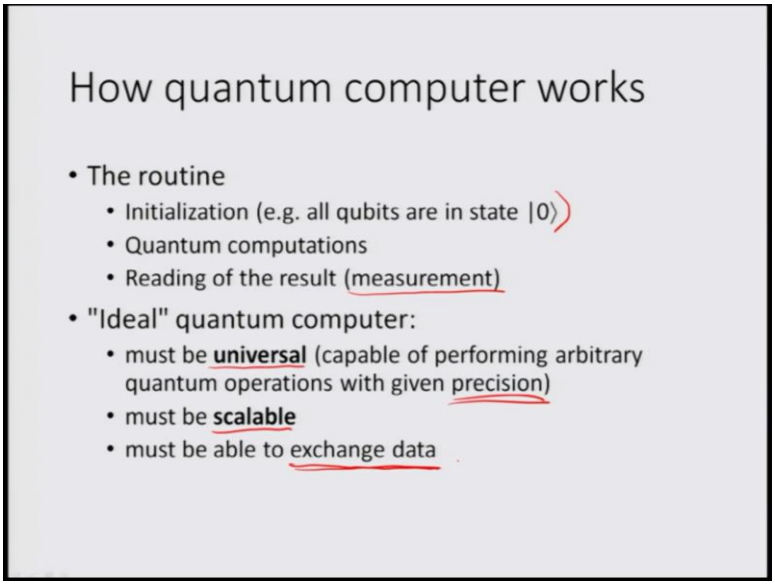
Implementation Aspects of Quantum Computing
Prof. Debabrata Goswami
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 39
Working of Quantum Computers: NMR QC

Welcome back. This being the final week we are looking at all the aspects of the course that we have covered in this particular area of quantum computing and quantum information. In the last couple of lectures this week we have covered the basics, now let us look at how we have gone ahead to look at the implementation aspects of quantum computing.

Some part of quantum information transfer which is also critical in terms of quantum information transfer and secured communication was discussed in the last lecture, in this lecture we will be looking at the computing part.

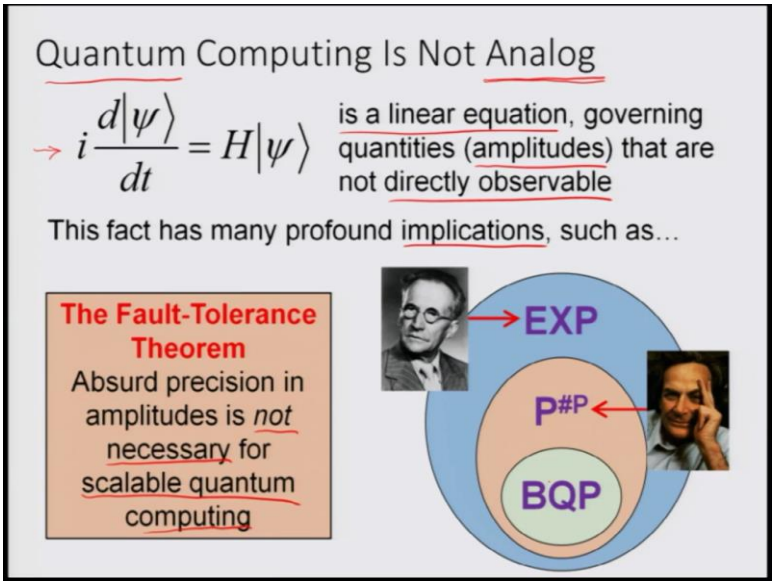
(Refer Slide Time: 00:58)



So, the basic point is how the quantum computer works that is the main part where we start from. The routine essentially involves initialization for example all the qubits are in say state 0, quantum computations which involve the gates and the different algorithms which are applied. And then finally, reading the result which is our main important part which brings it back to the classical world which is measurement.

An ideal quantum computer therefore, must be universal, which can be capable of performing arbitrary quantum operations with given precision. It must be scalable, this is one of the biggest difficulty in terms of quantum computing as of today as we have discussed several times in this course and it must be able to exchange data. And that is another part where it becomes critical that we are able to understand how quantum data can be connected or communicated, and in that regard quantum teleportation or associated methods are extremely important.

(Refer Slide Time: 02:20)



It is important to understand at quantum computing is not analog. Quantum word essentially implies that we are looking at discreet aspects and when we are evolving the state or the property, we are essentially using he quantum nature of the system which means that we are utilizing Schrodinger equation or associated similar equations in the statistical concept which is a (Refer Time: 02:49) equation, where we have instead of the wave functions we have the density matrix.

All of which in terms of evolution essentially involve a linear equation, governing the quantities which in these cases essentially the amplitudes that are not directly observable, and therefore it is far from being analog. That is one of the most important point which often comes out as a misconception should be cleared. And the power of the computing therefore is not to be misjudged with the fact that the principle of analog computation and its power can be related to how a quantum computer works.

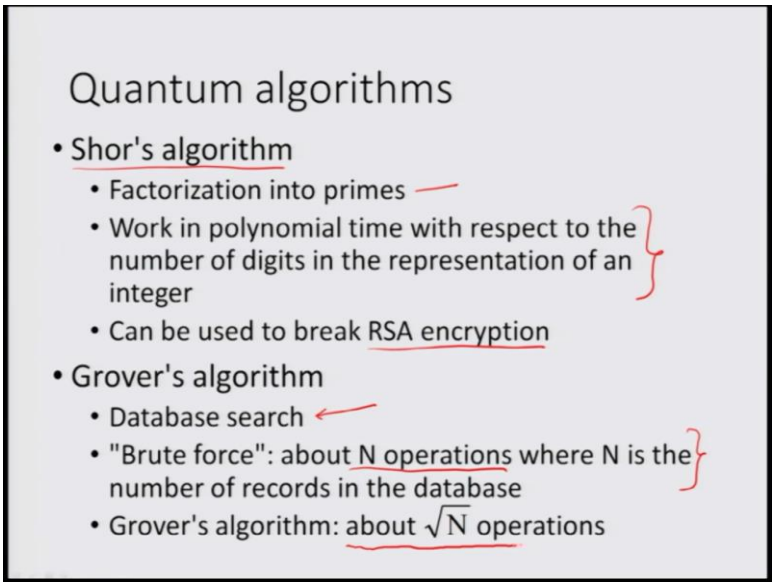
So, we should be clear on this point all the time. However, we should in fact that is one of the very important aspects, which means that this fact has many profound implications, Such as, the fault tolerance theorem, which means that absurd precision in amplitude is not necessary for scalable quantum computing. So this is actually one of the aspects which ensure the advantage of quantum computing and definitely makes it benefit over hat fact that it is not analog.

