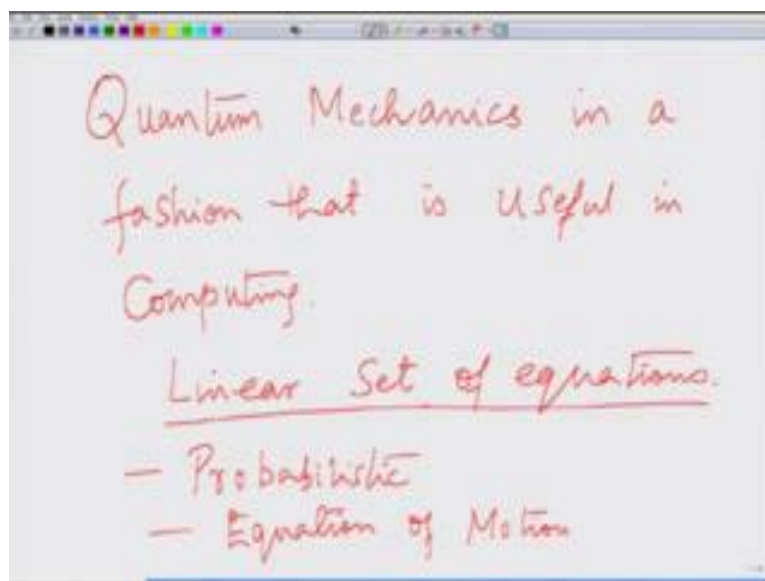


**Implementation Aspects of Quantum Computing**  
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**Department of Chemistry**  
**Indian Institute of Technology, Kanpur**

**Lecture – 2**  
**Introduction: Technical Details**

Today, we will learn Quantum Mechanics, in the way that is necessary for quantum computing.

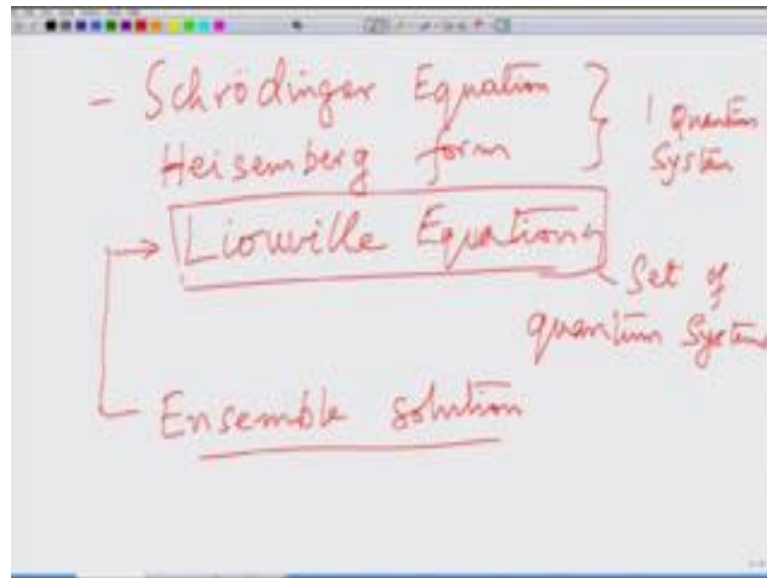
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So, quantum mechanics in a fashion that is useful in computing. So, what we will do is, we will be making our quantum mechanics the Linear set of equations. So, the way you have learnt quantum mechanics earlier that might be slightly different from the way we will be approaching quantum mechanics now.

Although the principles and everything else will remain the same for the benefit of utilizing this in terms of computing we will set it up in way. So, that it can have set of linear equations that can be solved, and that is the approach that we will do right now in terms of quantum mechanics. So, what are the main aspects of quantum mechanics? One of the main aspect is that it is going to be Probabilistic, next is it will have Equation of Motion, which is different from the classical one.

