get to the two-dimensional vector space, just for simplicity till now I was talking about n -dimensional vector space.

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Two dimensional vector space

- Orthonormal basis is $|\phi_1\rangle, |\phi_2\rangle$
- Suppose we have non-orthogonal basis $|e_1\rangle$ and $|e_2\rangle$, we do Gram-Schmidt orthogonalisation:

$$|\phi_1\rangle = \frac{|e_1\rangle}{\langle e_1|e_1\rangle^{1/2}}$$
$$|\phi_2\rangle = \frac{|e_2\rangle - |\phi_1\rangle\langle\phi_1|e_2\rangle}{N}$$

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But I will now confine myself to two-dimensional vector space and try and clarify a couple of notations and then you know how to do it for a n-dimensional vector space. So if you remember we had two basis in the last lecture, one was a orthonormal basis and the other one was a non-orthogonal basis right. So let me just proceed with this example.

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2-d vector space

$|\phi_1\rangle, |\phi_2\rangle \rightarrow$ orthonormal basis

$$\left. \begin{aligned} \langle\phi_1|\phi_1\rangle &= 1 \\ \langle\phi_2|\phi_2\rangle &= 1 \\ \langle\phi_1|\phi_2\rangle &= 0 \\ \langle\phi_2|\phi_1\rangle &= 0 \end{aligned} \right\} \langle\phi_i|\phi_j\rangle = \delta_{ij}$$

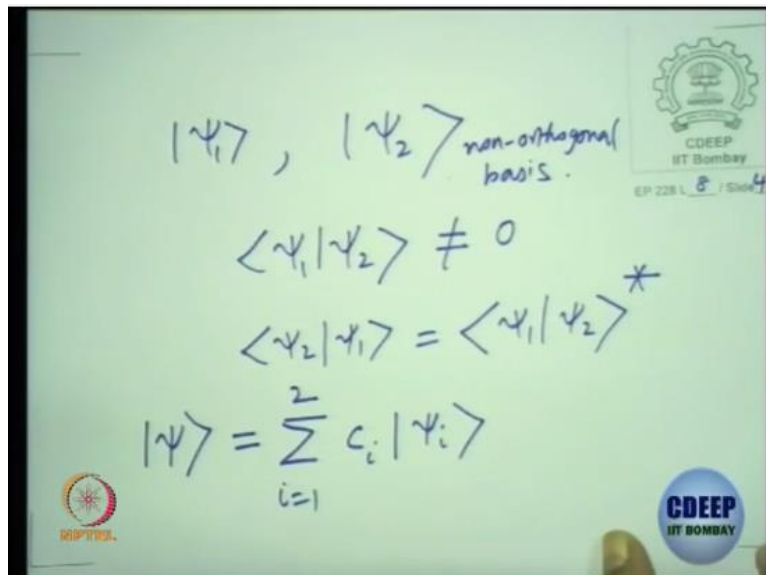
$i, j = 1, 2$

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So we call $|\phi_1\rangle$ and $|\phi_2\rangle$ to be orthonormal basis. When is that? When the inner product of $\langle\phi_1|\phi_1\rangle=1$, $\langle\phi_2|\phi_2\rangle=1$ and $\langle\phi_1|\phi_2\rangle=0$, $\langle\phi_2|\phi_1\rangle$ also=0. This can be compactly written as $\langle\phi_i|\phi_j\rangle=\delta_{ij}$. For a two-dimensional vector space, i and j will be 1, 2. Both i and j will take 1 and 2, this is a compact. Now you see the generalization, if I go to n dimension, there will be n basis vectors not two basis vectors.

And it will satisfy this orthonormality condition, so this is normalized, this one is orthogonal. So now what we would like to do is we could also have a non-orthogonal basis right.

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So we call that as $|\psi_1\rangle$ and $|\psi_2\rangle$. Why is it non-orthogonal? If you try to find what is $\langle \psi_1 | \psi_2 \rangle$ this will not be 0 okay and $\langle \psi_1 | \psi_2 \rangle$ will be in principle the star of this. So this is the meaning of saying this is non-orthogonal basis. What is the meaning of basis? If you want to write any arbitrary state, I could use once I call this as basis, I can use some complex coefficients on $|\psi_i\rangle$ for a two-dimensional vector space it is 1 to 2.

So this is the superposition of the basis states which will give you any arbitrary state in the two-dimensional vector space. So this is why this forms the basis set but this is not orthogonal and then what did we do? We wanted to get to the orthogonal basis from the non-orthogonal basis. This is what we were doing in the last lecture and some of you were asking me which should be the starting vector?

Any of these two vectors I can choose in the two-dimensional vector space and in the n-dimensional vector space the starting vector could be any of those n basis vectors. There is no requirement that I have to start only from this vector to do the Gram-Schmidt orthogonalization okay. So just for convenience, we say $|\psi_1\rangle$ to be proportional to ϕ_1 with normalization.

If suppose this is normalized, then $|\psi_1\rangle$ itself will be the first vector and you find the second vector by taking the projection, that is what you do right, this is what we did last time. So let us redo it here.