So, in terms of the complexity that we had originally mentioned, what we are looking at is we essentially have the capability of the exponential space or exponential way of looking at the problem in terms of how the Schrodinger equation looks like and that is the parallel nature of the problem, and that is one of the reasons why some of the problems which are otherwise difficult to look at can be thought of in the exponential domain.

In practicality, however as Feynman pointed out most of the problems that we will be dealing with are going to be super polynomials; in the sense that we can paralyze the system in such a way that we get the advantage of working in a domain where the quantum system itself evolves because we are using a quantum processor and so the laws of physics. And that was the basic vision of Feynman would be better described and processed by using the quantum computations. BQP by the way is bounded quantum problems or bounded quantum polynomial.

So, these are basic principles I just wanted to mention once more before we go ahead with the implementation concepts because we have to be clear n how we are going to go ahead with this implementation part, where we are going to go and apply quantum computation and quantum principles.

(Refer Slide Time: 06:20)



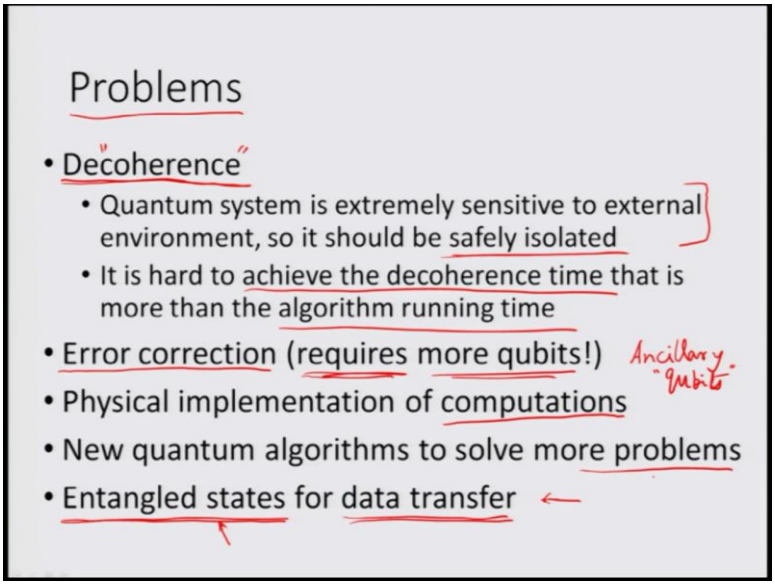
The quantum algorithms which have been the most celebrated once as we know are the Shor's algorithm, which enables factorization into prime and this can work in polynomial time with respect to the number of digits in the representation of an integer. So, this is basically the principle of the factorization that is achievable through Shor's algorithm. Given this advantage can actually be able to break the RSA encryption. Because the RSA encryption is based on the principle of factorization of a very large number which is typically takes a very large time and so prime factorization principle application into encryption; essentially means that we chose a large enough number whose factorization would be extremely difficult in proper classical computers and therefore it becomes encrypted.

In quantum sense however, this could break the RSA encryption because of the advantage of factorizing using the quantum algorithm. The other very important algorithm which is useful for quantum computation is the Grover's algorithm, which is the best application in terms of database search and since most of the problems that we deal with essentially involves finding the solution from the set, which has the solution already present it amounts to essential database searching.

The brute force technique for doing a database search requires about N operations, where N is the number of records in the database and as which means that as the problem size becomes larger it becomes increasingly difficult to do or to address a problem. Grover's

algorithm on the other hand which utilizes quantum super position principle, can be done can be achieved in about root N operations.

(Refer Slide Time: 08:47)



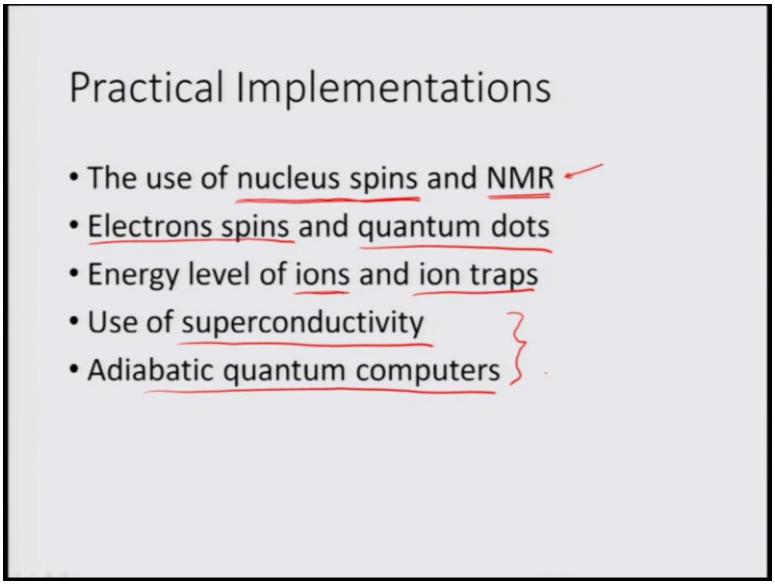
Some of the major problems that we have quoted over and over again in terms of quantum computing, quantum bill formation, quantum teleportation and associated properties of using quantum concepts is one of the major aspect being Decoherence. Quantum system advantage or the parallelism often is attributed to the fact that the system behaves coherently and does the work in a way so that it can all be processed together. Wherever the coherence part of the problem gets into compromise because of various difficulties, we have difficulty of losing the quantumness of the system.