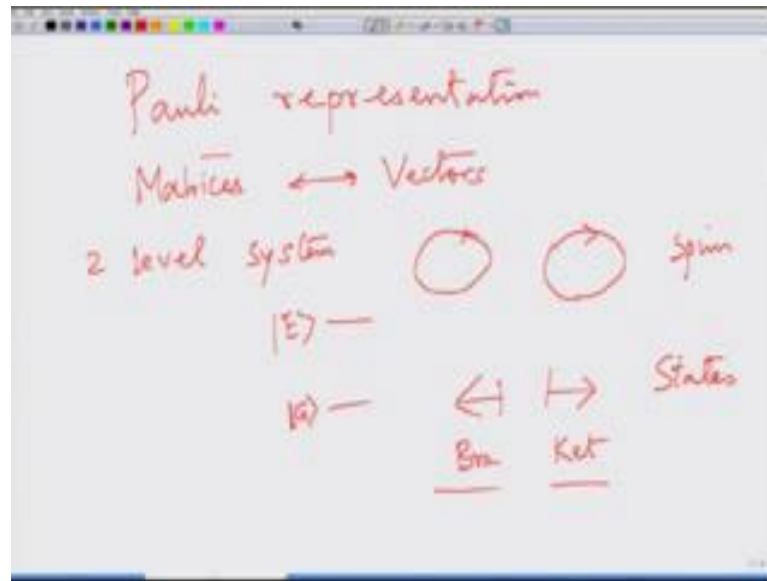
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And the equation of motion, here is the Schrodinger Equation. Now the equation motion the Schrodinger equation can also be expressed in terms of Heisenberg known as Liouville Equation, or when you have a set of quantum systems then it is more. So, each of these expressions essentially are going to give rise to the quantum mechanical solutions, which are of use to us. So, when we start with Schrodinger equation as we have done before, or the Heisenberg form they are essentially one and the same, and the Liouville equation is the form, which is using more than one system. Schrodinger equation has a Heisenberg form essentially for 1 quantum system whereas, when you have an ensemble or a set of quantum systems, then you will be using the Liouville equation. Now for all practical purposes when we will look at quantum computing Liouville equations become most important, because we are actually trying to see how an entire set of problems have been solved simultaneously.

And then Liouville equation is the one where you have all the processes working together. So, it is an Ensemble solution. So, in some sense this is the one, which takes into account additionally the effect of statistical mechanics. So, right now is the right time to tell you about this, because you have seen both quantum mechanics and statistical mechanics before and we are just combining them to get our final expression, which is a Liouville expression which is an ensemble approach of dynamics. So, when I set moves what is going with it?

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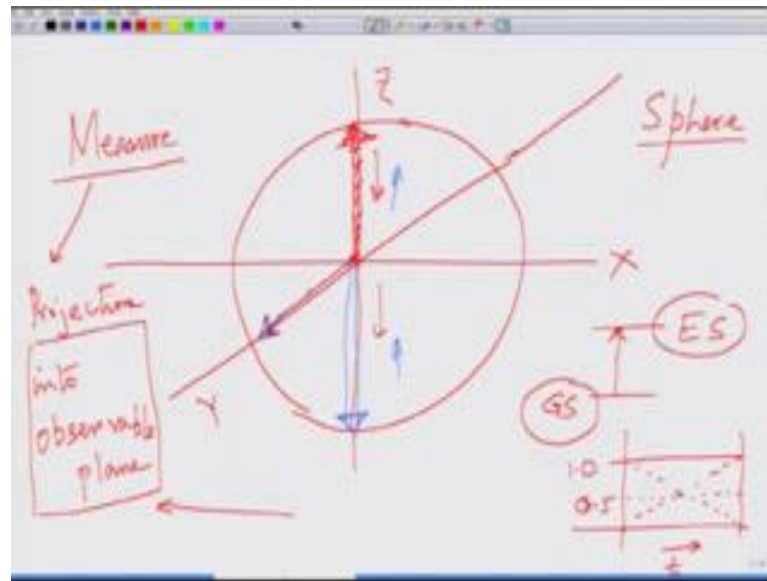


So, there are a few things which we need to do here, one is to use the Pauli representation. So, the Pauli representation is something which actually uses matrices, which can be equated to vectors, and these help you in picturizing what you are doing in quantum mechanics right. So, a 2 level system for instance, which can be as simple as spinning one way, versus the spinning other way or 2 states of a system, say ground state or in an excited state, these can be represented in terms of both matrices and vectors and the convention used is going one way or going the other way. So, this is known as the Bra, and this is known as the Ket in total it closes and becomes a complete set.

So, this is the representation which goes, which gives an overall idea that is see technically there is no pictorial understating of this, but it helps you in understanding the (Refer Time: 06:27) a lot more if you take this approach. So, that is what we are going to do we are going to use the bracket principle and put it in a way. So, that all the mathematics we write get short form. So, that is where we start off, so, it can be as simple as a spin system or it can be states that we are looking at. So, that is how we represent the quantum mechanical systems from where we started.

So, the first principle that we want to look at is to see how we can represent this. So, whenever you want to represent a vector, we are used to our 3 dimensional picture, which will essentially have is sphere.

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And in this sphere the vector can be either in one of the directions or it could be in the other direction. So, you have to choose, which one where it is either it is on 1 dimension if I choose to call it Z then I have the X and Y in these directions say Y and x, it depends on the convention we choose how it is going to look like, but the vectors can essentially rotate in this frame right. So, this is simply a sphere in which we can assume a vector to have different directions. Based on this simple principle you can define how your quantum system is going to be. So, technically whenever you are measuring one of the different conditions of quantum systems the measurement is in one of the directions. So, either you are measuring along the Z X plain or Z Y plain, or if you would like you can make measure along the X Y plain typically that is not what it is, because our convention is that we will be having our Z axis along the direction where the vector is going to align for us. This is the vector which is quantum vector for you, right.

