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

Lecture - 44 Futuristic Aspects of Implementing Quantum Computing-1

We have been doing a lot of introspection of the entire course in this particular week, as this is the final week of our course on quantum information and quantum computing and mostly the implementation part of it. In doing so we went through all the basics, we went through the implementation aspects that we have looked into in this course, now as the final part of this course is coming to an end let me try to give an overview of some of the aspects of the problem that we are in particular dealing with.

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So, in our case we are basically starting with the same principle that we have discussed throughout this course the ideal two level systems, which essentially forms the qubit, for most of the systems that we have discussed in this particular case.

The main point of our work have been focusing on the idea of using light as 1 of the three as 1 of the key ingredients for doing the quantum computing. So, that is why we distinguish ourselves from the rest of the work which is going around. So, in the simplest possible sense some of the earlier maths that you have looked in is summarized in this particular slide, where the interactions and the way the system evolves is being looked at

in terms of an ensemble of the system that is been looked at and that is interacting with the applied field in most cases for our particular case it is optical.

It is also important to mention that as we have developed during this entire course, any system that can interact resonantly with assists with an applied field whether it is radio frequency or it is electromagnetic or it is magnetic, they all have similar interaction features and they end up producing Hamiltonian interactions which are sort of what we go ahead with describing the system. The most important part which we discussed in this course was also the fact that whenever we are looking at a practical aspect of the problem, we are not looking at a single quantum system and so instead of solving the schrodinger equation, we always end up solving the Lionville equation which is how this entire process evolves with time and under the condition where the two states are being interacted with not just a resonance single photon excitation.

But with the resonant several photons adding together to give that excitation, a picture similar to the 1 shown here is often used and the simple picture for a multi photon process as long as it does not create any other complicacy, works quite well in terms of describing what is going on; with these basis many of the discussions which have been also made in this course are relevant to the kind of work that we are doing and have been developing over the years.



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You have also seen these kinds of features as we discussed during the course where the ground and the excited states keep on oscillating with the typical Rabi frequency based on the interaction with applied field, and as the field is not in resonance, but goes away from the exact resonance point to other frequencies which are non resonant with the two states that we are looking at the fall off of the population goes in this particular fashion, and in this theoretical limit the idea has been taken that there is nothing, but a pure two state system which is being excited and therefore, beyond a certain range of detuning, there is no resonance available and. So, it falls off in terms of excitation of the system going from ground to the excited.

However, it is important to note that there is a range over which the effect of the pulse is still there, because we are not really talking in terms of delta functions, but we are talking about actual width of these lasers or pulses that we are talking about and these fourier definitions often always help us in defining and finding out as to how far the excitations can exist even when they are not exactly on resonance. So, all these are important concepts to understand as we address and work with quantum systems and qubits in particular.

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There are effects of the actual profile of the laser, which is often not very importantly looked at, but the consequence of that is the idea of solitons, which I think I might have mentioned during propagation of laser pulses through optical fibers and others while we were doing the laser concepts, but there are certain shapes of which are more resistant or which maintain their shapes as they interact with systems and so hyperbolic seek and for example, is a better shape in that respect with as compared to let say the Gaussian 1 and so there are different principles which keep on working at every respect of the application of interaction in these kinds of areas of research.

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So, in general the ground state excitation of a laser pulse also has to be thought of an envelope profile, which is having a carrier frequency and in the carrier frequency included laser pulse for instance looks like this and when we often for convenience right only the amplitude profile we take a look and write it this way which automatically removes the carrier frequency of the laser, which goes into the resonant excitation of the field and most often we go into the rotating frame where this carrier frequency of the laser is considered to be the frame in which the system is rotating or revolving.

And therefore, we can only work simply by using the amplitude profile of the laser beam, instead of wondering instead of worrying too much about the frequency of the laser for instance. So, the populations and how they work are important aspects to understand, because that is how laser matter interaction plays which play a major role in some forms of quantum information and computing can be relevant in these kinds of understanding and studies.

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So, the model therefore, is built on this principle that if you have a simple single photon case, where the resonance is when the exact gap of the energy between 0 and 1 state is provided otherwise given the fact that there is a bandwidth does it with the laser even if the laser does not exactly match the bandwidth match the energy gap between 0 and 1, the two states can be connected through dipole interactions and excitation can occur and because of that a detuning factor delta may come in and that is how all these discussions appear.

If multiple pulses are possible to interact simultaneously then we can get two photon or multi photon cases and at every point there will be some aspects related to the line width and the exact energy gap differences that are allowed because of the way these interactions go. So, the resultant is that we were able to see the effect of these interactions in our last lecture where we looked at how the energy used to flow from the excite state to many other state and for simplistic real molecules that are real we actually saw how IVR can really be modeled and that can that information and their ideas can in fact go ahead to form the principle of adiabatic interactions to get to cases where they can be utilized for computing.

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One of the simplest applications we discussed was the idea of using Taylor series expansion of the instantaneous phase of the electric field.

