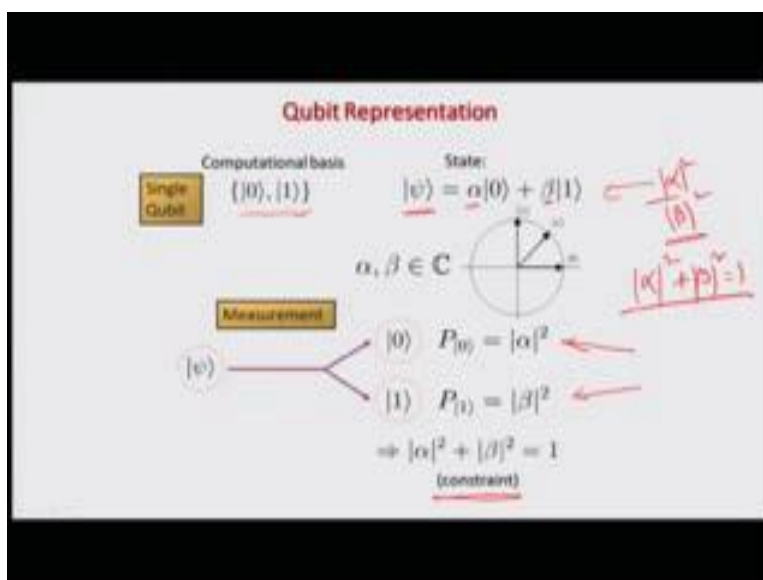


Implementation Aspects of Quantum Computing
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Lecture – 14
Concepts in NMR Quantum Computing

We have been discussing about NMR quantum computing, we have gone through the basics of how NMR operates? Is basic spectroscopic ideas? How it has become such a popular device of a spectrometer to start with?

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Now WE will be looking at it in terms of quantum computing, How the quantum or the qubit representation comes and we will discuss from there. So, the Qubit Representation for the NMR quantum computing, actually in general the first few may not be exactly for just NMR it can be for any case, is that a single qubit has the computational basis which is given as the 0 one kind of a representation and that takes on to the states.

So, the computational basis is based on the states 0 and 1. The wave function is represented as a combination of the basis sets 0 and 1. So, the alpha and beta represents the corresponding amounts. So alpha squared, beta squared (Refer Time: 01:30) are the

corresponding amounts of 0 and 1 state, that is their basis states which are there in the final state.

So in terms of how it is represented we have already discussed, this is how it looks like that it is a block sphere in which we have the state basis sets with certain proportional representation probabilities of alpha and beta square which are being used. So, at any point of time it will be alpha squared plus beta squared is equal to 1 that is the total amount of amount which is there. Which is what happens when you make a measurement it will give rise to either 0 or 1 with the probability which will be represented by their individual amounts; and So, that is always is the final constrain that exist when you are looking at the qubit representative. So, a single qubit will be represented by the individual basis sets, which will be constrained by these parameters. All possibilities exist however, whenever the measurements are made that as a probability of one versus the other, in the way that the constraint has been designed.

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Qubit Representation

2-qubit state: $|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$
 $\Rightarrow |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$

Basis states: $|00\rangle, |01\rangle, |10\rangle, |11\rangle \rightarrow |0\rangle, |1\rangle, |2\rangle, |3\rangle$

n-qubit quantum computer $\rightarrow 2^n$ states $|0\rangle, |1\rangle, \dots, |2^n - 1\rangle$

$|\psi\rangle = \sum_{i=0}^{2^n-1} c_i |i\rangle \quad \sum_{i=0}^{2^n-1} |c_i|^2 = 1$

Handwritten notes on the right:
 $|0\rangle \otimes |0\rangle = |00\rangle$
 $|0\rangle \otimes |1\rangle = |01\rangle$
 $|1\rangle \otimes |0\rangle = |10\rangle$
 $|1\rangle \otimes |1\rangle = |11\rangle$

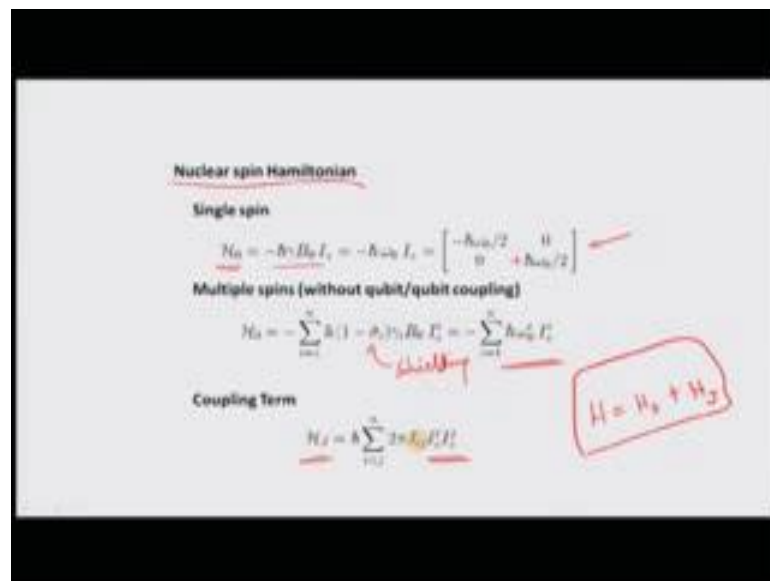
Now, for 2 qubit representation, we have similarly the (Refer Time: 03:12) a product of these individual states, which is represented by 0 0. If it is any one of the other then it is represented in this fashion. So, this is one kind, this is one it is of the other kind and depending on the fact that we can distinguish between 1 this with respect to this, will

have the different 4 different possibilities.

So, these are the 4 different possibilities and they have their own probabilities of their existence α^2 , β^2 , $\alpha\beta$, $\alpha\beta$, $\alpha\beta$, $\alpha\beta$, $\alpha\beta$, $\alpha\beta$ and some of them would always be equal to 1 because the total probability has to be 1. So, in general for n qubit quantum computer we have 2^n states, basis states and they can be represented therefore, by the wave function which would be having all possibilities of their independent basis sets with the α_i as their particular contribution. So, the probability of each of them being present is α_i^2 sum over all of them.

So, this is how the qubit representation goes, in case of the nuclear spin Hamiltonian which is what we will be using in case of NMR.

