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

Lecture - 3 Linear Vector Spaces - II: The Two-Level Atom

(Refer Slide Time: 00:07)



In my last lecture, I spoke to you about linear vector spaces and introduced the properties of a linear vector space. In particular, we discussed a two dimensional linear vector space. We shall continue our discussion on linear vector spaces today, using a specific example the two level atom.

(Refer Slide Time: 00:36)



So topic is linear vector spaces. This is the 2nd of the lectures on linear vector spaces, with particular reference to the two level atom. Let me, quickly recapitulate some of the salient features of what I said last time.

(Refer Slide Time: 01:08)



We had a 2 dimensional linear vector space. The basis vectors were chosen to be orthonormal. Each of them was normalized to unity and they were orthogonal to each other. If we used column vector representation for these basis vectors, we could have well represented e x by 1 0 and e y by 0 1. We could use the Dirac notation, and perhaps

refer to these basis vectors as ket 0 and ket 1. I want to emphasize that the 0 here does not stand for the null vector, this does not mean the null vector.

Earlier on when we discussed the properties of a linear vector space, I said that there is a null vector in the space, and on an addition with any other vector it leaves the vector unchanged. Also introduced, the scalar, the number 0 which multiplied with any vector in the space gives me 0, this ket does not represent the null vector, nor does it represent zero it is merely a label. It is a label for a basis vector and this is another label for this basis vector, in the case of the two level atom.

(Refer Slide Time: 02:45)

I have two basis vectors, I could refer to them as ket 0 and ket 1, or in the paralons of atomic physics they are usually referred to as ket g and ket e. So, g and e are merely some symbols, denoting that this is the lowest energy state of the atom or the ground state. And, this is the 1st excited state of the atom and that is why the symbol e. The point that I am trying to make is that, if energy is the observable in the system, which is indeed the way we are going to work with it.

Once a measurement is made on the energy, the system collapses either to this state with an energy Eigenvalue E g, or to this state with an energy Eigenvalue is E sub e. Denoting by H, the observable energy I have used H because H is the Hamiltonian, and from classical physics you would know that the Hamiltonian operator would represent the total energy of the system. Ket e and ket g are Eigenvectors of h with Eigenvalues E sub e and E sub g. A general state of the atom can be expanded in terms of these two basis vectors.

(Refer Slide Time: 04:53)



So, the general atomic state can be written in this manner and if indeed the state is normalized.

(Refer Slide Time: 05:07)

So, if the states psi were normalized to 1, then it automatically follows that mod a square plus mod b squared, equals 1 where a and b are complex numbers. Of course, here I have selected orthonormal basis states. This is 1, this too is 1 and ket e and g are orthogonal to

each other. This obviously, follows from this fact because this is obtained by simply taking the complex conjugate of this object. Now, I could give matrix representations in that case I would write this as: 0 1, 1 0 and that is 0. I could give matrix representations for all these and obtain for you for instance in this case that 0 1 row with 0 1 column vector is 1.

So, I have this orthonormal basis and these basis vectors are chosen in the context of this physical situation to be the energy Eigenstates of the atom. Now, having said that what are the various operators that I can make with these two basis vectors?

 $t_{av} = s_{pacea} - II = 1 = 0$ $(b)^{2} = 1$

(Refer Slide Time: 07:01)

Here, are the list of operators, that is an operator. In matrix notation, this is simply going to be and this is going to be the matrix. Similarly, I can write the other matrices, this is one of the operators that I can form with ket g. It is evident that these two are Hermitian operators, because when I take the dagger, that means interchange the rows and the columns and take the complex conjugate of all the entries that simply gives me the same operator.

Similarly, this is another Hermitian operator. Of course, I can have combinations of these operators, I can for instance think of the operator you will notice, that I use operators and observables interchangeably and I could give matrix representations to the operators. Similarly, I can have an operator of this form, these are evidently Hermitian operators. There are more operators that I can think of:

(Refer Slide Time: 08:48)

I can have the non-Hermitian operator e g and g e, this object is clearly the Hermitian conjugate of the dagger of that operator. I can think of combinations of these and so on. So, I can form a set of operators given the basis vectors. We now see, how the operators are formed using the basis vectors. Choose the basis, the basis should be physically relevant to that system. In the atomic system and experimentally measurable quantities say, energy of the atom, here is a two level atom. So choose the energy Eigenstates, ket e and ket g as the basis states. This is just a convenient choice, you may have many more sets of basis vectors that can be chosen. And I will discuss various possibilities later on, in subsequent lectures.

