## Quantum Mechanics- I Prof. Dr. S. Lakshmi Bala Department of Physics Indian Institute of Technology Madras

## Lecture - 4 Linear Vector Spaces - III: The 3-level atom

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In this talk I will discuss more properties of linear vector spaces. This is the 3rd talk on linear vector spaces that I am giving. Let me quickly recapitulate some of the essential features of what I have already discussed. Most of the time we were talking about a 2 dimensional linear vector spaces and I had basis vectors e x and e y. This was on orthonormal basis so they were normalized to unity and they were orthogonal to each other. All vectors in this space can be expanded as a superposition of these 2 basis states. I could have chosen the following basis. For instance, I could have selected e x prime, which is e x plus e y by root 2 and e y prime which is e x minus e y by root 2.

The root 2 is there purely for normalization purposes. Because you can check that e x prime dot e x prime is equal to e y prime dot e y prime equal to 1 and e x prime dot e y prime is of course, equal to e y prime dot e x prime and that is 0. The point is the following.

(Refer Slide Time: 02:21).



If we started by representing e x as 1 0 and e y as 0 1 which has been our notation in terms of column vectors. Then it is easy for you to check, that e x prime is 1 by root 2 1 1 and e y prime is 1 by root 2 1 minus 1. So, how do I go from e x to e x prime and e y to e y prime? These are unit vectors in the linear vector space and clearly I should have operated on e x with a suitable matrix to get e x prime. It is clear that the matrix 1 by root 2 1 1 minus 1 will do the job. I have spoken about this object even in one of my earlier lectures and you can easily check that e x prime for instance, can be written in this manner.

Similarly, e y prime now, this matrix is very important in logic gate operations. As I have mentioned earlier it is the Hadamard gate, it is also unitary you can see that this is a unitary matrix in the sense that this matrix with its dagger when multiplied is equal to the identity matrix. It is also equal to h dagger h dagger means transpose, complex conjugate. Interchange the rows in the columns and take the complex conjugate or every element of course, here all elements are real and so the second part of this prescription is not really needed, but that is the Hadamard matrix.

All quantum logic gate operations are reversible operations and unitary matrices are used to describe these logic gates. You can reverse it if you can suitably implement h dagger and therefore, make it identity which means no operation has happened as a net result on the state that one begins with. In general, we have gone from one pair of orthonormal basis to another pair of orthonormal basis set.

(Refer Slide Time: 05:19)

In general suppose, phi is normalized to 1 in this case it could well be e x. And phi prime is also normalized to 1. This could be e x prime. It is clear that I have operated with phi, with some operator u in this particular example it was the Hadamard operation to give me phi prime, u is an operator that acts on this state to give that state. So, phi prime bra in the Dirac notation is simply phi u dagger. Therefore, phi prime phi prime is equal to phi u u dagger, u dagger u sorry, phi and the fact that this is 1 clearly implies that u dagger u is equal to 1. In other words, it is a unitary operation that has brought about this change of basis so that the orthonormality property is preserved in both the old and the new basis set. Now, what happens to operators when they go from the old basis set to the new basis set? (Refer Slide Time: 06:55).



Consider for instance this operator. In the parlance of column vectors, it could well be the operator 1 0 1 0. When we talk about 2 level atoms, it could well be the operator e e or g g. Whatever, I say now can also be extended to operators like e g, but just for purposes of illustration I would consider an operator like this. So phi prime, phi prime is u phi phi u dagger. So, the transformation that we have brought about on the operator phi phi is this unitary transformation. (Refer Slide Time: 05:19) In other words, when the basis state changes to u phi, the corresponding operator is flanked by u on this side and u dagger on that side.

When operators are changed and basis states are changed to go to a new basis set and therefore, correspondingly new operators this is the way the unitary transformation is implemented. You flank the operator with u on this side and u dagger on that, the basis states themselves have transformed in this fashion. (Refer Slide Time: 05:19) So, a change of basis is implemented through a unitary transformation and such change of basis has preserved the orthonormality properties.