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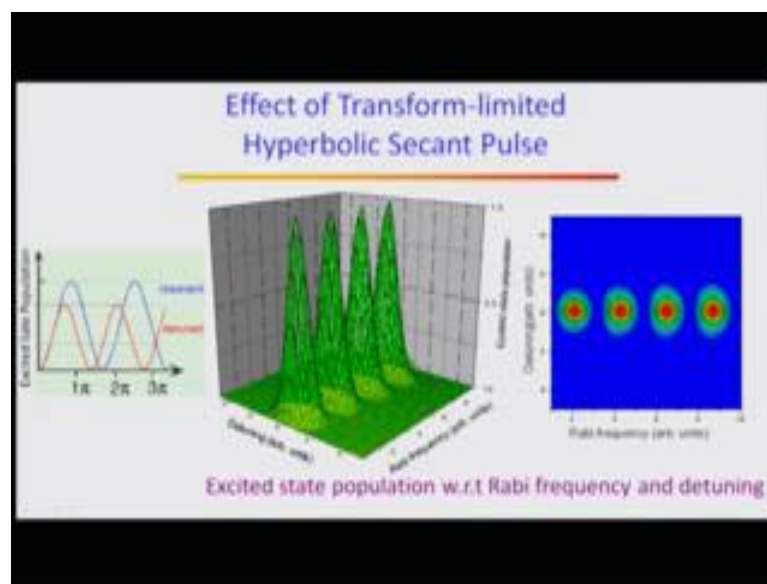


For a single spin the Hamiltonian is given by the interaction that we just talked about the energy gap $\hbar \omega$, $\hbar \omega$, $\hbar \omega$ of z which is equal to minus $\hbar \omega$ over 2, minus $\hbar \omega$ over 2 plus $\hbar \omega$ over 2, and this is the Hamiltonian that we work with. For multiple spins without coupling can be simply written as a continuous form of the same

way, where this is the δ_i is the interaction is the shielding due to each of them. So, this is the shielding as we had discussed due to the other electrons present and we can have the final Hamiltonian in the same format.

There are as we mentioned when the field intensities are higher, these coupling terms which are due to the spin spin of each of them which comes in separately, which is the h_j . So, in most cases the total Hamiltonian is (Refer Time: 06:26) of as the spin coupling term independent H_{naught} with, the coupling term spin spin coupling term which is H_j of j this is how the total Hamiltonian is looked at when you are looking at the nucleus spin Hamiltonian.

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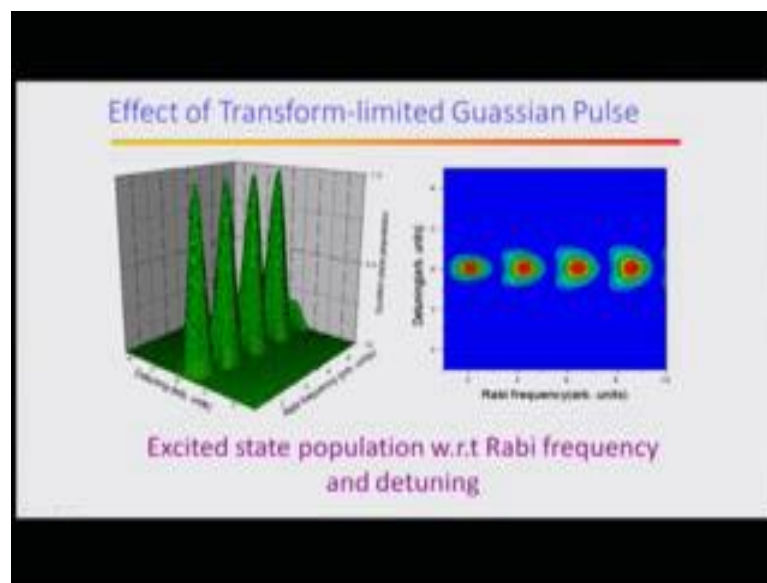


If you go ahead and do calculations with this and look at the (Refer Time: 06:50) and conditions and solve how the populations change for each of these states the excited state which is (Refer Time: 06:58) state, in find that they basically oscillate between the ground and excited states and they go through these Rabi oscillations, where the area under the applied field is the one which determines how it is going to go into the excited state or not and it is going to go back and forth between the ground and excited state, that is because they are the 2 states are coupled, such that going into one case with the right amount of energy would also have mean that one at the energy exist for a long enough

time, it will also be able to bring it down and so on and so forth.

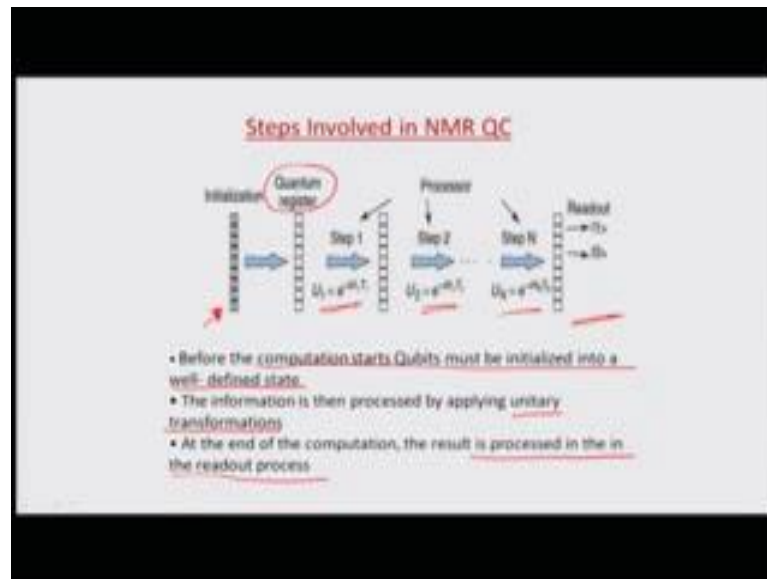
So, it can flop and that see Rabi flopping principle excited state energy and depending on how it is applied all these kinds of parameters can be looked at, this is a particular case where the shape of the field is hyperbolic secant this is supposed to be one of the exact solutions.

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The Gaussian is another way of looking at the field, where a rectangular applied field which is also done mostly the assumptions are rectangular because you turn on and turn off nothing but can be perfectly rectangular.

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So some of these other cases also been looked at, in terms of how this works the steps involved in the NMR quantum computing, we have an initialization step as because the before the computational starts the qubits must be initialize to well defined state. So, that is our initialization step.

The information is then processed by applying unitary transformations. So once the initialization is properly done we are having our quantum register and once we have our quantum register which has the information in that set that we want to start our computing n we apply the unitary transformations one after the other.

So the first step would take it to the application of one unitary transform into the other and so on and so forth and the end of the computation the result is processed and in the read out process, processed in the read out process. So, this is our final read out process which is been looked at as the final output.

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Initialization:

Quantum algorithms generally assume or demand that qubits can be prepared in a pure state, usually the ground state.