Given those basis vectors I can form all these operators and combinations of these operators. Some of them are Hermitian, and some of them are not but non Hermitian operators such as these also have a physical significance. They perform a certain operation on the atomic system. And we shall see pretty soon, what kind of operations are performed by these operators?

In this context, I wish to recall the algebra of the spin matrices because that is particularly relevant in the problem of the two atomic two level atomic system.

(Refer Slide Time: 10:58)



The spin matrices, were defined in this way, S y is h cross by 2 sigma y and S z is h cross by 2 sigma z. The matrix representation for these let me recall are as follows: these are the matrix representations. There was an algebra of the spin matrices, and I pointed out that that is the general angular momentum algebra. In the sense, the same algebra will be satisfied in the context of orbital angular momentum.

(Refer Slide Time: 11:46)

For the moment, I will refer to these as the algebra of the spin operators S x, S y and S z. And to remind you of the algebra, there is a cyclic relation like this the commutator of S x with S y is i h cross S z, S z with S x is i h cross S y and S y with S z is i h cross S x. I could equivalently define S plus and S minus as, S x plus or minus i S y and the algebra can be written in terms of: S plus S minus and S z in the following manner. What has that got to do with the atomic system? We will see that right away. Consider for instance the action of, let us say e g this operator on this state on either ket e or ket g.

(Refer Slide Time: 13:08)



So, let me consider the action of this operator for which I can give a matrix representation. Recall, that ket e was represented by the column vector 1 0 and bra g was represented by the row vector, 0 1. The action of this operator on ket g which is the same as the action of this matrix, and this matrix I write right here on 0 1, is simply ket e because the action of this matrix on that column vector is 1 0 which is identical to ket e.

I could have easily found this, without writing out matrices by realizing that this object can be expanded, using the fact that g is normalized to unity, ket g is normalized to unity and therefore I will have ket e. If we realize that this is simply the scalar product, that leaves behind the state ket e and that is what it is. Similarly, if I take the Hermitian conjugate operator, g e and if it acts on ket g, it is clear by the same kind of argument that because ket g and ket e are orthogonal to each other, this is 0.

(Refer Slide Time: 14:54)



So in my picture, I have the two levels of the atom and there is this operator, which I will denote by S plus. You will realize that I am doing this from hindsight because I will show soon, that this S plus is the same as the S plus that I got here. So, the operator e g takes the ground state to the 1st excited state. The operator g e, brings down the 1st excited state to the ground state. And to complete the story, when the operator S plus acts on the excited state. It simply destroys it, it annihilates it and when it's Hermitian conjugate acts on the ground state, it simply destroys it. So, I have this two level atomic system, where I have formed two operators non Hermitian conjugate of S plus and this is the role of these operators, to raise a state or to lower the state. If you look at this .and you put in the matrices for S plus and S y and find out the matrix representation of S plus.

(Refer Slide Time: 16:51)



You will find that, the matrix S plus is precisely this 0 1, 0 0. You can do that right away and check out that that is indeed true apart from a factor h cross, if you use matrix representations for S plus and S minus.

(Refer Slide Time: 17:19)



You find that S x plus i S y is, let me put in the h cross as well and that simply gives me which is precisely, what I have here apart from the h cross. And therefore, I can do by a similar procedure, I can find out that S x plus i S y, which is S plus is simply h cross e g.

(Refer Slide Time: 18:10)



So, I just have to write h cross e g is S plus and h cross g e, is S minus. S minus is h cross g e. We have therefore, discussed the job that these two operators do.

(Refer Slide Time: 18:30)

We now know what exactly is the role played by e g and what is the role played by g e. Let us look at an operator like e, e. I could do this by writing matrices explicitly, as in the earlier case, but I think we will do well to use the Dirac notation.

(Refer Slide Time: 18:57)



And find out happens when, this acts on states it is clear that because e is a, normalized vector normalized to 1. You just retrieve ket e and when e e acts on g that is 0. Similarly, this operator, acting on g gives me the same state and this operator acting on the 1st excited state gives me 0. Now, from this, it is evident that when the operator e e acts on a generic ket, which represents a vector in the linear vector space, it simply gives me a ket e.