So, what we doing is we are saying that this is the representative vector based on which we can have this. So, if it actually goes completely the other direction then we call that this is a flip. So, essentially it has gone from 1 state to the other state. So, it can be through this in between step or it can just show the observation when you make you will essentially see the observation will be that the upper one, the arrow in the upper direction is shrinking whereas, this is growing or vice versa this is growing, and this is shrinking sorry, this is shrinking and this is growing. So, this is how its related either this is shrinking and this is growing, but in the middle there is always this other state where the

system can be present while this shrinking and growing is going on, which means that there is this other plain X Y plain, if I do not measure that, that is the plain were the quantum vector if we look at it that way can reside infinite, in infinite possibilities and that is one of the biggest advantages of looking at how the quantum system it was. So, I am making an analogy to a classical system.

In a classical system you have vectors you have pictures that you can draw. So, I am trying to make that analogy right. So, we all know for sure that there is no way of representing a quantum system in this particular way that I am trying to do right now, but it turns out that they have a very strong correlation at least in understanding. The picture is that when we measure, we only measure it in one way or the other and that particular act which we call as measure is essentially the act of finding the projection in a particular plain. So, as long as I define my principles in a way that we are able to understand what we are saying there is no problem. So, if we can define that a projection is a measure of my quantum system in the plain which is my observable plain, so, projection into observable plain.

So, projection into observable plain is my measurement once I do that then I will see for instance in this particular case, that either the vector is shrinking in one direction or growing in that direction and correspondingly in the opposite direction it is becoming the opposite. So, if it is simple 2 state system which essentially make sense that my process where I am having a motion form let us say the ground state to let us say the excited state, if I measuring the excited state quantity, it is going to increase, when I push the system going towards excited state and correspondingly the ground state will go down.

So, if I make a simple measure of how let us say then my total probability is always one, I will always have a picture, which will look like I do not know how you define thinks, but let us say in terms of time I have a change which can be as simple, as a simple linear change one going down and the other correspondingly going up. So, there will be point of time when everything will be 50-50 write here is where half and half of each of the 2 states are available. So, this is gone down by 50 percent this is grown up by 50 percent.

At no point of time therefore, is any loss or any kind of event, but this is relying on the fact that we are making measurements all the time, if I make only one measurement and do not make the other measurement then there is always this possibility that while this is

going to the other side there is a chance that it can also be in the in between case and this is the power, which is very different from a classical system because, in a classical system it will always be what I just showed you whenever something disappears it always appear on the other side. Here since there is no line of action that you can draw from one state to the other you can only make a measurement and comment, which is basically a projection whenever you make the measurements, which is a projection you will have this story exactly as I mentioned which is the classical answer, but unless and until you complete the measurements, all the other possibilities exists, which means that at any point of time nothing may be on the upper side or the lower side they are all actually processing at the very middle and if you measure at that point of time.

Student: Sir is it represented at 0.5 probabilities (Refer Time: 14:50).

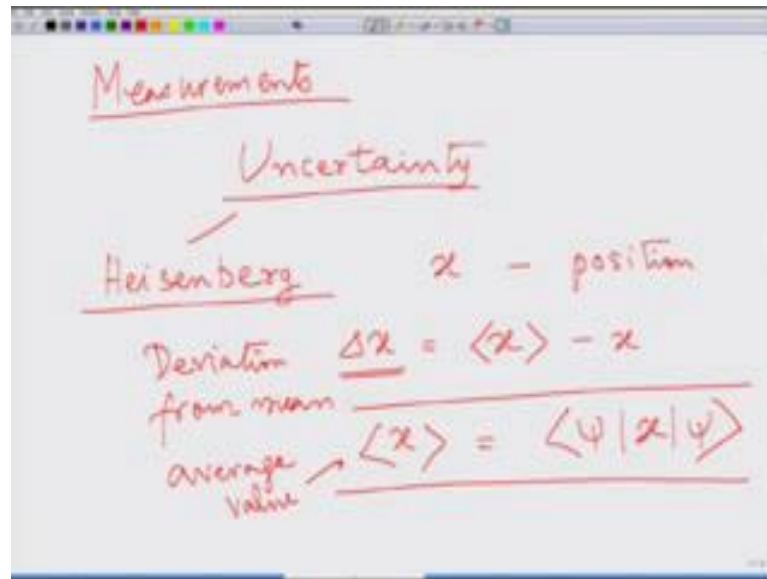
No, the point is when it is processing in the middle it can go either way whenever, you make a measurement either it will be possibly going into the Y dimension I mean plus Z dimension or the minus Z dimension, if it is exactly sitting in the middle, if it is processing exactly in the middle then the probability of it going one way or the other is 50-50. So, either you will see 50 percent going one way, 50 percent going another way, and since you are never making one measurement you are making an large number of measurements you will get a probability, which will give you a 50-50 split of that two. So, which will confirm exactly with your classical answer and that is the beauty of it, so, which means that I can now say that my quantum system will give me the classical answers, whenever I make a measurement. So, this point is extremely important otherwise you cannot have anything known as computing with a quantum system.