Nuclear spin are in thermal equilibrium at room temperature, and subject to a reasonable static magnetic field is in a highly mixed state and is given by the density matrix

$$(1+x)/2 |0\rangle\langle 0| + (1-x)/2 |1\rangle\langle 1|$$

where the polarization $x = \omega\hbar/2k_bT$

Requires creation of effective pure states, with a density matrix of the form

$$\rho = \frac{1-a}{2^N} I + a|\psi\rangle\langle\psi|$$

The initialization process for quantum algorithms, generally assume or demand that the qubits can be prepared in a pure state usually in the ground state. Nuclear spins are in thermal equilibrium at room temperature and are subject to a reasonable static magnetic field in a highly mix state and is given the density matrix and so this is a situation where generating a perfect pure state which is basically the perfect ground state is a very hard job and so, it requires creation of effective pure states with a density matrix of the form of something like that where it is not exactly all of them are in the ground state, but there are but it is done in such a ways. So, that they effectively are able to generate the same kind of result.

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Pure State
All the spins in same direction
All energy levels except one have zero populations
Such a state is difficult to create in room temperature.

Pseudo-Pure State
We create a state in which all levels except one have Equal populations. Such a state mimics a pure state.

So, in reality all the spins are in the same direction is what a pure state is suppose to be, essentially you want everything to be alpha. But that is sort of like what you would be wanting. So, if you are talking about 2 spin case, you would like all your 4 states to be at the 0 0 conditions. The pseudo pure state is the one we create a state will which all levels except one have equal population.

So, basically this is the condition where we can actually have a situation where everything if they can be balanced out, then all the levels except the one have equal populations then it mimics a pure state because that is the state which essentially has the property which is not going to be the same as the others and therefore, that pseudo pure state was pretty much the same way as a pure state would have occurred because the other populations are balanced out in terms of having equal populations because all energy levels except one have 0 population such a state is very difficult to produce in case of room temperatures for NMR condition.

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Pure States:

$$\text{Tr}(\rho) = \text{Tr}(\rho^2) = 1$$

For a diagonal density matrix, this condition requires that all energy levels except one have zero populations.

Such a state is difficult to create in NMR.

Pseudo-Pure States

Under High Temperature Approximation

$$\rho = 1/N (\alpha I + \Delta\rho) \quad \text{Here } \alpha = 10^8 \text{ and } U \ll U^* + 1$$

We create a state in which all levels except one have $1/N$ populations. Such a state mimics a pure state.

So, in the pure state technically demands that $\text{Tr}(\rho) = \text{Tr}(\rho^2) = 1$, for a diagonal density matrix this condition requires that all energy levels except one have 0 population such a state too is difficult to create in NMR. So, what is done is that under high temperature approximation pseudo pure states are taken, where we create a state in which all levels except one have equal population such a state mimics a pure state.

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Pseudo-Pure State

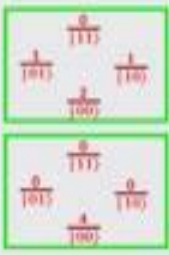
In a two-qubit system:

(i) Equilibrium:
 $\rho = 10^6 + \Delta\rho = (2, 1, 1, 0)$

(ii) Pseudo-Pure
 $\Delta\rho = (4, 0, 0, 0)$

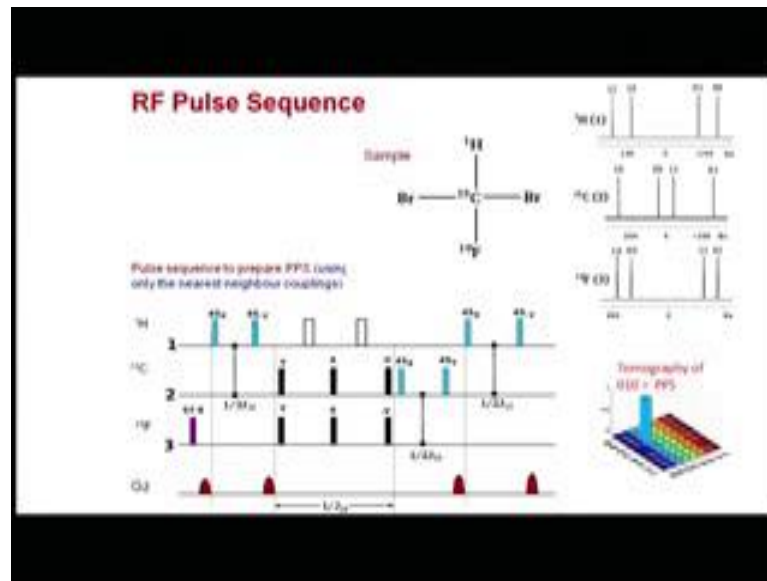
How to Create ?

- (i) Spatial averaging ✓
- (ii) Temporal averaging ✓
- (iii) Logical labeling ✓
- (iv) Spatially averaged - Logical labeling ✓



So for example, alpha can be a very high number in this case for instance, but as long as it is not going to create an issue it is going to work out. So for a 2 qubit system in equilibrium, we can have this situation where that pseudo pure state would therefore, the equilibrium condition is like this where every possible case is existing by the, pseudo pure state is the one which will work for us where its 4 0 0 0 it is going to work out for us how to create; this is can be done by spatial averaging, temporal averaging, logical labeling or spatially average logical leveling principle.

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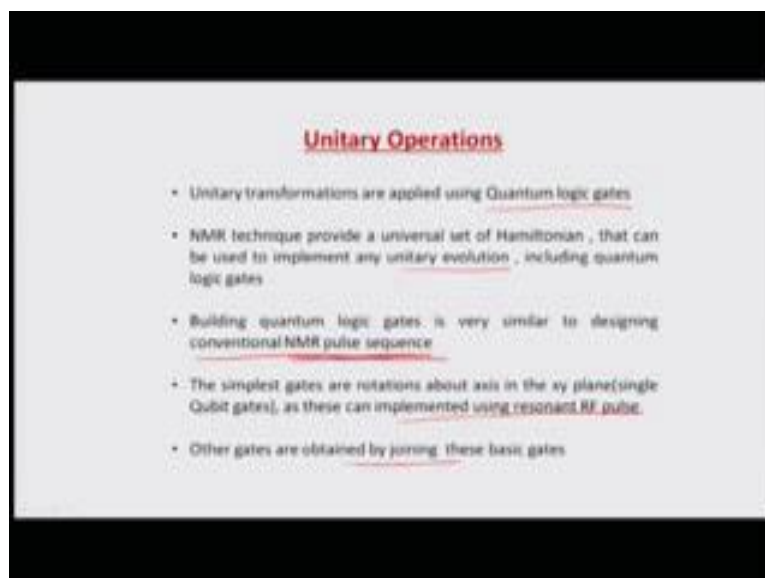
So, method for preparing effective pure states therefore, can be done by logical labeling which consist of applying a pulse sequence that rearranges the thermo populations such that, a subset of the spins is in an effective pure state. Something like this for instance, there is one some molecule penta, fludo, butadienyl, cyclopentadienyl, dicarbonyl complex in thermal equilibrium, the same spectrum after preparing in effective pure state is looks like this; this is courtesy of some of the work which been carried out in IIC Bangalore Professor Anil Kumar's group.