(Refer Slide Time: 08:48).



In general, for any basis state phi prime is u phi. This is true for all the basis states that are involved and it is for all operators. If this is an operator it goes to a new operator prime, the relationship between the primed basis state operator and the unprimed one comes about in this manner, where the same unitary operator is used for both the transformation of the basis set and for the operators. Under such a unitary transformation or change of basis, what happens to Eigenvalue equations?

Suppose in the unprimed basis, ket psi is an Eigen state of some operator o with Eigenvalue a. In the primed basis o goes to u o u dagger and psi goes to u psi and since a is just a number, I can pull it out and put it here and this is 1. So, this object is o prime, this is psi prime and this is psi prime. Eigenvalues do not change under this unitary transformation. So, all that I have done is multiply this whole thing by u and insert a u dagger u in between and recognize this as the new operator, that is the operator in the primed basis and this as the new state. So, under a unitary transformation, Eigenvalues continue to be whatever they were numerically. What about the commutation algebra?

(Refer Slide Time: 11:20)

So let us look at the spin matrices which we are now familiar with. I have the commutator S x, S y, is i h cross S z and this is the cyclic relation. This is an operator, because it is a commutator of 2 operators. Let us recall that this is same as S x S y minus S y S x. If I flank this operator with u on this side and u inverse on that side, obviously I will have to do the same thing on the right hand side. Remember that u inverse is a same as u dagger because this is a unitary operator. Expanding out the commutator, the left hand side is simply this object where I can well insert a u inverse u here because this is the identity. I could do the same thing here by inserting a u inverse u.

(Refer Slide Time: 12:42)

This is the corresponding operator in the primed basis. This is S y prime, this is clearly the commutator of S x prime with S y prime and that is equal to i h cross s z prime because this object is S z prime. So the commutation algebra does not change, under a unitary transformation which brings about a change of basis. The basis set that I want to work with for a given problem largely depends on my convenience and what would be suitable for the physics of that situation.

Indeed if I have to work on the plane of this table. I could have chosen e x and e y to be two orthonormal vectors at right angle to each other in so many different ways. Each of them is a convenient basis set and I will move from one to the other through a unitary transformation in general. And if I were dealing with objects which have only real elements in them, it would correspondingly be an orthogonal transformation and the unitary matrix would simply become an orthogonal matrix. We could do better.

(Refer Slide Time: 14:40)



Let us look at a specific unitary transformation and understand something more about the physical properties of the spin matrices  $S \times S y$  and S z. So, let me consider this unitary operation, e to the minus i theta S z where theta is a parameter, it is a constant and it can take values 0 to 2 pi any value it is fixed, it is a constant parameter. So, u dagger which is a same as u inverse is simply e to the i theta S z. Let me see the effect of the unitary operation on S x for instance.

So, what is u S x u dagger? Well that is the same as u S x u inverse. This operator is unitary because S z is Hermitian and this is just a constant and e to the i times a Hermitian matrix, it is a unitary matrix. Of course, there are many ways of simplifying this I could have used the Baker Campbell Hausdorff relation or variance or cousins of the b c h Baker Campbell Hausdorff formula, but instead for our purpose right now, let me do this by brute force.

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So I first consider e to the minus i theta S z, S x.

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I am just looking at this part of it. Make a brute force expansion, but before that I realize that S z is h cross by 2 sigma z and just for convenience of notation I am going to call theta h cross by 2 as alpha. So, basically I have to find out e to the minus i alpha sigma z, h cross by 2 sigma x because S x was h cross by 2 sigma x e to the i alpha sigma z and this is the part that I am going to look at first. I can make a series expansion of the exponential.