The facts that whenever, you make a measure you will always get the solution, which is guaranteed classically you will be able to use this as a computing device otherwise it is not possible. Because we have gone through a few of the initially preliminary discussions, where we had said that there was this presumption that what is a point of a quantum computed to never work because, it is always probabilistic there is no answer, which is going to be correct because every time we will get a random answer that is not the point. But here is not really random you will always get what you are supposed to get classically also is just that that until you make the measurement all the other possibilities exist and that is the thing, which you can take advantage of. If you can take advantage of

that then quantum computing is useful otherwise it is just like a classical computer. So, that is the basic point here which we would like to stress.

So, now that we have sort of understood this let us go over a few of the important points, which is in terms of measurements first things to understand is uncertainty.

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So, whenever you have a measurement in quantum system it will be associated with uncertainty, and this uncertainty was devised by heisen berg, this heisen berg uncertainty principle essentially is just a measure of the deviation that can happen from the average measure at any point of time you make a measure that deviation it can have from the most or the average measure is what is known as a heisen berg measurement uncertainty.

So, in other words, so say for example, you are measuring a position X right, if you are measuring position then the associated uncertainty delta X for the position will be given by the fact that you have say an average position minus the position that you measure at any point of time, that is your uncertainty right. Every time you will not get the right value which is your average value, but there will be some deviation from there as long as you can the point, which is important in the uncertainty principle is that there are properties of this uncertainty, which can be correlated and that gives you the advantage or gives you the limits of measurement. This particular deviation, deviation from mean, but the more used uncertainty parameter is the squared deviation from mean. So, that is given by typically at any point time if you want to write what this average value means,

it means this is my measure. So, this is my parameter that we; so, position we want to measure associated with a wave function which is my side and with respect to the wave function I get the average value of position as  $\langle x \rangle$  right.

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The image shows a whiteboard with handwritten mathematical equations in red ink. The equations are:

$$[\Delta(x)]^2 = [(x - \langle x \rangle)^2]$$

$$= \langle x^2 \rangle - \langle x \rangle^2$$

Below these equations, the text "Square deviation" is written and underlined. To the right, the equation  $\Delta x = [\langle x^2 \rangle - \langle x \rangle^2]^{1/2}$  is written, with "RMS deviation" written below it and underlined. A small "M" with a horizontal line underneath is also present at the bottom right of the whiteboard.

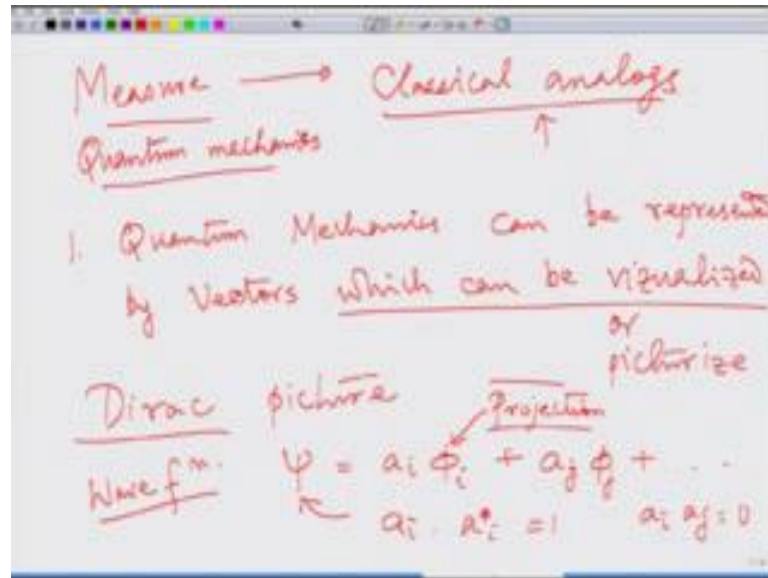
Now, this average position can have a deviation, which is mostly done in this form squared 2, say I have  $X$  minus. So, this is the square deviation, so this particular deviation is the square deviation or the variance and what you are more used to is the route mean square deviation, which is basically the square route of this. So, this is your route mean square deviation, so, whenever you make a measure. So, if I want I can replace this  $X$  which is position in my case to any measurement where value or parameter, which can be  $m$ ,  $m$  representing any measurement. So, this measurement can be position as a I just showed you  $x$ , it can be momentum, it can be energy anything that you want to measure. Now, some of these measurements are not possible to be had done simultaneously, now this is coming from quantum mechanics.