Quantum systems are extremely sensitive to external environment, so it should be safely isolated. So, one of the biggest issue about quantum computing implementation is the concept of safe isolation. It is hard to achieve decoherence time that is more than the algorithm running time; this is another big problem of these entire field which is that it is hard to achieve decoherence time that is more than the algorithm running time. The other important aspects which are related could be attributed to also decoherence part is the fact that it requires corrections and the corrections could be due to loss of coherence, due to many other errors and so it requires the principle of error correction, which means that it would essentially require more qubits then it is required to just simply look at the problem from first principles.

And that is the reason in most of the implementation aspects we have been encountering ancillary qubits. Such ancillary qubits are critical in ensuring that the error correction part of the problem is properly taken care of. But, the requirement becomes harder as more and more qubits are necessary for achieving fault tolerant computation. Physical implementations of computations have always been one of the challenges. New quantum algorithms to solve more problems is another area where a lot of efforts have been dedicated as we know there are only a few limited quantum algorithms which take advantage of the quantum nature of the system.

As far as the data transfer processes concerned as we mentioned for quantum systems, entangled states are necessary which are critical in ensuring quantumness of the problem. And so making of entangle states and preserving them for data transfer is another very important area of quantum computing which needs to be addressed while quantum computing parts is been looked at. So, these have been some of the basic problems or hurdles in the path of achieving quantum computing to the levels that we are actually interested in.

(Refer Slide Time: 12:48)



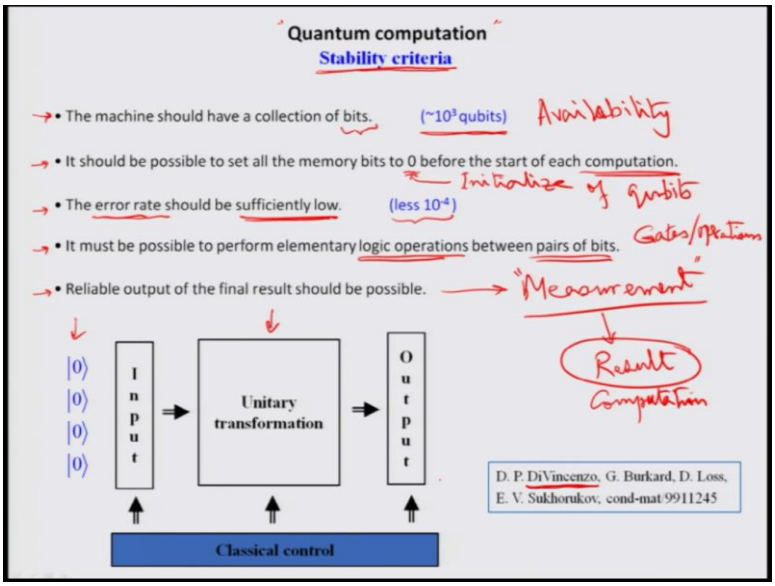
Still a lot of practical implementations we have discussed in this course and some of them are listed here; one of the first implementation of quantum computing in a very successful manner has been the use of nuclear spins and that have been utilized in a machine known as NMR, which is the principle which is used in terms of measuring or

manipulating nuclear spins known as the nuclear magnetic resonance spectroscopy.

Since this technology has been already available in spectroscopic sense for identifying molecules and has been utilized very often in chemical and biological systems and has made a huge advancement in the area of spectroscopy, this particular technique became the most handy way of showing the first few implementation principles of quantum computing. We have also talked about electron spins and quantum dots in the process of implementations; the energy levels of ions and ion traps are the other very important areas of quantum computing implementations, which we have discussed; use of super conductivity is another very important area where quantum computing has been brought into and adiabatic quantum computers are the ones which are finally, made some of the commercial implementations possible in most recent times.

So, by using these two principles of super conductivity adiabatic quantum computation principle as well as isolation from the environment the first commercial quantum computing came into being.

(Refer Slide Time: 15:05)



One of the most important features which enabled the principle of quantum computation has come due to the effort put in by Di Vineenzo wherein he was able to come up with the stability criteria that are necessary for minimally ensuring quantum computation can be achieved.

So, he had a few set of rules which are often known as the 5 sets of rules provided by Di Vineenzo and those are listed out here; the machine should have a collection of bits, which is the basic requirement of starting the quantum computing process, recommended bits for doing the large computing would be in the range of 1000 qubits, which we know that we are not yet there in that terms in reality to use a 1000 qubits in all practical senses; commercial processor cleaning 1000 qubits are now presently available; however, for most of the application experiment that have been made possible with them as we have discussed earlier all the 1000 qubits have not been effective utilized as we just mentioned in the previous slides that ancillary qubits are an extremely important part of quantum computing to ensure error corrections can be done.