So, again has another way which is temporal averaging consists of adding up spectra multiple experiments, each experiments starts with a different state preparation pulse sequence consist of c naught hence, not operations and then these spatial averaging case which uses a pulse sequence containing magnetic field gradients to equalize all populations.

Now these are all practical principles for us, when we want to learn how to do this in terms of real applications or just for the case of understanding how NMR quantum computing does. It is just to understand that it is not a case which is very simple, but it turns out that there are ways of making sure that you can get to a result, which would be sort of like what you would be expecting or where you would be starting off as a simple

case.

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Now, Unitary transformations are the ones which are applied using quantum logic gates, NMR technique provides a universal set of Hamiltonian that can be used to implement any unitary evolution including quantum logic gates. So the building of quantum logic gates is very similar to designing, conventional NMR pulse sequence and therefore, it is as something which has been possible to be done. As I mention before in the principle of the NMR was that, you would be essentially applying RF pulses to do the operations where you do spectroscopy with it.

In this particular case instead of doing that as a spectroscopic tool, you would be essentially designing logic gates which are the NMR which are in tune with designing the NMR pulse sequences that is used for spectroscopy in the conventional NMR case. The simplest gates are rotations about the axis and x y plane single qubit gates and these can be implemented resonant RF pulses, other gates are obtained by jointly using these basic gates.

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Unitary Operations

Single Qubit Gates

X-gate: $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ Y-gate: $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Z-gate: $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ S-gate: $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$

Two Qubit Gates

CNOT: $CNOT = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$

90, 180, ωt , ω , t , ωt . Lo Area dimensionless

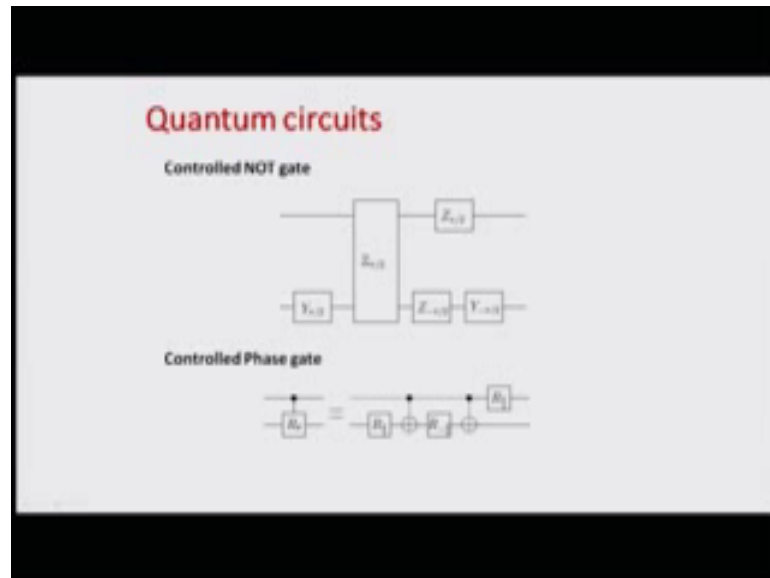
Now so for example, the unitary operations for single qubit gates, can be as simple as the x gate, the y gate, z gate or the s gate all of which are the simple single qubit gates that we have already known the 2 qubit gates are of the ones which have the Hadamard, which had a result of 90 degree pulse in the y dimension, and a 180 degree pulse in the x dimension.

Now, just for clarity let me actually tell you that these pulses, these 90 and these are essentially measured with respect to the area under this and this is these are on for a certain time on off and this is the omega which is being applied. So, omega t the area under this pulse, omega t the area is a dimensionless number and this dimensionless quantity is being represented by 90. So, basically it is pi by 2, pi or some of this depending on the product of these 2 numbers.

So, that is how the Hadamard gate turns out to be a sequence of 90 degree along the y axis, and 180 degree along the x axis. So there are 2 axis that can be utilized. So, the field is propagating along the z dimension as we have discussed this is the z dimension applied field, b or h whichever way you look at it and the x and y are the ones along which the RF is being applied. So, the coils could be used along these dimensions and that is how these coils are been applied for the RF pulses of 90 pi, 180 pi and so on so

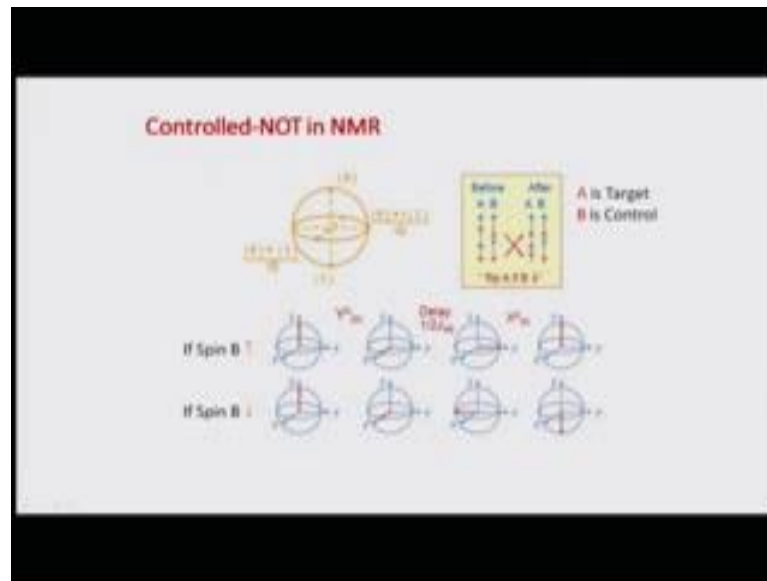
forth.

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Controlled NOT is of a different kind of gate which is being discussed here. So the quantum circuits can have controlled NOT, which can go along and provide all the different directions of applying the fields, there can be controlled phase gates which are just rotation gates and depending on how these pulse sequences are been used, it can generate these kinds of gates. So in controlled NOT in NMR essentially works in the principle that, you are applying these fields applying these so that they can undergo the spin flips and if they are going spin flips then you see the z pulses something like that.