This is the part which we have already learned, but we have revised here because this is the part which is very critical in terms of the quantum picture. In the classical picture there is no reason to expect that there will be any complimentary amongst measurement. So, I have arbitrary precession of measuring say position, velocity, momentum, all the measurements that we want to; however, in quantum mechanics this is not true. We have to have only a few parameters, which are allowed now this is



coming because as I have been telling the character of quantum mechanics says that we are not going to have the path laid out for us. We can only measure one point and we can make measurement the other point, we cannot actually have a continuous evolving measurement possible because every time you make a measure it is a classical unit.

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So basically the definition of measure is that I am converting all my quantum aspects into classical analogs they need not be the same thing.

A classical analog is not classical it essentially means it has a correspondence to a classical principle that is all. So, measurements in quantum mechanics has a classical analog in terms of saying that I am able to say that every time I make a measurement I am actually able to correlate to my classical conception. So, that is the whole idea here. So, what I will doing going to do about this we are going to see how we can use these principles to go further. So, the first principle we introduced here was the fact that, quantum mechanics can be represented by vectors which can be visualized. So, that is our first concept which we said. Second concept we said that every time you make a measure, you are making a measurement implies correspondence to.

Student: Sir, basically measure (Refer Time: 25:29).

No, visualize means you can picturize or maybe I should use the word picturize, or picturize. See, otherwise quantum mechanics has no way of understanding how it is

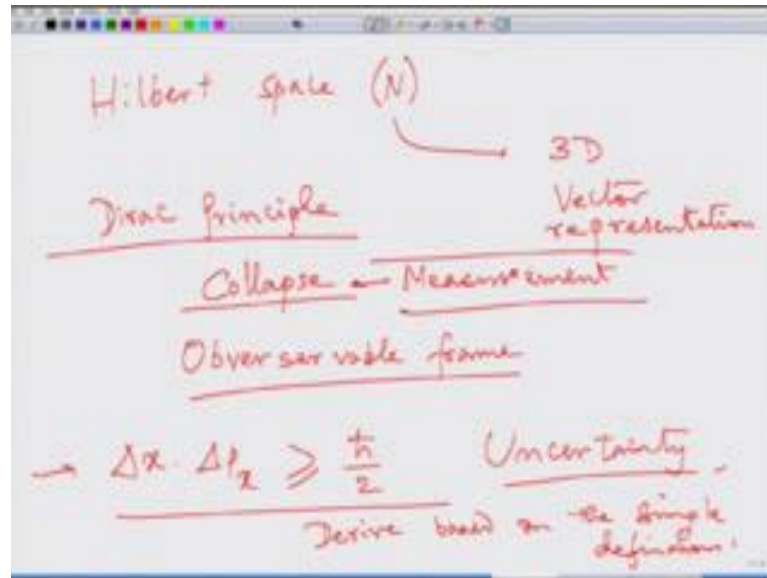
right, I mean in if I quantum mechanics is supposed to be only a math you are not able to say for instance understand, how the quantum mechanics parameters are going to be one way or the other because, wave function for instance there is no physical analogy of wave function I cannot feel a wave function, I cannot have any aspect of wave function; however, if I can somehow have certain kinds of wave functions come together they will end up producing results which is measurable right. So, that is that certain kind that we are defining. We are saying that these wave functions are nothing, but ways of representing vectors that is another way right. So, I have actually in the exact Dirac pictures. So, what we are trying to build up is a Dirac picture, so, let me actually tell you the exact way Dirac picturized it. In the Dirac picture the wave function  $\psi$  is consisting of as with everybody with say many coefficients  $i, j$  let us say equalized, fine it can continue it is a super position of many different wave functions right, that is my wave function  $\psi$  final wave function it has many other wave function.

Now the idea was that no matter how it happens the wave function we looked at it when we were doing it earlier also the wave function. So, this is the wave function was supposed to be normalized, which means that no matter what happens if you take this square of the wave function which is something which you consider as the probability function that is having a maximum value of 1 because, that is what a probability does. So, wave function has no meaning, but the probability function which is the square of the wave function has a meaning and therefore, it can have values ranging from 0 to 1. So, the Dirac picture is essentially takes this and puts it in a different prospective saying that in that case this wave function, if you wanted to look at it that way should have a connection to how all these parameters adopt to give rise to the final answer.