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$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, |\psi_2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|\phi_1\rangle = \frac{1}{\sqrt{2}} |\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|\phi_2\rangle = \frac{1}{\sqrt{2}} \left\{ |\psi_2\rangle - \frac{\langle \phi_1 | \psi_2 \rangle}{\langle \phi_1 | \phi_1 \rangle} |\phi_1\rangle \right\} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$N = \frac{1}{4} (1+1) = \frac{1}{2} \Rightarrow \sqrt{N} = \frac{1}{\sqrt{2}}$$

So we define $|\phi_1\rangle$ to be $|\psi_1\rangle$ but this may not be normalized, you have to normalize it. So we are doing the Gram-Schmidt orthogonalization. Take one of the two states, just normalize and call it to be the first basis vector. How do I find $|\phi_2\rangle$? $|\phi_2\rangle$ will be the second non-orthogonal vector but subtract the component along $|\phi_1\rangle$, so that is what you will do. So typically you do this is what will give you the component along $|\phi_1\rangle$.

The inner product of the state $|\psi_2\rangle$ with $|\phi_1\rangle$ will give you the component along $|\phi_1\rangle$ but this is a scalar, you have to get a vector equation. So I can put the $|\phi_1\rangle$ this side or I can put the $|\psi_2\rangle$ this side okay. So this is a number and this is a column vector if you give a two-dimensional vector space. So if we are in two-dimensional vector space, I can denote $|\psi_1\rangle$ to be a b and then you can find out the fact.

Let us give the a and b some specific value, we can take it to be $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. So then $|\phi_1\rangle$ will be what? Is that right? There will be a by $\sqrt{2}$ because of the norm, clear. This is a representation and we use this to find this. So if I want to find $|\phi_2\rangle$, I need to take $|\psi_2\rangle$, $|\psi_2\rangle$ in this notation I could take to be $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. If I take that, then you can see this is $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and this is $1/\sqrt{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ with $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ that give you $1/\sqrt{2}$.

So do this and after you do this, whatever is the numerator result I need to whatever is this let me call this to be some new state and you have to take the norm of the inner product of that

state with itself. You understand what I am saying right and then take the square root and you should get the $|\phi_2\rangle$. What do we expect here? What do we expect? We will get $1/\sqrt{2}$ that is what I expect.

Can you please do this algebra and check. This will be $\begin{pmatrix} 1 \\ 0 \end{pmatrix} -1/2 \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. So $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and then $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ with $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ right. What happens? That is 1 and this is 1/1, so you will have 1/2 and a -1/2 right. Numerate but that is not normalized right, if you do that, it is $1/4 (1^2+1^2)$ but 1/4. So this gives you what normalization some N on $1/4(1+1)$ which is 2/4 which is 1/2 implies square root of n is $1/\sqrt{2}$.

So you get the state is $1/\sqrt{2}$ types, so very simple, try to do it for a simple example like this and get a feel of it but in this process there is something which I wanted to tell you. What is it we see here? This piece what is that piece? I just said few slides ago is an outer product but what is the operation of this outer product? It projects the component of an arbitrary state along the ϕ_1 direction.

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$|\psi\rangle = \sum_i c_i |\phi_i\rangle = P_1|\psi\rangle + P_2|\psi\rangle$
 $|\phi_1\rangle\langle\phi_1|$
 $= \text{projection operator} = \hat{P}_1$
 $\hat{P}_1|\phi_2\rangle = 0 \quad c_1 = \langle\phi_1|\psi\rangle$
 $|\phi_2\rangle\langle\phi_2| = \hat{P}_2 \quad c_2 = \langle\phi_2|\psi\rangle$
 $\hat{P}_1 + \hat{P}_2 = \mathbb{1}$

So this outer product is a projection operator is $|\phi_1\rangle\langle\phi_1|$ is a projection operator which is going to be a matrix operator. If this operates, so let me call this as and \hat{P}_1 put these operators with a hat. This is the convention which we follow; do not confuse this with momentum. It is some projection operator. \hat{P}_1 suppose I do it on $|\phi_2\rangle$ what is this zero or nonzero? Zero. So that is a definition of a projection operator.

If you have n basis set, if you define a projection operator with projects onto a specific basis $|\phi_1\rangle$ that when operates on the other orthonormal basis it is going to be 0. It is the definition of a projection operator. So you can also similarly define for a two-dimensional vector space, a projection operator \hat{P}_2 . You can define a projection operator \hat{P}_2 . $\hat{P}_1 + \hat{P}_2$ The sum of the projection operators should be like an identity operator.

In two-dimensional vector space I am specifying myself. In the two-dimensional vector space, the two projection operators can be summed up to be identity. So whenever I write an arbitrary state $|\psi\rangle$, I could write this as, as I said I could write it as some $c_i|\phi_i\rangle$. I could also write it as projection operation $\hat{P}_1|\psi\rangle + \hat{P}_2|\psi\rangle$ because $\hat{P}_1 + \hat{P}_2$ is identity. The state ψ is same as this.

And this state ψ can also be written as a superposition of the basis states with complex coefficients. Now tell me what is c_1 and what is c_2 ? c_1 will be $\langle\phi_1|\psi\rangle$ is the outer product $|\phi_1\rangle\langle\phi_1|$. What is c_1 ? c_1 will be $\langle\phi_1|\psi\rangle$, c_2 will be the state $|\phi_2\rangle$ will come here in this outer product, so what is c_2 ? $\langle\phi_2|\psi\rangle$ okay. So if you understand this concept in the two-dimensional vector space for you to do it for any finite dimensional, infinite dimensional vector spaces, this theme is the same.

Only thing is the number of projection operator will increase right. You would not have this 2, depends on the number of basis or the dimension of the vector space and any arbitrary state can be written as either this linear combination or this thing. Let me stop here.