Where the phase was actually in expanded by using the Taylor series and then his derivative gave rise to the frequency sweep, which resulted in shape pulses and the application of those and their interactions with this is model systems can be understood in terms of an ensemble of states by using the Lionville equation.



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And that is typically the result of all these experiment all these theoretical models which have been described and discussed in many of the lectures previously; and the convenient unit for many of the interactions are often in terms of Rabi frequency which essentially has the connection of how well the two states are connected as well as the intensity of the applied field. Both of them together define the Rabi frequencies mu dot E over h cross; mu is the coupling constant, E is the applied field and h cross is the plancks constant. So, that is how typically these parameters are placed so that they can be related to how the actual interactions as well as the theory can be looked at between each other.



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Once again the sweeping which results in adiabaticity can be looked at as a result of different shapes of the pulses and the complex shapes of certain pulses are much more are complex; laser pulses have very specific interactions and one of the interesting ones is hyperbolic secant with hyperbolic tangent frequency sweep, because it essentially results in a rectangular inversion profile. So, this principle where the population is being looked at with respect to the applied energy and the detuning applied field and the detuning is often called as the inversion profile and the shape of the inversion profiles often enables to understand how the interaction goes and it is important when these interactions are well defined rather than they are Oscillating or changing, because once they are well defined they can be utilized for certain applications.

For instance, a perfect way of taking one state to the other precisely all the time is for instance applying a not gate, but if a simple pulse is applied to a Gaussian pulse without any other property a changing of the laser is applied to a two level system it will start flopping. So, the Rabi flopping which means the population will go back and forth between ground and excited state, so we will it will not really undergo a clean not gate, but an oscillation and so for generating simple gates which are abuse, it is important to have interactions which can be predefined in a certain way and can be utilized in terms of computational principles; that is the basic idea behind the start of these kinds of applications in this format.

Ideal Two Level System PI Pulse Effects 0.08 Eig[1] ρ11 0.0 Im[1.2] units) Ab Coherence Term (arb. Real[1,2] 0.0 Real[2,1] 0.02 0.04 -0.5 Im[2.1] 0.06 Eig[2] 0.08 -1.0 40 10 20 30 50 60 70 Time (fs)

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So, under these kinds of implications and the pulses interaction with the system can be looked at a little bit more and completely, and even under the condition where there is an ideal two level system the effect of the pi pulses can be understood in terms of realizing how the coherence terms. Now that we know that in a just density matrix, the diagonal elements represent the population and the off diagonal elements which are rho 1 2 and rho 2 1 essentially represent the coherence of the system, those are not observables; however, for simulation these are important parameters which can be looked at and to in order to understand what is going on with the system. So, by looking at these it is possible to understand how the different pulses affect the interaction of the system, which is to be used as a qubit.

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So, here is the model of looking at the off diagonal density matrix elements that is in other words looking at the coherence of the system under the impact of an applied field. The population may oscillate as in this particular case it is only a simple pulse, which is been provided without any modulating field associated with it. So, there will be a Rabi flopping and that depends on the pulse area of the interacting pulse with the system and the interesting part here which cannot be an observable, now this part population part is an observable the part which is not an observable is the coherence part and it can be modeled and understood in these terms.



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And by using the principle of adiabatic passage where the frequency is being changed slowly from below resonance to resonance and to beyond resonance, the population can be made to follow the applied field.



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And so these ideas can be demonstrated and understood in the same way as the principles are built up and it is possible to see that these principles are really well followed as the applications are being made to these kinds of understandings and the model is being checked at every point through simulations and applications.

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So, based on these understandings and checking it through many different intensity patterns and the conditions, we have managed to distill a few of the important aspects which is related to probing the coherence and coming from the off diagonal elements of the density matrix. And as expected all absorptions are associated with dispersion and this is known from spectroscopy as it is known as the famous Kramer-Kronig relationship, all absorptions are composed of the real part and the imaginary part where the real part corresponds to the dispersive and interaction and the imaginary part is corresponding to the absorption of this applied field and which results in there are be flopping and this is coupling through absorption.

In case of the adiabatic process coupling is through that dispersive part, so there is no absorption process and so there is no population flopping. So, this is the key concept of the adiabatic process, which means that the adiabatic process essentially works through the interactions through the dispersive part and so no absorption process occurs and no population flopping is seen.

Whereas, in case of the resonant interaction absorption, Rabi flopping occurs because the coupling is through absorption; so the benefits of such understanding of theoretical models and study is the fact that we can quantify the two level character in a multi level system which is very important, it is almost like saying that we are tracing out the density matrix to get the information about the rest of the system. Off-diagonal (Refer

Time: 18:16) symmetric elements switch from real to imaginary and the excited process changes from being resonant to completely adiabatic and this is one of the most one of the interesting observations that was observed as a result of such a study. So, some of these fundamental ideas that we have been discussing has profound implications as expected, and these were the models to test and find that they do in fact, confirm to these understandings.