So, this particular wave function can be connected to the total observable issue which is composed of many different (Refer Time: 28:38). So, at any point of time if I actually align it such that only one of the aspects is going to be there, then it becomes a pure function. So, in other words if I can have a  $i$  and say a star  $i$  come together. So, that that becomes one then everything else a  $I, a, j$ , they all should banished this is what happens. So, I am in other words I have actually taken a projection along my  $\psi$  direction my  $\psi_i$  direction that is my projection. So, this is basically the Dirac picture when I am actually taking any state and picturizing it in this manner. So, I can take the extreme of saying that this entire vector picture this entire wave function picture can be accommodated in

the vector mode, where I am picturizing this and then I am deciding how I am going to take the projection along with dimension, and that is why this sphere picture only works for just the beginning understanding.

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A real quantum system has something called a Hilbert space, where the space is can be infinite right all the possible numbers of wave functions can be there. So, it can be in infinite side. So, for us to visualize again becomes completely impossible, because we do not know anything more than 3 dimensions if you tell me anything better than sphere I do not know higher dimensions sphere I have no idea right, but the Hilbert space is an extension of this idea into a mathematical world. So, we are just connecting the mathematical world to an understanding which we can understand. So, we are saying that to a picture which we can understand. So, we are saying that we are actually taking an n dimensional space to a space which is understandable to us. So, this Hilbert space of n dimensions is being brought down to a 3D space, which is my vector representation just for understanding, but it turns out that this Dirac principle of doing the whole picture.

Student: (Refer Time: 31:17) 3D dimension and we are cutting n minus 3D dimension to get 3D dimension picture.

No, we are not cutting anything, we are just saying that there can be n dimension, but whenever, I am interested in understanding how the picture is evolving I am only able to

draw it in 3 dimension right that is the only way I can represent, I cannot understand anything more than that that all now it is up to you if you want to.

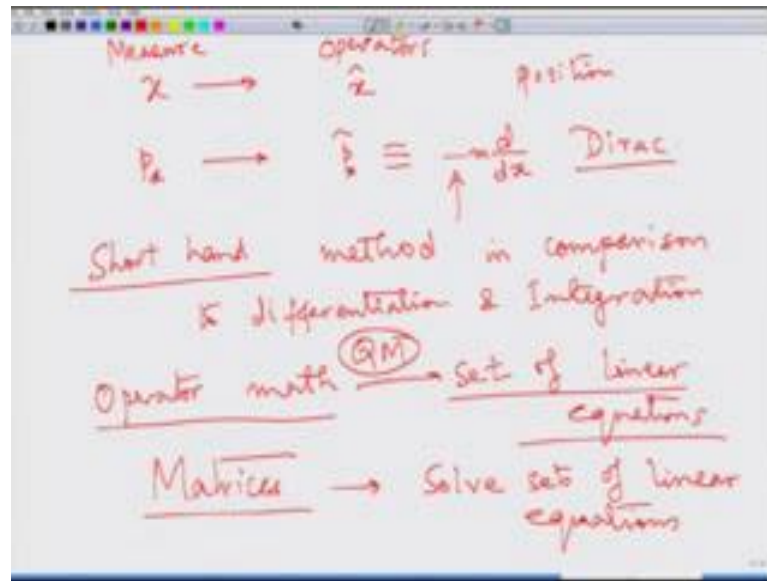
Student: (Refer Time: 31:49).

Simplify, we not doing anything. So, all I am saying is that at any point of time whenever it take a slice or a projection it is not in any of the n dimension its only in 1 dimension, which is my measure because lab frame ultimately is corresponding to only the 3D that is right here. So, we are always collapsing. So, the keyword here is collapse. So, this idea of collapse is the fine idea of the measure. So, measurement corresponds to collapse. So, you will be see hearing this term too many time in quantum computing and that is why our quantum information, that why it is important to know it right off at the very beginning, what is the principle of collapse? The collapse is nothing that you are just going to take this entire n dimensional object into observable region observable frame. So, we are just creating an observable frame.

So, our observable frame of reference is letting us collapse the system for measureable quantity, now in this regard we are also already introduced you to the idea of uncertainty were we have said that every measure has some level of or some bit of deviation from the mean value did you take the square of that, but you will find this that it is the actually difference of the square of the means with respect to the. So, basically it is a mean square deviation, because you are taking the average of the squares minus the mean square to get to the squared deviation value. So, based on that you can actually construct something has your uncertainty and the beauty of the quantum system is that there are measurements, which cannot be made more accurate than a certain quantity and that was given by heisen berg, which basically state that if you take complimentary measures say position and momentum along that same direction then you cannot have each of them being measured at with arbitrary position. There is a limit to the maximum value that you can do that it is often represented by  $h^2$  or  $h$  cross square, so this is uncertainty.

You can actually derive this, so, I leave this as an exercise how to derive this based on this simple derived, based on the simple definition. So, I leave this part as an exercise to show that this momentum and the thing can be done, because you have been exposed to the so,  $X$  is position which means that the operator.