(Refer Slide Time: 17:21)



So e to the minus i alpha sigma z, sigma x is simply 1 minus i alpha sigma z plus minus i alpha the whole square by 2 factorial sigma z square plus the next term and so on and this multiply sigma x. But then I understand the following sigma z square is simply the identity operator. You can explicitly check this out by substituting the matrix 1 0 0 minus 1 for sigma z. I will also need to find sigma z sigma x. Sigma z sigma x is i sigma y.

Remember that I could use the matrix 1 0 0 minus 1 for sigma z and 0 1 1 0 to sigma x and that is the same as i sigma y. Therefore, e to the minus i alpha sigma z sigma x is 1 minus i alpha sigma z. The next term is simply the identity operator here. Sigma z square is identity and therefore, this becomes sigma z, that is an infinite series and that multiplies sigma x. Just looking at the 1st few terms is going to tell me what is going to happen and I can now group term suitably.

(Refer Slide Time: 19:09).

So, this is equal to sigma x (Refer Slide Time: 17:21) times 1 minus i alpha the whole square by 2 factorial plus minus i alpha to the power of 4 by 4 factorial and so on which is the x cos alpha. And then I have sigma z sigma x which is i sigma y. So, this object is sigma x cos alpha plus minus i alpha sigma z sigma x which is i sigma y plus minus i alpha the whole cube by 3 factorial sigma z sigma x which is i sigma y plus so on. It is very clear that this object is simply sigma x cos alpha plus sigma y sin alpha.

This is a matrix, this is just a number, this is another matrix. I am expected to find (Refer Slide Time: 16:20) e to the minus i alpha sigma z sigma x times e to the i alpha sigma z. And therefore, it is simply equal to sigma x cos alpha plus sigma y sin alpha multiplied by e to the i alpha sigma z. Since we are dealing with matrices the ordering is extremely important. We should be careful that sigma x sigma z is not confused with sigma z sigma x. Once more I can make an infinite series expansion of this and I have this sigma z squared is identity; sigma z cube is merely sigma z and so on.

(Refer Slide Time: 21:43).

That tells me that the whole object simplifies to sigma x cos alpha plus sigma y sin alpha (Refer Slide Time: 19:09) 1 plus i alpha sigma z plus i alpha the whole square by 2 factorial and so on. So, there are terms which do not involve sigma z and it is clear that that is 1 plus i alpha the whole square by 2 factorial plus i alpha to the power of 4 by 4 factorial and so on which is simply cos alpha. (Refer Slide Time: 19:09) And then the rest of the terms, would multiply sigma z and if I pull out an i sigma z.

I just have alpha and then I have an alpha cubed by 3 factorial and so on which is i sigma z sin alpha. So, basically this is sigma x cos squared alpha plus sigma y sin alpha cos alpha. I have a sigma x sigma z and that is a minus i sigma y. So, that just gives me a sigma y sin alpha cos alpha and then I have a sigma y sigma z which is i sigma x, but that is an i out there so that is a minus sigma x, which is simply sigma x cos 2 alpha plus sigma y sin 2 alpha, but remember that theta h cross by 2 was alpha and therefore, this is simply sigma x cos theta h cross plus sigma y sin theta h cross.

Remember that theta itself has dimensions. It can be written in terms of h cross inverse, because it figured in the exp1ntial it was e to the i theta S x or S y or S z. And therefore, we have cos theta h cross coming up now, but the h cross should cancel out because theta is some number by h cross. Let us set h cross equal to 1 for the moment for convenience..

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And then I find that in general I have shown this particular transformation, that e to the minus i theta S z S x e to the i theta S z is equal to S x cos theta plus S y sin theta. But this rings a bell this is very reminiscent of the way, x y and z transform to x prime y prime and z. If I did a rotation about the z axis, by an angle theta you will recall that if we have axis x, y and z and a rotation were performed about the z axis by an angle theta x goes to x prime which is x cos theta plus y sin theta, y goes to y prime which is minus x sin theta plus y cos theta and z itself does not change.