Similarly, if I replace all the e's by g's, I find that the operator g g here would simply project out b, which is the component of the state in the direction of the basis vector, g. In other words, this is a projection operator

(Refer Slide Time: 20:18)



And I have identified e e and g g as, projection operators which project a generic state in the direction of ket e or ket g, depending on which operator is used. So, these are the projection operators.

(Refer Slide Time: 20:46)



So Now, we know what exactly these two do needless to say,

(Refer Slide Time: 20:55)



That if I now consider the operator e e plus g g, that is, simply going to play the role of the identity operator. It is obvious because while one of them gives us the component along e the other gives us the component along g, and therefore we can assemble both together and make the full vector. To go back to our matrix notation, just to keep correspondence with it. This object is simply going to be and this is going to be represented by this. You can easily check that this is the identity operator, that is the identity operator. That is a 1 0 out there.

So, you see the sum over operators formed like this from the basis states, that sum adds up to the identity. In other words, in general this is an example of a statement which says that let phi i, i is equal to 1 2 as many as there are basis states, be a complete basis set. Then, summation over i, phi i, phi i is equal to the identity operator. And here, in our problem i simply takes values 1 and 2 phi 1 being e and phi 2 being g. And therefore, this relationship is evident, this is called the completeness relation and what I have demonstrated to you is the completeness relation in the context of the atomic system. Now, let us proceed and see what the other operators mean. (Refer Slide Time: 23:43)

So we know what this operator is, this operator is merely the identity operator. Now, let us consider this operator:

(Refer Slide Time: 24:04)



So, I now start with the operator minus g g and I wish to know what it is. Already, I know what S plus and S minus are, suppose I find the commutator of S plus and S minus in this language. That is the same as trying to find the commutator of e g, apart from an h cross with g e. I pulled out h cross squared because there was an h cross with this operator, and there was an h cross multiplying this. The way to do this, is to make it

work on some basis state and see if the algebra that we have is indeed state independent. So, let us consider the commutator of S plus with S minus acting shall we say on the state e.

So this is the same as h cross squared. Suppose, I expand the commutator since, the commutator is a b minus b a, where this is the operator a and that is the operator b and this is supposed to act on ket e. So, we take a look at this, this is 1, this is 1 and I can write it as e e minus g g acting on ket e. And low on behold that is what I was trying to find but I do know that this commutator S plus S minus is 2 h cross S z and therefore, I understand that h cross by 2, e e minus g g is equal to S z.

(Refer Slide Time: 26:02)



So, I have found out what exactly this is h cross by 2 e e minus g g is S z, e e plus g g is the identity, h cross e g is equal to S plus, h cross g e is equal to S minus. And of course, I can form e g minus g e and so on. So, returning now to the construction of further operators. Let me consider S squared.

(Refer Slide Time: 26:50)



I define S squared as S x squared plus S y squared plus S z squared. The simplest way to find out what S squared is, is to realize that this is h cross squared by 4 sigma x squared, plus sigma y squared, plus sigma z squared. But, this is each of them is the identity operator. You can explicitly check this, by putting in the matrix representations for sigma x, sigma y and sigma z. Therefore, S squared is 3 h cross squared by 4 times the identity operator. It is obvious that S squared commutes with S x, S y, S z, S plus, S minus and so on, because it is essentially the identity operator.

Let me look at Eigenstates of S squared and S z or S squared and S x or S squared and S y but it is conventional to look at the Eigenstates of S square and S z and pretty soon we will understand what the purpose of this is.

(Refer Slide Time: 28:11)



It is clear that when S squared acts on ket e, it simply gives me 3 quarter h cross squared ket e and S squared acting on ket g, gives me the same thing. I would like to, write this as half into half plus 1, like this. I would like to write this in general as S squared, acting on an Eigenstate, gives me S into S plus one h cross squared Eigenstate. And in this case, this state could be either ket e or ket g and S is equal to half.

Now, let me look at S z acting on ket e. It is obvious, that this is the same as h cross by 2, e e minus g g, acting on ket e, and that is just h cross by 2 ket e. There is no contribution from this term, because this inner product is 0 whereas, from this term one realizes that, that inner product is 1 leaving behind ket e. I can do S z acting on ket g and that is just going to give me minus h cross by 2 ket g. I therefore, realize that the two basis states in question ket e and ket g are common Eigenstates of S squared and S z.