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So, in order to derive that you need to go back to your term of operators, so the  $x$  which is position is an operator, which is  $x$  and in terms of operators we always put small  $\hbar$  (Refer Time: 35:43) on the top of it just for you. So, this is my measure and this is generated by my operator which is in this case this is position similarly, there is momentum  $p_x$ . Now this can be generated by an operator which can be simply written as  $\hat{p}_x$  this thing, but it has a meaning to it and we have to know how that, what does that correspond to right.

Now, you might remember it from your earlier studies this nothing, but  $d$  by  $d$   $x$   $m$   $d$  by  $d$   $x$  right, that how did you get it and why did you use the minus sign there is the little bit of a history to it. Right now if you use either plus or minus you will get the same answer for almost everything, but there is a reason why the sign minus was chosen by again these are all this operator math was given by Dirac this entire operator math for doing quantum mechanics was given was derived by Dirac. The reason of this entire math was required, because he is the one if you remember who introduced who was able to solve the entire go beyond the schrodinger equations to be able to show that spin quantum number can also appear as a suggestion rather than being (Refer Time: 37:37) as was done before him by Pauli and others.

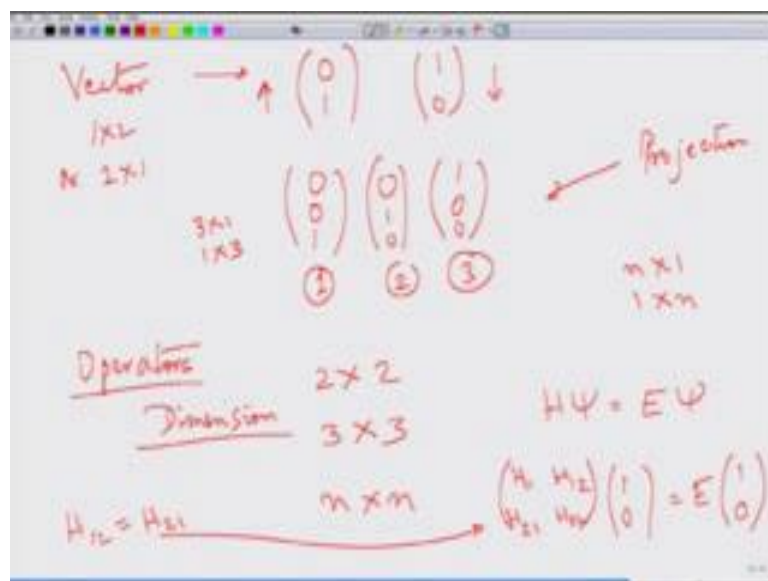
So, the exclusion principle and all of those principles are very nice, but mathematically how do you arrive at it was given by Dirac based on all these principles and here to use

the idea of an operator math to get this to work, principally this is a very short hand method. So, is this short hand method in comparison to differentiation let us say comparison to differentiation and integration, and this particular operator math makes everything into a linear algebra. So, this operator math also serves the purpose transform quantum mechanics into set of linear equations.

So, the differentiation equations or the equation, which look more complex are converted into a set of linear equations thanks to the operator math that is been introduced by this approach. So, for this particular purpose of quantum computing will definitely be using operator math, because there is a way we can go ahead and do this some of you might have been exposed this earlier operator math because the eigen value, eigen function equation that you have used before is nothing but an operator math kind of an equation. It is a short hand notation equation and is very simple because it actually takes this entire approach and solve the equation solve simultaneously.

Now, whenever you talk about set of simultaneously linear equation what is the next thing that you need matrices, whenever you need to solve sets of linear equations you need simultaneously linear equation you need the matrices, little bit linear equations first thing first how will you represent a vector as a matrices.

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So, for the simplest vector, which is only 2 levels, which represent only 2 states it can be a this is my 2 vectors, this represent vector going let say up down or vice versa it is up to you how you chose it now that is how it is.

So, vectors can be measurably represented by this if you have 3D vector then instead this it will become 0 0 1 1 0 0 right. So, similarly you can choose one the thing, which you can immediately see is that we are choosing only one. So, this is already proving that I am going to consider projections. So, this are my three different cases 1 1 2 and 3