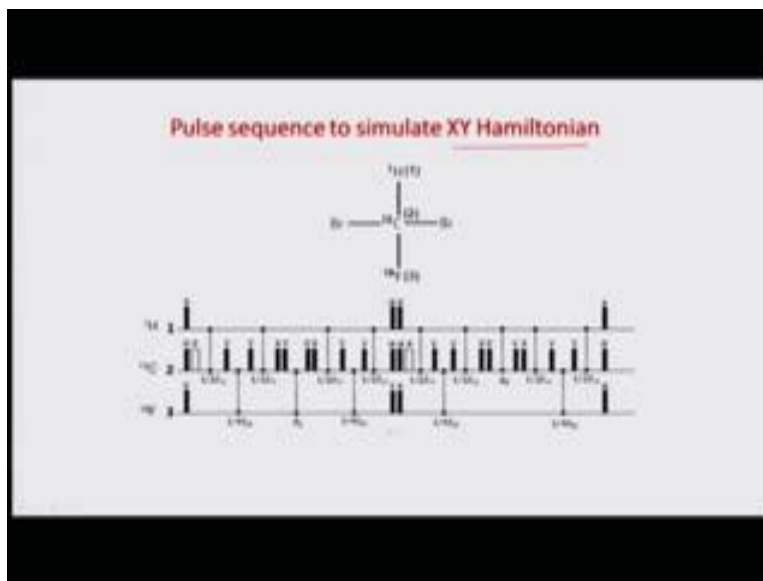
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So here for instance, if the spin B is up, then it under goes this possibility of putting one through the other and then there is delay which is very important because this delay essentially allows the system to relax. If you are in the z dimension, if you are put it back in the x dimension, it can fan out and relax and that delay is the one which takes care of the fact that it will be actually utilizing that as a part of its pulse cycling. So, here it is a y 90 degree pulse followed by a delay to give the half coupling j a b coupling, and then it is again an x a 90 degree pulse.

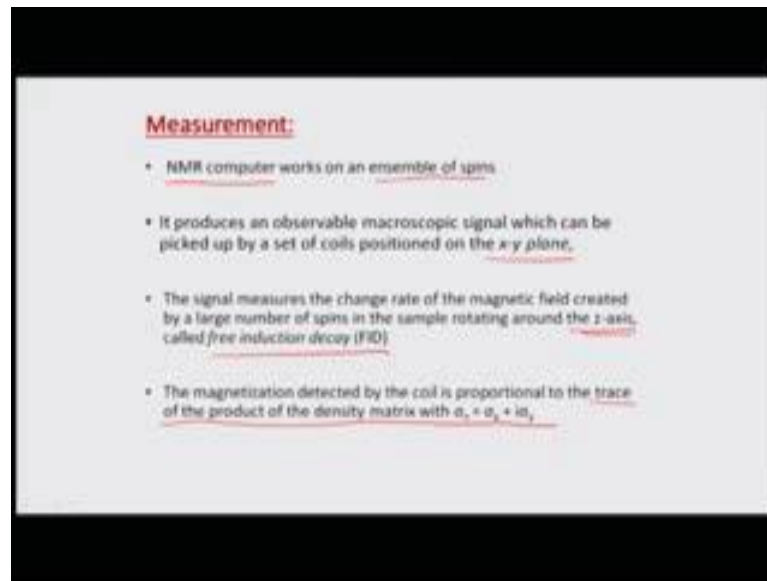
If the spin B is down, then you provide a different way of doing this possibility. So, this is sort of like if you have this 2 spin system then you have a flip a if b is down and vice verse. So, this is how generally RF pulse sequence would look like for instance when a real situation, for a carbon 13. So, if you notice the carbon 13 is one which has the spin, proton as the spins and flurine 19 has the spin. All these 3 are spin which are going to interact in terms of this spin cases, we have 3 different cases and based on these 3 it is being used to the RF pulse sequences to do this kind of (Refer Time: 20:14).

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So, these are basically certain examples coming from research which we are not going to discuss in detail, we are just showing it to you so that you understand that it is possible. We will perhaps not be able to get into the we get will not be able to get time to get into the details of, these are just to show that these things in reality workout and this is how they kind of look like where you are providing the pulses and how they are coming in different windows and timescales and how they interact and how you get these things to get to the simulation of what you are looking for. So, this is the case to show you can generate x y Hamiltonian and so on and so forth for a molecule of this kind.

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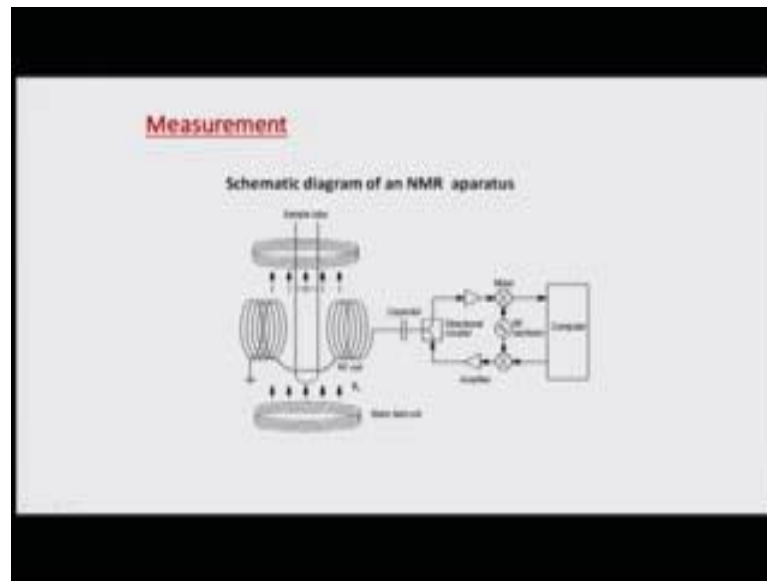


Measurement:

- NMR computer works on an ensemble of spins.
- It produces an observable macroscopic signal which can be picked up by a set of coils positioned on the $x-y$ plane.
- The signal measures the change rate of the magnetic field created by a large number of spins in the sample rotating around the z -axis, called free induction decay (FID).
- The magnetization detected by the coil is proportional to the trace of the product of the density matrix with $\sigma_x + i\sigma_y$.