The manner in which S x has transformed under this transformation is simply reminiscent of the manner in which x transforms under rotations by an angle theta about the z axis. You can work this out and show in a similar manner that S y prime is minus S x sin theta plus S y cos theta. And if you considered e to the minus i theta S z, S z e to the i theta S z it is clear that S z commutes with this and therefore, S z itself does not change.

What I have shown you now is simply this that S x S y and S z transform the same way as x y and z do under a particular transformation. In this case, this is the transformation under this unitary transformation S x transforms like the x component of a vector, S y transforms like the y component of a vector. Similarly, you can show that S z transforms like the z component of a vector. I could have taken S z here and put an S y and an S y there then it would have transformed like the z component of a vector.

(Refer Slide Time: 27:35)

I therefore, define an object s which is a vector, which can be written as S x e x plus S y e y plus S z e z. It is to be noted that this is an operator or a matrix. The matrix is merely a representation for the operator, so is this and so is this. These are unit vectors so in some three dimensional space, remember that we have used basis states  $1\ 0\ 0\ 1$  and so on quite independent of position or momentum or angular momentum.

So, we really should not be confusing this three dimensional space (Refer Slide Time: 24:28) where the basis vectors are e x e y and e z. We really have no business to confuse this with the usual position space, where too you can define basis vectors and denote them by e x ,e y and e z. So, this is an internal space that is really nothing to do with position or angular momentum or linear momentum. But in that space S x S y and S z transform like components of a vector under this particular transformation. (Refer Slide Time: 24:28) The general transformation is of the form so unitary transformation.

If the transformation is about the z axis that is, if it is in the s y plane it is given by e to the minus i theta S z. If it is in the y z plane it would correspondingly be e to the minus i theta S x, and if it is in the S z plane the unitary operator in question will be e to the minus i theta S y. So, already we have an object where the coefficients of the unit vectors are not numbers, which is most probably what we are used to till now.

But these are operators is a matrices. In general when one talks about an object transforming as a vector, first of all one has to say: what is the transformation law that

we are talking about? What is the transformation? Is it rotations in space? Is it a transformation of this kind? (Refer Slide Time: 24:28) Where the operator itself is of this structure so one first defines the transformation law then studies what happens to objects under that transformation law.

Remembering that under unitary transformation the u is on this side and u dagger or u inverse is on that side and then looking at the resultant object. An object could transform as a vector under a set of transformations, it need not transform as a vector under some other set of transformations. So, it is very important when discussing whether an object is a vector or not to state what is the transformation that one is looking at.

In any case, this object s is a vector to that extent I can define sigma as sigma x e x plus sigma y e y plus sigma z e z and that too is a vector (Refer Slide Time: 24:28) under a transformation where S z is replaced by sigma z and so on. The point is the following space rotations for instance, rotation by an angle theta it is easy to see that if one rotates by an angle theta 1 about the z axis followed by an angle theta 2 about the z axis, the net result is also a rotation about the z axis and some other value theta 1 plus theta 2. In that sense the closure properties obeyed.

Associativity is also there, because I could have done a space rotation in this context by theta 1 plus theta 2 and followed that up with a space rotation by theta 3 or I could have first done theta 2 and then followed it up by a rotation by theta 1 plus theta 3. So, there is an associativity property. For every rotation there is a unique inverse, because if I rotate by an amount theta in the clockwise direction, I could well de-rotate it by a different angle so that there is no net rotation. There is a unique identity which is 0 rotations.

Therefore, I find that all group properties are satisfied here except that I cannot write down for you the set of group elements, because it is not a finite set of elements, it is not a discrete set of elements it is a continuous group of elements. Because this parameter theta can continuously go from 0 all the way back to 2 pi and all of them are elements of this group of transformations. So, this is an example of a continuous group or a Lie group, in contrast to discrete groups.