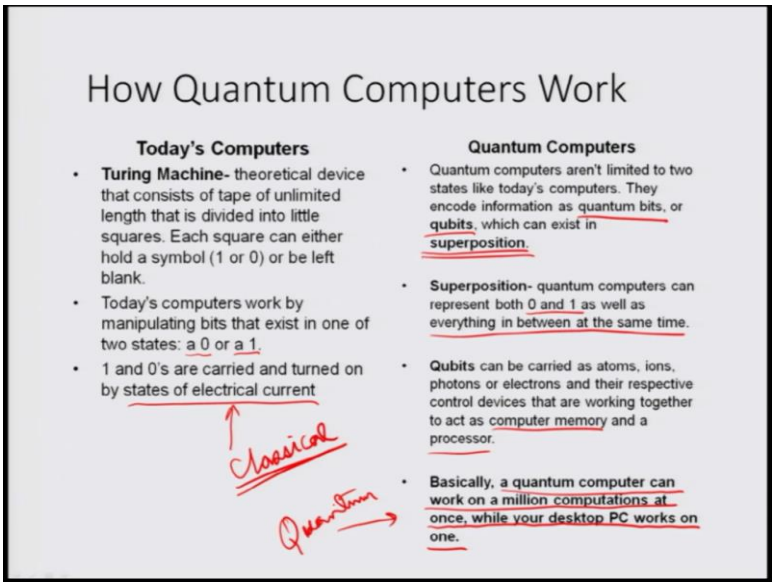
So, currently although about 1000 qubits or even more could possibly be available, the actual use of 1000 qubits for effective computation in terms of the power coming from 1000 qubits is not really available in that sense; however, the first point that the machine should have a collection of bits in our particular case qubits is definitely the first criteria. Secondly, it should be possible to set all the memory bits to 0 in other words initialize before the start of each computation, this is also extremely important as it is important to know how to go about the computation cycle; otherwise once computation cycle over a particular problem is over the computer becomes un usable.

The third important parameter laid down by Di Vineenzo was that the error rate should be sufficiently low and in some sense there was some numbers given by them in their initial several work, which comes out to be about less than 10 to the power minus 4 to make sure that the computation becomes effectively fruitful. It must be possible to perform elementary logic operations between pairs of qubits to ensure that computation is possible; otherwise just having a lot of qubits which could be initialized is not going to really have any computation, go ahead with any kind of advantage. There should also be a reliable output of the final results; otherwise the computational concept does not become useful so this last part is associated with measurements.

So, in other words essentially it can also be simplified to availability initialization or initialization of qubits, then logic operations which implies principles of gates, logic gates or operations which could lead to computations and finally, after the process of computation is over we would like to have the measurement made so that we can get to the results which could be called computation. So, these are the basic set of 5 rules which

are often used nowadays and they go by Di Vineenzo rules; pictorially such a system can be shown in this kind of a graphical term, wherein we have the input which goes in to the unitary transformation systems, which can be controlled if necessary by classical concepts and then finally, to get to the output which can be the result leading to computation. So, that is the basic idea behind the quantum computation that can be utilized to ensure that it is a computation of use.

(Refer Slide Time: 21:27)



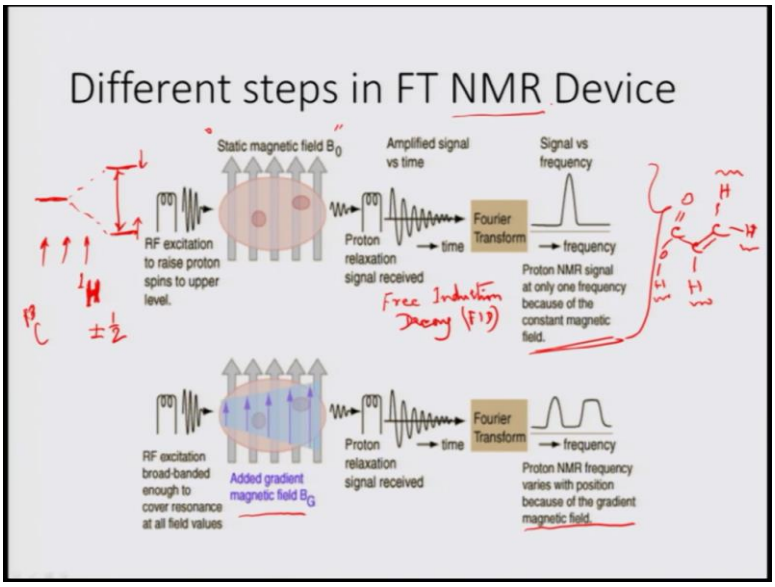
Now, in order to realize how this is in relation to today's compute, here is a sort of a comparison; today's computers essentially are based on Turing machines, which is the theoretical device that consists of a tape of unlimited length that is divided into little squares each symbol each square can either hold a symbol 1 or 0 or be left blank. So, that is very basic concept of the classical Turing principle of a computer, the classical computers work by manipulating bits that exist in one of the 2 states either a 0 or a 1. 1 and zeros are carried and turned on by states of electrical current that is basic idea behind today's classical computer.

In terms of quantum computers are not limited to 2 states 0 or 1e like the classical computers they encode information as quantum bits or qubits which can exist in superposition. Superposition essentially means are the quantum computers can represent 0 and 1 as well as everything in between at the same time. The qubits can be carried as atoms, ions, photons or electrons and their respective control devices that are working

together to act as computer memory and a processor. So, the net result essentially results in a quantum computer can work on a million computations at once while our desktop PC works on one.

So, that is the basic promise of a quantum computer the extreme parallelism, but as we have been saying all the time this has to be harnessed and that is the basic or the major issue about the implementation of quantum computation.

(Refer Slide Time: 23:49)



So, let us start with the very first one in terms of implementation which we looked at; which definitely is the concept of the Fourier transform NMR machine, which was able to be used to show the some of the most important steps in quantum computing. So, the principle of Fourier transform NMR device lies on the fact that the system can interact with the applied radio frequency excitation, to raise the proton spins to the upper level.

So, in order to make the proton spins affected by this kind of an action, what is necessary is that the spins become non degenerate, because almost all nuclear spins have similar energy unless and until they are subjected to static strong magnetic field, which results in splitting of the states based on the applied magnetic field. So, once the static magnetic field be 0 say is applied, it will be able to split the otherwise similar nuclear states into two different states depending on their aligned with the field or being aligned opposite to the field. So, the one which is aligned along the direction of the field will be lowered in energy verses the ones which are opposite the direction of the field will have the higher

energy.