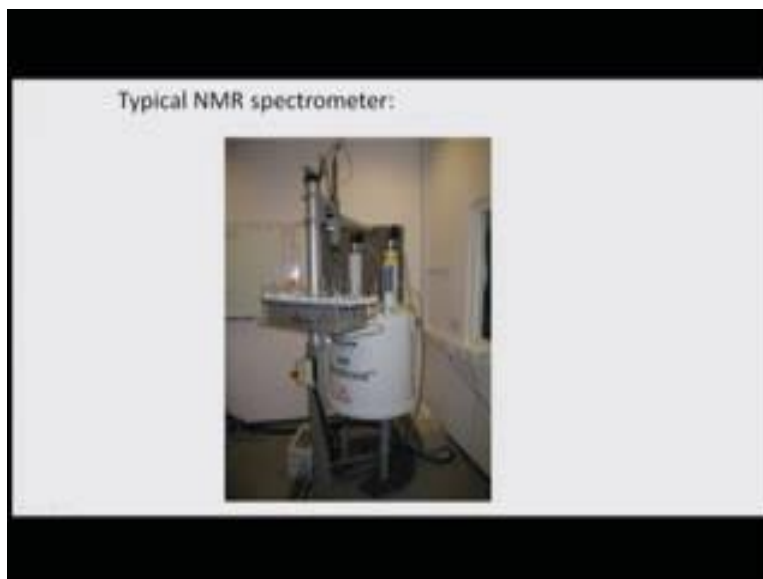
So the finally, NMR computer also works with the idea that you are working (Refer Time: 21:00) ensemble of spin, which is why the measurement principle is very very important. It produces an observable macroscopic signal which can be picked up by a set of coils positioned in the $x-y$ plane. The signal measures, the change in the rate of the magnetic field created by a large number of spins in the sample rotating around the z axis called the Free induction decay as we had mentioned earlier and this free induction decay is then Fourier transform to get to the result. The magnetization detected by the coil is proportional to the trace of the product of the density matrix with the sigma plus, which is basically $\sigma_x + i\sigma_y$. So, this enables the in detection of the magnetization which is being read by the coil as it is a proportional to the trace.

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In terms of measurement the schematic of the diagram looks like this, you have the sample tube which has the liquid sample in it, which is being subjected to the static magnetic field. So B_0 has been showed here and these are the RF coils which are along their dimension which gives raise to the x y plane and the capacitor filters the signal out there is a directional coupler and with which we can actually have the signal being controlled and provided through the RF oscillator by the help of a computer.

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So, this is how a typical NMR spectrometer this is 300 mega hertz, (Refer Time: 22:33) spectrometer looks like there are many different versions of it now a days there are 800 mega hertz NMR spectrometers which are very powerful compared to these, and it can be a lot more interesting work with it.

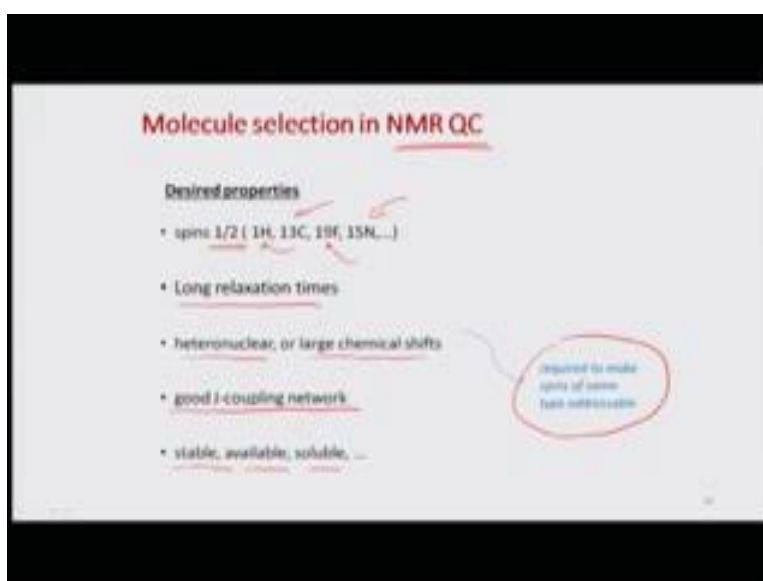
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Molecule selection in NMR QC

Desired properties

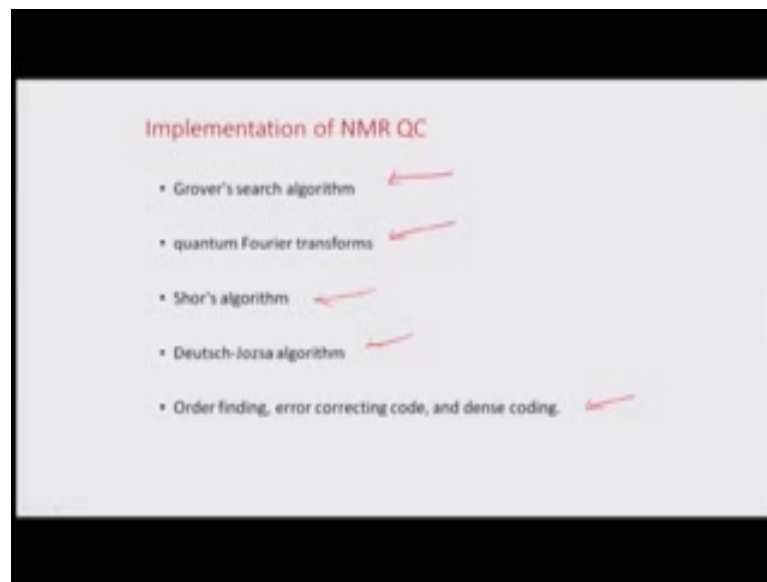
- spins 1/2 (^1H , ^{13}C , ^{19}F , ^{15}N ...)
- Long relaxation times
- heteronuclear, or large chemical shifts
- good J-coupling network
- stable, available, soluble, ...