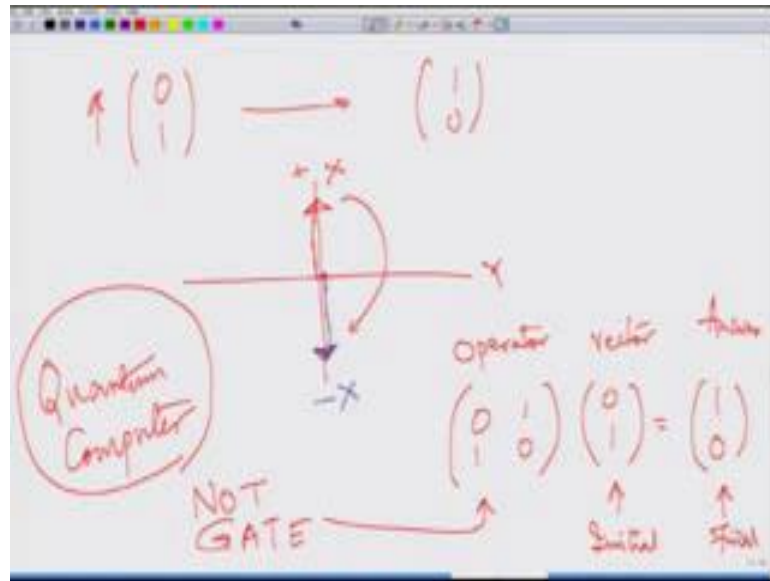
So, correspondingly whenever I had chosen the vectors my operators will have the same kind of matrices forms. So, whenever I deal with a vector which is only going to be 2 by 2 I will have corresponding operator which will be. So, this is a if I have a 1 by 2 vector or a 2 by 1 vector, then I need at 2 by 2 operator similarly, if I have a 3 by 1 or 1 by 3 vector then my operators are going to be 3 by 3 and so on and so forth. So, in principle you can have n by 1 or 1 by n vectors and correspondingly I can have n by n operator dimension. So, this is my dimension.

So, this is how you set it up. So, this kind of gives you the idea of where we are leading to the simplest one that you know is the schrodinger equation  $\hbar \psi = e \psi$  and if you are allowed to replace them by the way we have done it here for the simplest case will be having 2 by 2 matrices giving raise to say this and the corresponding matrices looking like this now generally, you know that this particular matrix is supposed to be a mission. So, what will happen is  $\hbar^2$  is going to be  $\hbar^2$ . So, that is the way the very first equation that you are a use to comes back to you has linear algebra and maths in terms of matrices and that how your computer get set up in one way or the other.

So, I am actually now taking you from your physic knowledge of quantum mechanics into a mathematical set, which you will give a computational way of looking at it. So, this is the first step trying to understand how we go about computing from a point which is pure physic on one hand and looks completely incompressible in many ways to a place, where you can relate it to the simplest possibility of classical computer.

Now, it easy to start with the two conditions 2 by 2 conditions, because there is directly corresponding to your bit parameters, because in computer also you are always going do bets and operations relating to bets. So, let us just look at couple of very simple examples.

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Let us, look at one simple case where we can connect computation to this kind of operations say you want to have the vector state of 0 1, which is a one direction go into the 1 0 state, which is going form. So, it is a 2 dimension case. So, this is my vector upwards. So, it can be X and Y I am going from plus X to minus X all right. So, this is my minus x. So, when I go from between this to two different cases what is it that is going to look like on my case.

So, what do I have to do, to get this happen? So, the idea is to find out a way how I can have 0 1 become 1 0, what will you do? What do you have to multiply this to give rise to this? So, this is my operator and this is my vector, which I am using and this is my resulting answer. So, this is my essentially this is my answer. So, whenever I finally, look at state of the vector I would be looking at this is my answer this is what my initial condition was. So, this is my initial, this is final, if I want to make this happen what is it that I have to do, what kind of operator do I need

Student: (Refer Time: 47:31).

(Refer Time: 47:32) is fine what are the elements, so, this particular operator that you will discover right now is something, which is a NOT Gate in terms of a computer right I just inverted. So, whatever was before has become the opposite right, so it is NOT gate. So, in order look at in this form all we have to do is to find out how an operator looks like for this. So, for those of you forgotten the rules of matrices multiplications is this



right this, plus this and the other way right. So, you should do that what is it that you will use to get this one.

Student: Second column is 1 0.

1 0.

Student: (Refer Time: 48:38).

With that work.

Student: (Refer Time: 48:48).

Would that what everything will work. So, this idea of been able to create results which are computationally useful is one of the first step in figuring out what is it that you would be requiring for a quantum computer.

So, I want it to just have you understand where we come from, when we are going to proceeding this direction there are lots of difficulty that we will find because, even for this simplest operations that you wanted to do. It is almost like a inverse operation right you have to actually look at what you trying to get from where you are and what do have to do in order to get there, this is what you have to keep on trying to get this, but nature does it in a much more simpler ways. So, we will casually do that in that easier manner and that is what we will try to do when we going to develop quantum computing ideas for doing this.

There are many hurdles and that is one of the reasons why we do not have one yet in reality seating everywhere, but we have been trying there are lot of attempt something which are going on. We are going to stop today here; we will pick it up from the next in this class.

Thank you.