So, once this separation of energy is set up for the nuclear states, the radio frequency excitation can be utilized to resonantly excite the nuclear field. Resonantly excite the nuclear spin from the ground to the excited state. So, this is the first step after this is done this was the simplest case is the case of the proton NMR as it can interact with the applied magnetic field, you have to have the nuclear state in such a way so that it can interact with the applied magnetic field. So, all the nuclei which would have an interaction possible with the applied magnetic field would be able to go into this mode of separation of their energies.

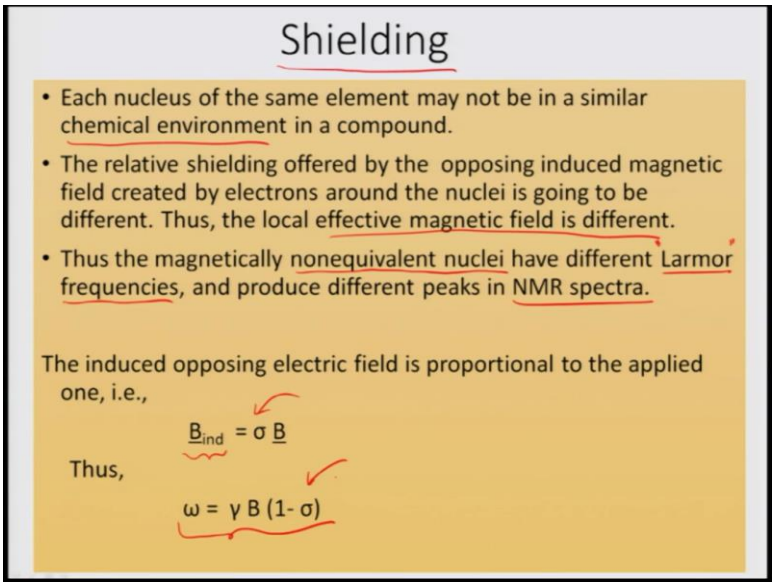
So, protons happens to be one of those which can undergo a plus minus half separation into the 2 cases where the spin is aligned in the direction of the magnetic field or opposite to the direction of the magnetic field. So, similarly carbon 13 also has similar properties and there are many other nuclei that we have used and we have discussed which have these properties which can interact with the applied magnetic field to split into 2 states. So, once the proton is excited the relaxation signal of the excited state can be amplified with respect to time and this process when the system is freely coming back to its normal state is known as free induction decay FID and once this signal is Fourier transformed then we get the proton NMR signal at only one frequency because of the constant magnetic field.

On the other hand if the added magnetic field has a gradient, then this can have different frequencies with respect to position due to the gradient magnetic field. The other way of looking at this principle is how you are changing the property of the system; whatever be the principle the very idea that a signal in terms of the Fourier transform of the relaxation of the excited state can be identified, it forms the basis of the NMR. Now this particular process is very subjective to the environment under which the proton or the nuclei is presented and so although all the protons would have otherwise given a single frequency signal upon Fourier transforming under this condition, considering the ideal case that all the protons are the same they are change in environment around the proton give raise to different frequencies and we have discussed this principle of NMR at length during our course.

Once the principle is understood it is possible to understand that different molecules can

have protons for instance under different environments due to the electron cloud around them are different. So, for example, just a carbon carbon chain having single and double bonds around them would have the protons facing different environments of electron cloud around them making the environment of the proton different from where their otherwise and similarly if they have other electron withdrawing or electron donating systems around them, they will also lead to changes in the proton environments that they will notice as they undergo this simple transformation and that is one of the basis behind the NMR spectroscopy, which is use for identifying the molecule per se.

(Refer Slide Time: 31:34)

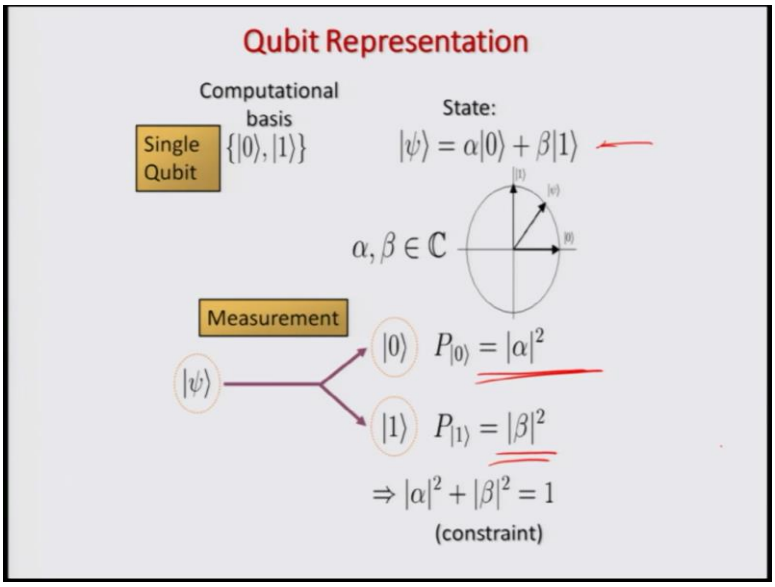


Now, the same principle which is otherwise known as shielding is the one which is utilized for this entire process. So, a few more words about this principle that I just discussed; each nucleus of the same element may not be in a similar chemical environment in a compound this is the basic idea behind whatever I was discussing until now. The relative shielding offered by the opposing induced magnetic field created by electrons around the nuclei is going to be different thus the local effect of magnetic field is different.