required to make spins of same both interactions



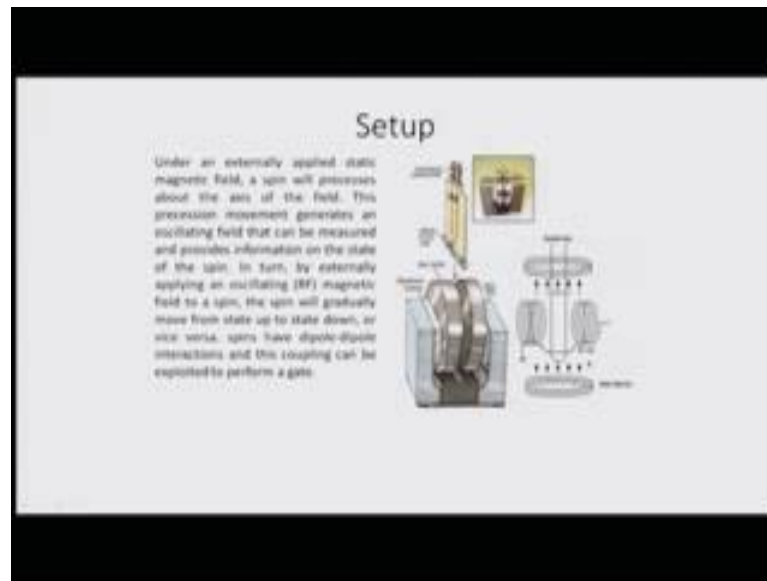
Molecule selection for NMR quantum computing have to be also done very carefully, desired properties are for the case of spin half systems which are say for example, proton carbon 13, fluorine 19, nitrogen 15, they need to have long relaxation times it could be useful to get hetero nuclear or large chemical shifts systems. So, that you can also use require to make spins of the same type addressable, you need to have good j coupling networks. So, that you can actually work with them and make them happen as and you want them to be stable available and soluble in the system that we are looking at.

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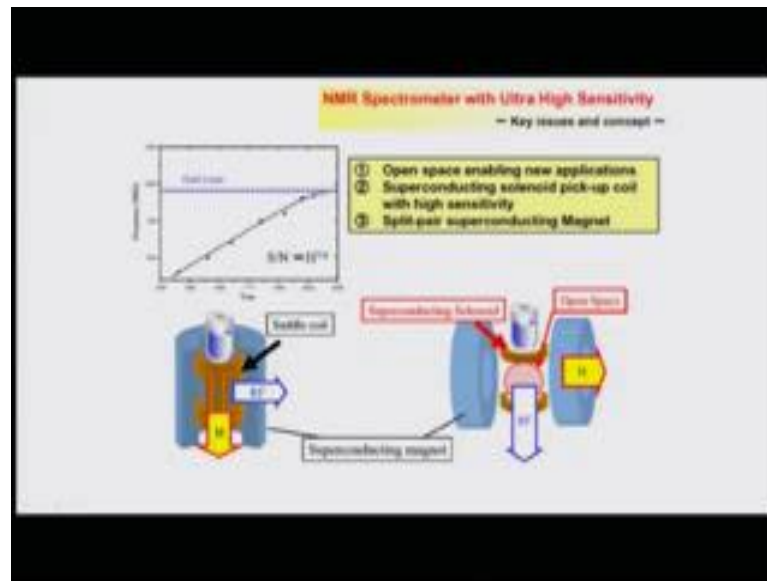
It has being shown with the NMR quantum computing, Grover search algorithm has been shown quantum Fourier transform has been shown, Shor's algorithm has been shown, Deutsch Jozsa algorithm was also been shown order finding error correction codes and dense coding has been shown.

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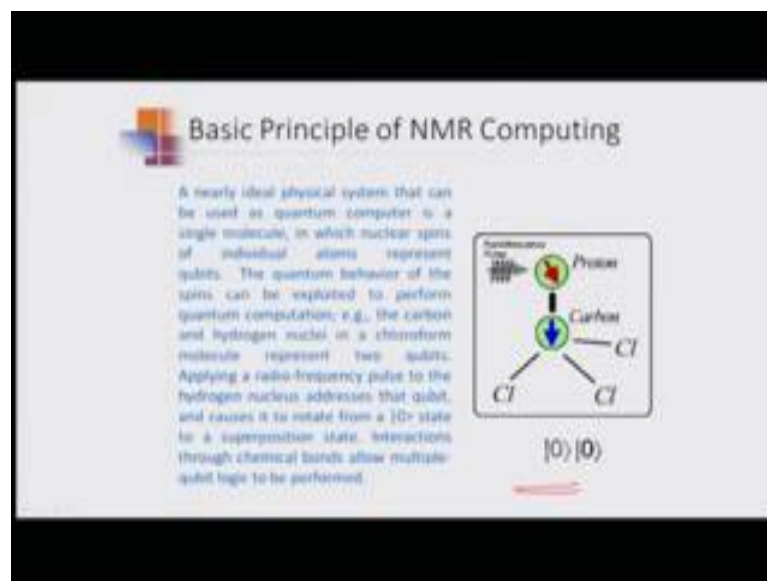
The typical setup essentially if you look at it a little bit more close has this kind of setup, which has this electric field as I just showed here. So, this is the magnetic pole pieces in which the this a permanent magnet and then there is this super conducting magnet which is also used along with, this to make sure that this one works properly. This is internal externally applying an oscillating magnetic field to the spin this spin will gradually move to the state from down or up and vice verse and this is how these gates have been done.

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So, ultra high sensitivity of NMRs have also been developed and people have working on this area also to try to see this can make things work better for NMR. The RF and the magnetic field availability is the most important thing in this cases, the signal to noise ratio is dependent on the amount of magnetic field that can be applied also. So, they have the magnetic field the better and so that is one of the sick ideas here.

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So, here is a simple cartoon of how things work. So in this particular case for instance the carbon and the proton in the chloroform as I had discussed earlier, have one of the proper molecules where used for 2 qubit system. One of the first molecules which is use for quantum computing to show Hadamard transform happen for by using this chloroform molecule, where the carbon and the proton was used and the radio frequency pulse was used to address the hydrogen nuclei and causes it to rotate to form a 0 state to a so position state, interactions through the chemical bond would allow multiple qubit logic to be performed. So, this was one of the first cases which we have shown.

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Implementation using Chloroform

CNOT- two-spin(qubit) experiments

- The nucleus of carbon 12 has no spin, chloroform used containing carbon-13.
- Carbon is arranged so that it definitely points up, parallel to the fixed magnetic field.
- The spin of the hydrogen can be parallel or anti-parallel to a vertically applied magnetic field
- A properly designed radio-frequency pulse can rotate the carbon's spin downward into the horizontal plane.