So, what are the Eigen values?

(Refer Slide Time: 30:11)



The Eigen values are the following: s is equal to half and m, where m is defined this way, takes values plus or minus half. This becomes very important particularly in the context of spin doublets like the electron. A model which I will talk about a little later. Returning to the two level atom, I find that there are two commuting observables: S squared and S z. By commuting observables, I mean that this commutator is 0, it is also true that S squared commutes with S x and with S y. But, since S x, S y and S z do not commute with each other. The only commuting observables that I can talk about are S squared and S z or S squared and S x or S squared and S y. It is conventional to use S z as the operator along with S squared.

What do we see from this? If a measurement is made, to find out the value of s and m, that means the Eigenvalues of S squared and S z, for clever experiment is made on the atomic system. On the state of the atomic system to, find out these Eigenvalues after the measurement simultaneous measurement of S squared and S z. We will get the values of s and m accurately.

Of course, you have to allow for human errors and for instrumentation errors but having said that you can get simultaneous values for s and m. The Eigenvalues of S squared and S z accurately, quantum mechanics tells you, that you can take a complete set of commuting observables and make a measurement simultaneously of the Eigenvalues, corresponding to all those observables, or the actual values, numerical values of these

observables, which are outcomes of the experiment that is performed. And you will find, that you can measure all these with accuracy, subject to human errors and instrumentation errors.

On the other hand, if you make a measurement of the Eigenvalues corresponding to S x and S y. Since, this is not a pair of commuting variables, if you make simultaneous measurement, you will find that you cannot measure both of them accurately, simultaneously. This is in fact, the preamble, to the uncertainty principle the Heisenberg uncertainty principle which I will talk about in more detail in a subsequent lecture. In this problem, we have these two commuting observables S squared and S z and therefore, it is possible to label the state of the atom in the following manner, by two quantum numbers, which I get as the outcome of suitable experiments.

(Refer Slide Time: 33:56)

There is this state e: which has a value of s equal to half and a value of m equal to half and the state g: which has s equal to half and m equal to minus half in units of h cross. So, I can do better than simply use abstract notation e and g for my states, I can start finding attributes, I understand properties of that state, I understand that these are states with values of quantum numbers given like this. I also understand that these are the only two quantum numbers in this problem that can be measured simultaneously, accurately. Quantum mechanics, does not forbid us from making measurements on observables simultaneously on any set of observables. The question is how accurate are your answers? And if you want accuracy, then there should be a set of commuting observables.

I would now consider another example. This does not pertain to the two level atom, it is a different example. It is about the spin doublet. Now, the reason why I wish to discuss it here, is because the spin doublet can also be explained using the same mathematical framework, that is a two dimensional linear vector space.

(Refer Slide Time: 35:29)



The spin doublet, in particular I can talk about the electron. An elementary particle which has got charge minus e and rest mass approximately 0.51 million electron volts by c squared, where c is the velocity of light and vacuum. Even as the electrons attribute is minus e, for the value of charge and the rest mass with this value, it can exist in two spin states. Spin is an experimentally measurable quantity, you could call it the up state of the electron, which is the half, half state that I spoke about here.

And the down state of the electron, which is the half, minus half state. Both these states are spin states of the electron, before measurement of the spin of the electron, the spin state of the electron would in this notation be represented in this manner. And after measurement, the system would collapse either to the up state, or to the down state. We will show later, that there are other particles, with spin s value given by 1, 3 by 2, 2 and so on, in units of h cross.

(Refer Slide Time: 37:18)

porton rnious +

In fact in the three dimensional world that we live in, elementary particles are classified as fermions and bosons, fermions have S equal to half 3 by 2, 5 by 2 etcetera. Half integers spin values, in units of h cross and bosons have S equal to 0 1 2 etcetera in units of h cross. What I have spoken about, in the context of the two dimensional linear vector space, is the physical system. A physical system, with S equal to half, which could live in the up state, which means m is equal to half, that is the Eigenvalue corresponding to S z, or in the down state where m is equal to minus half, which is the Eigenvalue corresponding to S z in the down state of the electron.

(Refer Slide Time: 38:26)

electron, proton, neutron - e, restman ~ 51 MeV

There are other particles which have spin equal to half for instance the proton, the neutron and many others. Now, examples of bosons and example of a boson is the photon.