Thus, the magnetically non equivalent nuclei have different Larmor frequencies the other name for resonant frequency that is attributed to the scientists who had first notice that, which produces different peaks in the NMR spectra. The induced opposing electric field is proportional to the applied one that is the induced magnetic field has a relation to the

effect of the surrounding, which is otherwise known as shielding and therefore, the frequencies will be dependent on the effect of the environment and this can shown to be in this manner.

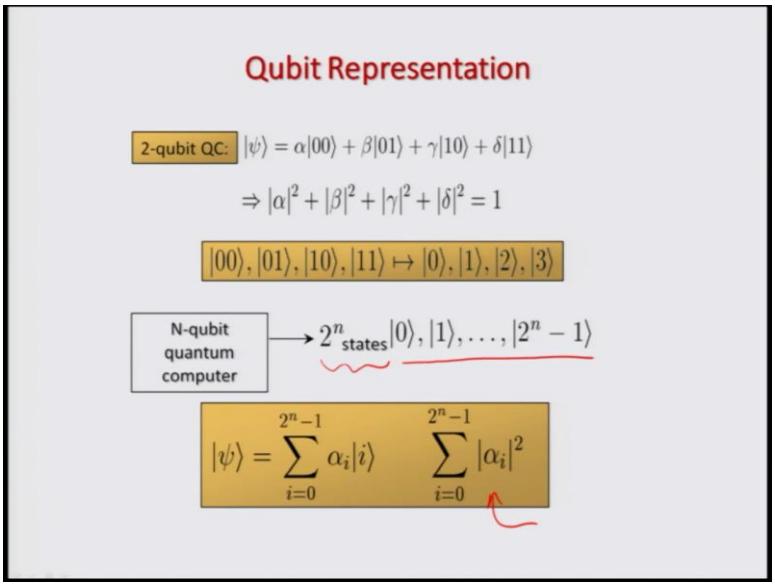
(Refer Slide Time: 33:03)



So, in these regards the qubit can be represented in this principle; a single qubit would have a computational basis which can be given by 0 and ones, where the state can have a representation as we know from all times a combined effect of both the basis states and that is the part which is the quantum part of the states that we look at and (Refer Time: 33:34) point of time when we make a measurement.

We get a probabilistic contribution of one of the 2 spin up or spin down in these particular cases for getting their result and the constraint which we have for all these cases the fact that the mod square of the probabilities in the both the cases has to add up to one that is because we are looking at a probability and the probability of finding the result is always going to be there and so it is going to add up to one all the time.

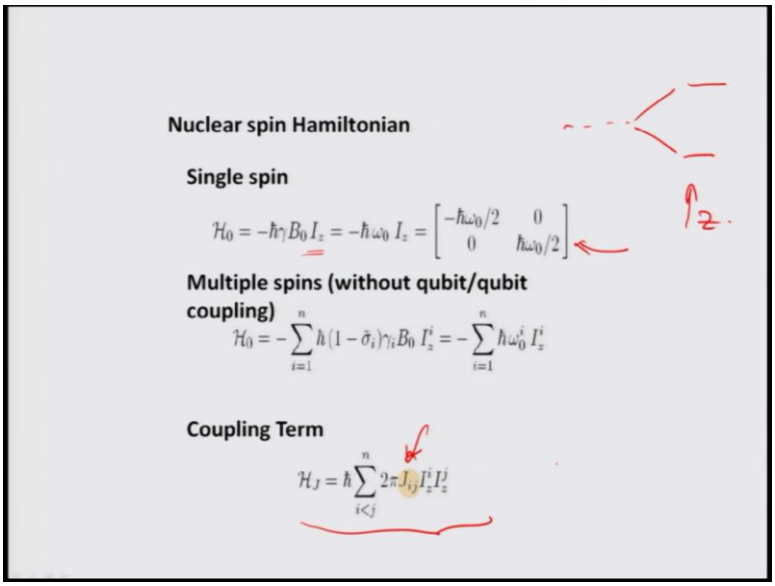
(Refer Slide Time: 34:16)



So, similarly if we end up getting 2 qubits which is basically 2 spins interacting, we can go back and see the same results that we have been discussing from all the times in terms of the contributions from their combined effect and as before their sums have to always land up to be one.

So, in case of N-qubit quantum computers, we definitely would have the 2 to the power n states, where each of these states are essentially being represented from 0 1 to all the way to 2 to the power minus 1 states and ultimately whatever we get is essentially connected to the contributions of each of these which corresponds to their probabilities, basically square mod square of each of the amplitudes.

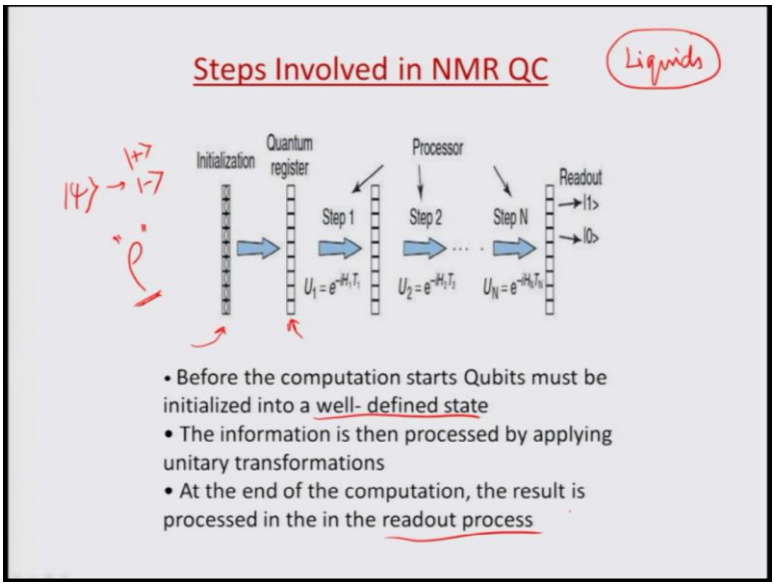
(Refer Slide Time: 35:19)



In terms of the nucleus spin Hamiltonian, which is what is the result of all these interaction, we have in this particular case the 2 states which have being affected because of the applied magnetic field and which are embedded in the splitting along the z dimension as we discussed; applied field being taken along the z or z dimension and therefore, we have this particular Hamiltonian which essentially looks like this.