ClC(Cl)Cl

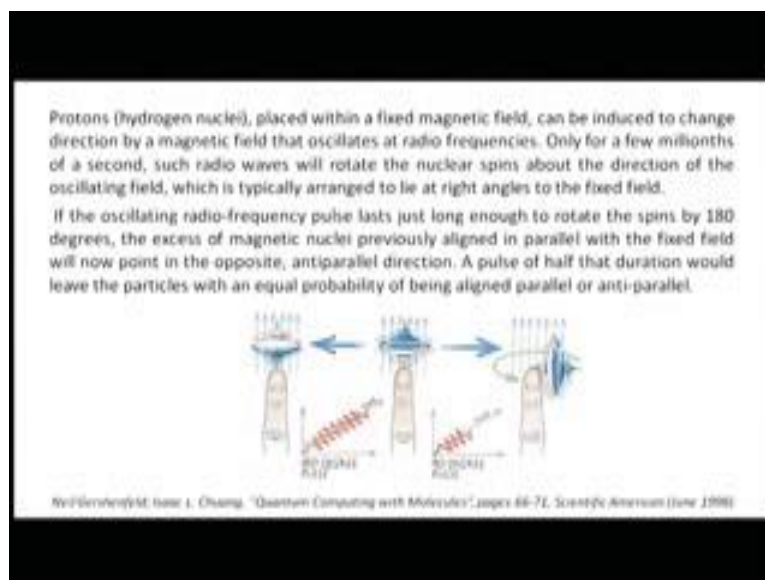
H ← Spin 1/2
C ← Spin 0
Cl ← Spin 0

I have already mentioned that carbon 12 has no spin; carbon 13 is the one which we would like. So in the case of for example in the chloroform that I just showed the carbon 13 and the proton shows this spin half case and these chlorines do not have anything, it is properly designed radio frequency pulse can rotate the carbon spin downwards to the horizontal plane and so on and so forth.

The geometry of the molecule is constrained because of the way the structure of the molecule is. The protons placed within the fixed magnetic field can induce the change of direction by magnetic field oscillates at radio frequencies as we have been saying only a few millionth of a second, such radio frequencies which rotate the nuclear spin about the

direction of the oscillating field, which is typically to try at right angle so the fix field.

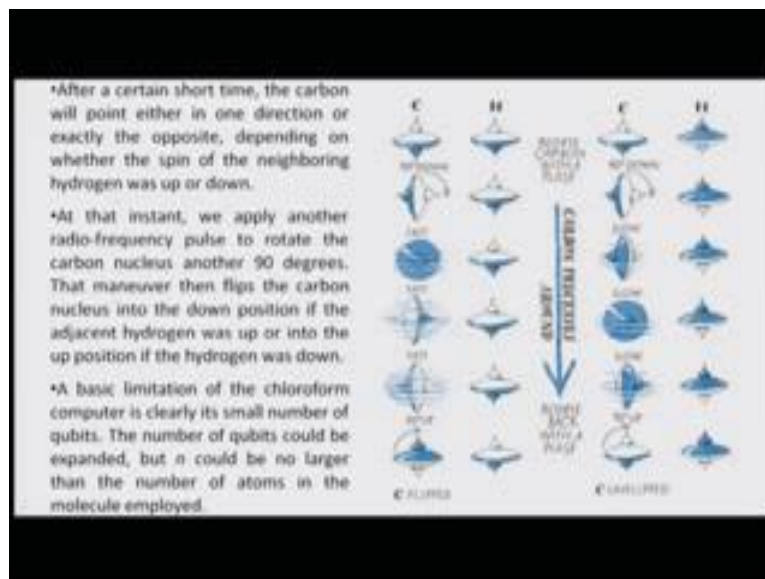
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So, that is how we had shown along the right angles hundred and 80 pulse, 90 degree pulse, it depends on how you are providing them at each point and they flip or they remain in the same place. If they flip then they actually precess wherever they are they will precess and that is what happens when you if the maximum precision is at 90 degrees place, if the oscillating radio frequencies (Refer Time: 27:07) just long enough to rotate spin per 180 the excess magnetic field previously aligned, in parallel with the fixed field will now point in the opposite anti parallel direction.

A pulse of half that duration will leave the particles in an equal probability of being align, parallel or anti parallel and that is the idea behind 180 pulse verses 90 degree pulse and that was the area under the pulse principle that I have been showing before.

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So, I mean in generally whatever I have shown until now is sort of shown here pictorially, which says that after certain short times is this is trying to explain whatever I said in pictorial form, the carbon will point either in one direction or exactly the opposite depending on whether the spin of the neighboring hydrogen was up or down, at that instant we apply another radio frequency pulse to rotate the carbon nuclei another 90 degrees that many over than flips the carbon nuclei into the down position, if the adjacent hydrogen was up or into the up position if the hydrogen was down.

A basic limitation of the chloroform computer, this is what we have been discussing lately is clearly in it is small number of qubits that is what happens in most of the NMR principles, unfortunately the number qubits could be expanded, but n could not be larger than the number of atoms in the molecule employed because this is a molecule only computer that is the point of how it works.

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7- Qubit Q-Computer by IBM

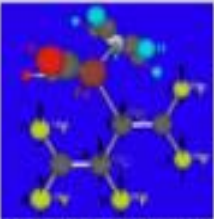


Diagram of the 7-qubit molecule
Alanine, an amino acid

- Most advanced model of QC
- Finding the factors of the number 15 with Shor's algorithm
- Nuclei of five fluorine and two carbon atoms interacting with each other
- Programmed by RF pulses
- Detected by NMR technique

So, this is how these sequences they have been showing in different ways, either by showing through animation or by showing the different stages this is how it goes and the celebration of quantum computing by NMR, one of the largest one has been the 7 qubit computer in IBM, where they use the 7 qubit molecule alanine an aluminum acid to factorize the number 15 which Shor's algorithm and this was done by Chwang while he was still in IBM and this he was able to show this with the help of nuclear of 5 fluorine and 2 carbon atoms interacting with each other, to provide this process of the Shor's algorithm where he was able to factorize the number 15. We have done the factorization of number 15 separately in this course to show the steps and so it will become clear that how he applied this with respect to NMR quantum computing by using this molecule typical.

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Difficulties in NMR QC

- Standard QC is based on pure states
 - In NMR single spins are too weak to measure
 - Must consider ensembles
- QC measurements are usually projective
 - In NMR get the average over all molecules
- Tendency for spins to align with field is weak
 - Even at equilibrium, most spins are random
 - Overcome by method of effective pure states

Difficulties in NMR quantum computing lies in the fact that the number of qubits difficult in scaling standard Q c is based on pure states in NMR single spins are too weak to measure. So, we must consider ensembles that is one of the biggest thing here which is different from the regular standard quantum computing principles, in a Qc measurements are usually projective in NMR we get the average over all molecular values, tendency for spins to align with field is weak even at equilibrium most spins are at random, that is one of the difficulties here.

However this is overcome by the method of effective pure states and that is the reason why I mentioned little bit one the effective pure state pseudo pure states which have been done. Some of these sections will again be dealt with a little bit when we do more on the theory side of these principles where we do, density matrices pure state pseudo pure states, how they interact how they operate and those kinds of things this was more to do with implementation aspects and with that I would like to thank you for today's class we will take on further aspects of quantum computing in the next session.

Thank you.