(Refer Slide Time: 38:43)

The photon, is an example that is light quanta, it is an example of a boson. And, it has spin 1. So clearly, the photon will not be described in the purview of this two dimensional linear vector space. In general, it is true that for a given value of spin, the 3rd component can take values minus s to plus s in steps of 1. This is a very important result in angular momentum algebra. And I will derive it in a subsequent lecture in detail, when I talk about angular momentum.

It would be pretty clear by now, that the Dirac notation is extremely powerful and it would be very cumbersome to use matrix notation all the time. In the sense of writing explicitly column vectors and matrices n by n matrices, as the dimension of the linear vector space increases and do an explicit matrix multiplication. The power of the Dirac notation, was what I was trying to bring about, in this context by trying to find out, what all these objects mean through their effect on the basis states. By using the Dirac notation instead of the matrix notation.

(Refer Slide Time: 40:32)



A good exercise would be to consider the 3 level atom, you could denote the energy Eigenstates as g, e 1 and e 2. Both in the case of the two level atom and in the 3 level atom, a question arises, if the only commuting observables are s squared and s z. How do you manage to find out the value of the energy? These are supposed to be energy Eigenstates and if energy does not commute with s squares and s z. How can we fix the energy Eigenvalues corresponding to the ground state and the excited state of the atom? The fact of the matter is that, the Hamiltonian or the energy operator in this problem can be written in terms of s z.

(Refer Slide Time: 41:31)

As also in this problem, look at it this way. Suppose I wrote the Hamiltonian as omega S z, where omega is a suitable constant, then the action of the Hamiltonian in the case of the two level atom on e, is going to be h cross omega by 2 e, and when it acts on the state g it is minus h cross by omega by 2 g. We would not like to have negative energies as the Eigenvalues as experimental outcomes.

(Refer Slide Time: 42:20)

So it is easier for us to say, that we can choose a Hamiltonian, which perhaps is of this form, omega S z plus h cross omega, times the identity operator. In that case, it is clear that I pickup an extra h cross omega from here, and therefore, I will have a net energy value 3 h cross omega by 2 e for the excited state. And for the ground state, I have h cross omega by 2 with the minus sign there, plus h cross omega. And that is the same as h cross omega by 2 g which is a positive quantity. So this is how I would construct the Hamiltonian for the two level atom. I would attempt to do a similar kind of operation. In the case of the 3 level atom the operators are easy to identify.

(Refer Slide Time: 43:25)



I have a set of operators as before e e, e 1, e 1 to show that this is a 1st excited state, g g and e 2, e 2 and non Hermitian combinations of this kind, e 1 g etcetera. The completeness relation, in this case would simply mean that: e 1, e 1 plus e 2 e 2 plus g g is really the identity operator. I could choose for e 2; the column vector 1 0 0, for e 1; the column vector 0 1 0 and for g; the column vector 0 0 1. This is a possible representation for the basis vectors, and in terms of these I can write out various operators for this system. I should be able to construct raising operators, that is operators which act on ket g and take it to ket e 1, act on ket e 1 take it to ket e 2 and lowering operators which will bring down the atomic levels, we should bring down this level here and this level there.

How exactly is this done? Well, normally in order to raise the system from a lower energy state to a higher energy state you pump in energy by getting the atom, to interact with light, shine light of appropriate frequency on the atomic system. So, that energy is provided to the atomic system (Refer Slide Time: 40:32) which perhaps is in the ground state enough energy for it to go into this excited state or that excited state and so on.

Similarly, when the atom gives energy out in the form of light quanta, that is photons it jumps from a higher excited state to a lower energy state, it could come from here right there or from here, here and so on.

So, there are very many possibilities and clearly these experiments are done, using light atom interactions. Many times, ideal laser light is used to make ket interact with the atoms in order to, take care of these operations and we just saw how exactly the operators, in the linear vectors space do the job of raising and lowering of the atomic levels. It would be a very good exercise, to try to interpret the various operators that one can form in the case of the three level atomic system, and I would urge you to do it, so that you get a complete understanding of what exactly happens in this system.

It is evident that, there are three basis vectors in this case and therefore, it is no longer the two dimensional linear vector space that we spoke about. The linear vector space is larger. It is good to check out all the properties of the linear vector space in this context. With this, I conclude my discussion on the two level atoms. And the next time, we will continue our discussion of the spin matrices with further properties of S x S y and S z and of course, the Pauli matrices.