Similarly, in the context of spins, the theta here can go from 0 to 2 pi and this too defines a continuous group of transformations. So, theta is the group parameter and as theta changes I get the entire set of elements which is a continuous infinity of elements. For such groups there is an algebra which is given by the generators of the transformation. The object sitting here next to the group parameter, the non trivial object, is the matrix or the operator whose exponential is responsible for the transformation.

So, this is the generator of the transformation. It is a unitary transformation and there are 3 such generators, instead of talking about e to the minus i theta S z. I could well talk about S z itself and therefore, I have three Hermitian matrices in this context S x, S y and S z which correspond to the generators of the transformation and these Hermitian operators satisfy this algebra, which is the Lie algebra corresponding to this group. I could equivalently have worked with S plus and S minus and S z and I have already mentild, the corresponding commutation algebra which S plus, S minus and S z obey.

(Refer Slide Time: 35:28)



This particular group is the s u 2 groups of transformations a special unitary group. Unitary, because I have been working with unitary matrices 2 because this smallest dimensional matrix representation for S x, S y and S z is 2 by 2 is the Pauli matrices or the spin matrices. Special, because a unitary matrix in general has determinant plus 1 or minus 1, and in this case it is possible to choose, all of them to have determinant plus 1 and that is what is meant by S u 2 the special unitary group of transformations (Refer Slide Time: 27:35) and you can see that the spin matrices naturally obey this S u 2 algebra.

You have now got a glimpse, of how group theory, comes in naturally into the framework of quantum physics, this is a simple example. I would now ask the question suppose, we went back to the 3 level atom problems that I very briefly described in my last lecture, is it possible to construct an S u 2 Lie algebra using this 3 level atom structure? Let me do that explicitly.

(Refer Slide Time: 37:03).



So, now I have 3 basis states, the ground state of the atom, the 1st excited state and the 2nd excited state. Of course, they are normalized to 1 and they are orthogonal to each other. I use the Dirac notation wherever possible so that you may familiarize yourselves with this very comfortable powerful and concise notation. What is the role of S plus? S plus is the operator which takes g to e 1 and e 1 to e 2. S minus is the operator that brings e 2 down to e 1 and e 1 to g.

Let me recall that these are energy Eigen states. This is the ground state or the lowest energy state, that is the 1st excited state and that is the 2nd excited state of the atom. And in this atom only 3 levels are of importance to us. So, what are the operators that I can construct with the basis states, g e 1 and e 2 which could represent S plus S minus and S z.

(Refer Slide Time: 38:54)



Now, those are simply done. S plus is the non Hermitian operator. I have written this just by inspection. Because I can see that S plus acting on g is e 1, because g g is 1, e 1 g is 0 and therefore, it is obvious that S plus acting on g is root 2 h cross e 1. The root 2 is there because I have tailored it to suit the commutation algebra. S plus on e 1 would be root 2 h cross this will not contribute and that will give me e 2. I know that s minus dagger is S plus.

So, I know what is s minus? S minus is root 2 h cross g e 1 plus e 1 e 2. I can find out the commutator of S plus with S minus by making it act on the basis states g e 1 or e 2 and the commutator S plus with S minus, would be 2 h cross S z. So, let me find that commutator.

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So, here we go. The commutator of S plus with S minus and as I said earlier these are done on some states. So, let me take this state g it should be a state independent algebra in other words, I could use ket g or ket e 1 or ket e 2 here and I should be able to get the same algebra independent of the state that is used. So, this just gives me 2 h cross square, the commutator of S plus with S minus which is just e 1 g plus e 2 e 1. The commutator of this with S minus which is g e 1 plus e 1 e 2 and of course, this commutator could act on g.

You can easily check the following, first of all the commutator of this with that plus this operator with that and so on. The commutator of e 1 g with g e 1 that is the first term, I have four such commutators the commutator of e 1 g with e 1 e 2 plus the commutator of e 2 e 1 with g e 1. These are operators, plus the commutator of the operator e 2 e 1 with e 1 e 2 and this of course, acts on the state g in my case, I could have chosen any basis state.