Whenever we have multiple spins without qubit, qubit coupling then they would essentially scale with respect to the applied magnetic field. The coupling term is the one which is represented by their spin, spin interaction which goes along with them which is the j j coupling in this particular case.

(Refer Slide Time: 36:19)



So, the basic steps involved in the NMR quantum computing goes along with those 5 principles that we basically discussed, the first part being initialization process of such spin states to be able to get to a condition where they can be put in the original starting phase. Now in this process a lot of these have to be treated by using the density matrix approaches because we are looking at an ensemble of states. And therefore, most of these NMR quantum computing pictures essentially use the density matrix approach although we start of by sing the fact that we are essentially using just one spin which can have the 2 possibilities of plus minus half.

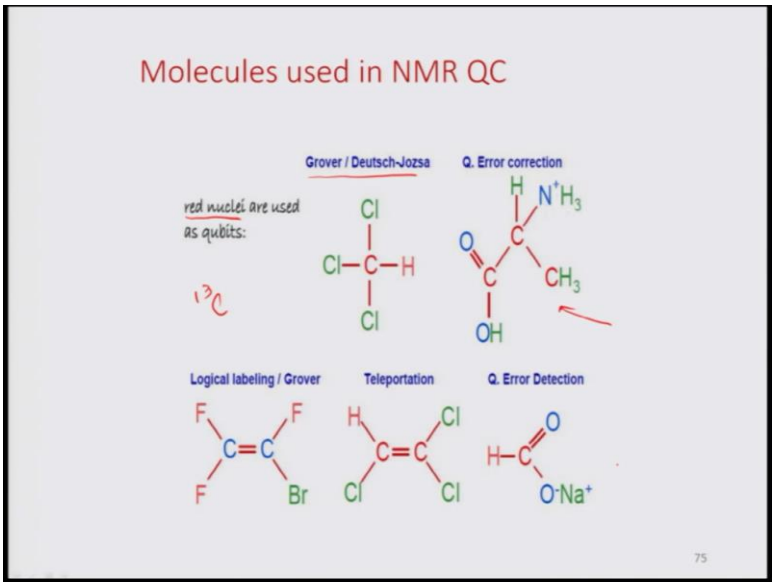
But since we are looking at a system which is going to have ensemble because most of these NMR machines that we are discussing now are in terms of liquids which have been looked at and the advantage of studying these in the liquid phase is the fact that the molecule by itself can behave as individual identity as the dipolar averaging around the molecule essentially goes to 0, as the rest of the molecules around them can have all possible orientations and they all essentially average out to 0 contribution.

So, the individual molecules itself can be looked at and so within the individual molecule the density matrix is found by the number of coupled spin states that have been put together. So, in some sense this is a average Hamiltonian theory which is applied for this entire process and we have mentioned some of it during our discussions, a lot of deep theory we did not get into because we were mostly interested in the implementation part

by using the NMR method. However, its suffice to say that the density matrix picture including average Hamiltonian theory is basically the idea behind this principle where before the computation is started qubits are initialized to a certain well defined state.

The information is then processed by applying unitary transformations and so the well defined state has the quantum register information, which is then undergoing the processors steps which are the unitary transforms and at the end of the computation the result is processed in the read out process and the readout in our particular case is the final Fourier transform giving raise to the measurement of the signal.

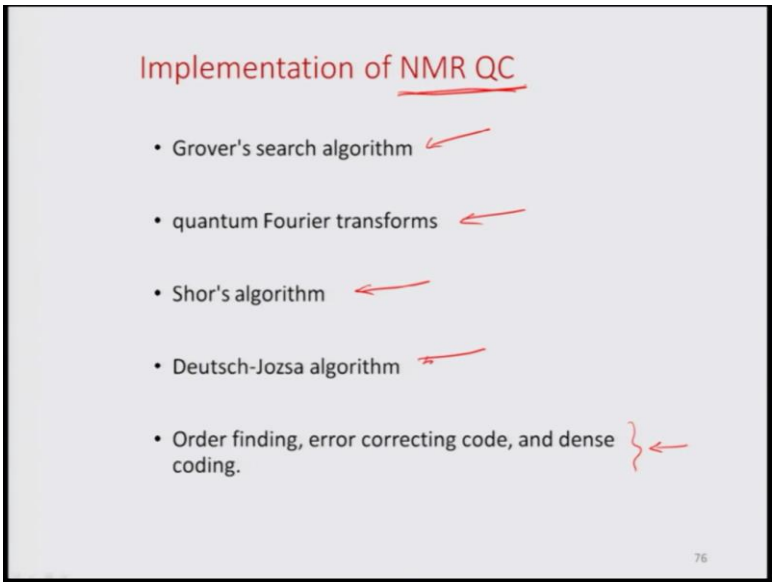
(Refer Slide Time: 39:45)



The molecules used in NMR quantum computing have been quite a few. So far example the Grover and the dj algorithm were able to be shown by using chloroform, where the each of these cases the red nuclei are the once which have been used as qubits. So far instance here the qubits are the carbon basically carbon 13 and the proton so 2 qubits. The error corrections quantum error corrections have been shown to be achieved y this kind of a molecule were we had the carbon been used as the qubits only the carbons not the protons.