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This can be simplified I leave it as an exercise to work this out and you will show, that the commutator of S plus S minus acting on g is simply the same as 2 h cross S z where I identify S z as h cross times e 2 e 2 minus g g. This whole thing acts on g. This relationship that S plus with S minus is 2 h cross S z holds and I can check this whether I use the basis state ket g or the basis state ket e 1 (Refer Slide Time: 37:03) or the basis state ket e 2 out there.

Similarly, I can check that S z with S plus or S minus is plus or minus h cross S plus minus. So, S z with S plus is plus h cross S plus, S z with S minus is minus h cross S minus. Now, this is the same algebra that we saw when we worked with the 2 level atoms. The point that I am trying to make is: if I Now give matrix representations for S plus S minus S z and therefore, for S x S y and so on, which can be written as linear combinations of S plus S minus. I will have 3 by 3 matrices, because the basis states here are 3 by 3 elemented column vectors.

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Let us start with ket e 2, e 2 is 1 0 0 for instance, e 1 then is 0 1 0 and g is 0 0 1. I am now working with 3 component column vectors and therefore, S plus was root 2 h cross S plus is written here it is e 1 g plus e 2 e 1. So, it is e 1 g e 1 ket is 0 1 0 g plus e 2 e 1. So, this matrix is simply root 2 h cross this plus that can be easily simplified. It is just root 2 h cross 0 1 0, 0 0 1 and 0 0 0 so that is my S plus. S minus is S plus dagger, you could do that explicitly or you could simply take the dagger of that matrix that I have just now got.

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So, I have the following. S plus is root 2 h cross 3 by 3 matrix with one sitting here and there. S minus is root 2 h cross  $0\ 0\ 1\ 0\ 0\ 1\ 0$ . I can work out S z and I will just get h cross, with 1, 0 and minus 1 on the diagonal, because this is my definition of S z. The point is this: the dimension of the matrix representation that you use for the operator depends upon the dimension of the linear vector space.

The dimension of the linear vector space is equal to the number of basis vectors that you need, in order to expand an arbitrary vector in that linear vector space in terms of these basis vectors. The matrix is nearly a matter of convenience. You use a matrix representation, in order to take care of explicit manipulations like finding the commutator or doing a matrix multiplication, addition and so on. So, the s u 2 group is really defined by the Lie algebra given by the commutator S plus S minus is 2 h cross S z and S z with s plus is plus h cross s plus and so on. (Refer Slide Time: 42:56)

The matrix representation is not that important. It could be represented by 2 by 2 matrices, by 3 by 3 matrices, as I have done now. (Refer Slide Time: 38:54) Because I have given you S plus S minus and S z (Refer Slide Time: 46:23) in terms of 3 by 3 matrices, from this you can find out S x and S y and check that indeed the algebra between S x S y and S z is satisfied. The matrix is nearly a representation. (Refer Slide Time: 42:56) The algebra of the operators is all powerful and this indeed is the s u 2 Lie algebra.

So, you could work with multi level atoms. So, if I had 4 levels then clearly I have a choice of basis states. I could choose the 4 componented column (Refer Slide Time: 44:46) 1 0 0 0 0 1 0 0 0 0 1 0 and 0 0 0 1. Construct operators the way I have done, find out the matrix representation for these operators and this algebra will be satisfied in any case. So with multi level atoms I could create for you an s u 2 Lie algebra.

The dimension of the matrix is governed by the dimension of the linear vector space. I have already said that I have chosen my basis states to be mutually orthogonal and normalize to unity. To begin with, all I needed for a basis was a set of linearly independent vectors in terms of which any arbitrary vector in the space can be expanded. I can always make them mutually orthogonal and normalize them to unity. The mutual orthogonalization is done by using the Gram Schmidt procedure, a procedure which I will describe in the next lecture.