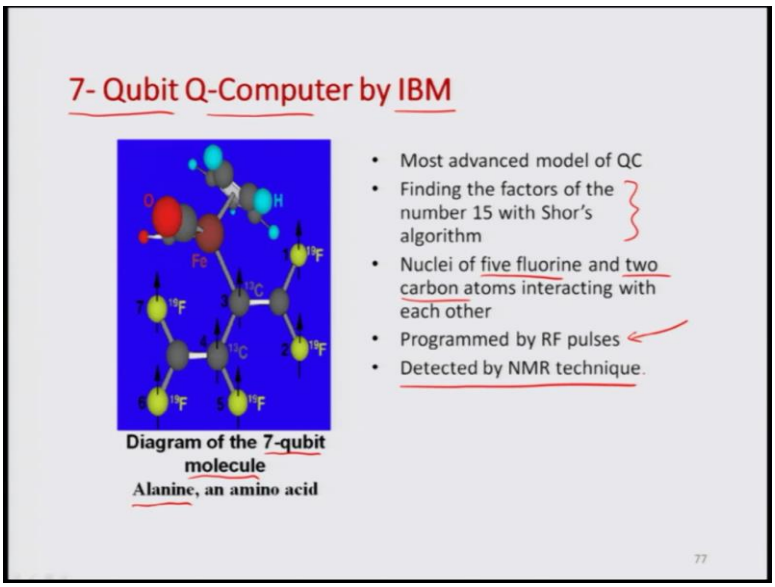
So, this way this is the 3 qubits system. Logical labeling and Grover's algorithm again has been utilized by using fluorine as the nuclei of choice for the NMR application. So, 1 2 3 fluorine; in terms of teleportation a proton and 2 carbons in this kind of a molecule and in terms of error detection a proton and a carbon has been shown.

(Refer Slide Time: 41:42)



So, several different molecules have been used for quantum computing using NMR and Grover search algorithm, quantum Fourier transforms Shor's algorithm, dj algorithm, Deutsch-Jozsa algorithm order finding, error correction code, and dense coding all these have been shown to be possible to be done by using NMR quantum computing. So in some sense NMR quantum computing has shown has shown a great lead in terms of major developments in quantum computing and so it has been one of the many studied areas of quantum computing.

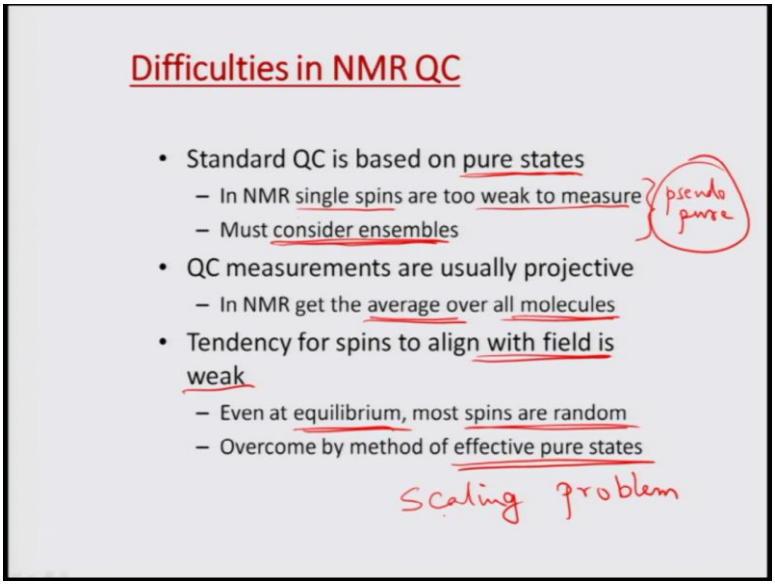
(Refer Slide Time: 42:01)



The best feet in terms of quantum computing was the implementation of Shor's algorithm by 7-Qubit quantum computer which was possible in IBM research by (Refer Time: 42:22) was working on that time over there, this use this molecule which is a 7 qubit molecule having an amino acid Alanine so the fluorine 19 has been used as one of the qubits in this case, 5 fluorine 19, and 2 carbon 13 makes the 7 qubit molecule for this particular case.

This has been used for finding the factors of the number 15 which Shor's algorithm and so these are the 5 fluorine and the 2 carbon atoms as we mention and the programming in these cases are essentially done with the RF pulses because those are the ones which enable the unity transforms and can be detected by NMR technique.

(Refer Slide Time: 43:20)



In spite of its great success one of the biggest difficulties have been the scaling problem in terms of NMR quantum computing and that is one of the reasons why though NMR is a great technique it cannot be an area which could be a next quantum computer for us. Typically the single spins in NMR are too weak to be measured, and as a result we have been always talking about ensembles.

So, that is one of the issues where quantum computing has always been more and more difficult and more and more involved whenever it has been an NMR quantum computer; it is so much simpler to talk about quantum computing in terms of pure states however, in these cases the best could have been done are known as the pseudo pure states because

they have been always cases where it had to be dealt with in terms of ensembles.

The quantum measurements are usually projective and in NMR get the average over all the molecules. So, once again the very idea of having one to one correspondence is a little difficult and so for smaller numbers of qubits, while there is always a correlation possible to be found as the number of qubits become larger and larger his correlation becomes more and more difficult and as such it becomes very difficult to implement quantum computing in terms of scaling the qubits for NMR.

There are also couple of others difficulties for example, the spins have an tendency to align with the field for example, the spins tendency to align with the fields is very is quite weak and that is a difficulty; because even at equilibrium most spins are random and therefore, most often we have to talk about effective pure states which is what the principle of pseudo pure states have been. So, all in all it is always an issue where scaling becomes a major problem for NMR quantum computing. And very often the signals to noise levels go below the quantum noise levels and so it cannot be scaled effectively.

So, this was one of the major aspects of quantum computing which was the first one to basically show the way that quantum computing can actually be possible in reality to be implemented and so NMR formed one of the basic backbone of starting to realize and go ahead with quantum computing. So, I first thought that we will first finish that part then going to the other implementation aspects and to the commercial one in the next lecture.

Thank you.