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These are also very important as we would like to make molecules as or qubits because molecules are richer in terms of handling as well as interacting as well as the number of states concerned and so they would become good quantum computing qubits.

However there are many challenges, one of the biggest challenge is the process of IVR which we discussed in earlier classes and there is also there is other important point that since molecules are not really two level systems, to know it is important to realize that in order to use the molecules as qubits we would need to demonstrate, a true two level nature of the molecules. So, for instance as I mentioned before all real molecules are going to be multi level and we have to find a way to see how we can understand their two level nature. Increasing decreasing time of the states have to be also very important as we would like to use them as our qubits.

So, this is a coming from the temporal side; the other important part is the isolation or controlling the molecules in such a way so that they can be made to interact under experimenter's discretion. So, that has to do with the spatial processing so that they can be under control as we interact or to work with them and this has been achieved through principles of molecular beams or in the gas phase, which is equivalent to the idea of atomic or ionic traps of environments were such possible (Refer Time: 20:53) exist.

Optical tweezers are the other interesting ways of doing it in terms of liquids and so they are also very attractive which we look at it, and we have developed the pulse optical tweezers in this context to make this possible. So, the ideas of control essentially exists both temporarily and spatially and they can be coupled at some point by using pulsed optical tweezers for instance where both temporal and spatial aspects can be put into action.

Adiabatic half passage in coupled systems: Adiabatic half passage in coupled systems: t<0: sweep to resonance 0-t<T: constant amplitude, μ -E/fi >> couplings to dark states 100° Ground State Dark States Time

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So, in this context is perhaps useful to also discuss about the half passage instead of the full passage that we discussed earlier, where the property of the laser is changed from below resonance to resonance and is held there; so that the property of the pulse is changed from below resonance to resonance and it is either kept like that or after a while it is switched off; so that the states follow to the point where they are coherent between the ground and excise state.

However the states which are going to create IVR or the dark states we take the energy away do not interact with the ground and excited states when they are coupled; this is one of the principles which we discussed before in terms of IVR and their control once the pulse is turned off they all go back into their original conditions.



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So, this is the work that I have already presented in one of the lectures in this week. So, I am not going to explain it once more, it suffice to say that it is possible to use these same principles and this is our work in particular which shows that it is possible to show molecules can be tuned to be working as qubits.

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And in terms of molecules realistic molecules, a lot more work can also be done to show that they all would be interacting in one way or the other depending on the other kinds of shapes that can be applied not just the ones where the pulse is just going to counter resonance and turn off and go through resonance in a very slow manner and so on and so forth.

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So, there has been some work in terms of looking at all the components, both real and imaginary components as it undergoes these changes. So, as to be able to understand how the coherence flows in these kinds of interactions and how the energy localization may be looked at as a function of the applied field.

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In this regard it is possible to bring the states to coherence by using the population to follow a pattern where the amplitude profile of the pulse is following the frequency profile, or may be undergoing a certain kind of a phase modulation, where this kind of coherence between the two states exists and the other states are not possible to interact because they are not able to get any interactions with them.

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In these kinds of cases it is important to find that the real part is important as we can see the off diagonal elements to understand how the coherence of this entire process is going and working.



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This particular idea of how molecules are interacting because of their many many states is also possible to understand in terms of another model of intra molecular vibrational relaxation, where it is not just a few state interacting with the original two states which get coupled due to applied field, but there are many other states which sort of interact in a different way and that particular model is shown here which is known as a tier model of intramolecular vibrational relaxation; where the energy of the states are sort of star interaction and the interactions keep on increasing as the number of states across keep on getting coupled more and more; such a model Hamiltonian can also be built and many molecules have such interacting Hamiltonians which can be further generalized to make a good model of the molecule.

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Using such models it is possible to have simple hadamard gate in molecules, which was also mentioned earlier in one of the lectures and this is the same slide that was used there to essentially show if that more than one state is coupled to the ground state, then they can all be simultaneously put to an equals position whereas, the dark states which are the ones which are not coupled through dipoles, but are going to interact with the excited states to take the energy away are kept at bay and not allowed to interact and so it automatically creates an equilibration of bright states. So, these have their interesting implications and perhaps can be utilized as qubits has been suggested by earlier work.

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So, one of the key features in all these interactions is the idea of having control knobs, where the spatial modulation is being used to get the individual molecular control in condensed phase and in case of gas phase one can use molecular beam conditions as we discussed before. The other kind of control that can be utilized in any kind any in many of these applications in terms of control knobs is the laser polarization.

So, one is the laser spatial modulation, the other one is the laser polarization and in terms of temporal modulation the simplest of all that we have been discussed is the frequency chirping. So, a natural question under these conditions to ask whenever we are looking at control knobs is how important are these parameters or control knobs in the in concept of molecular control, because the idea of the molecular control is intimately connected to the concept of quantum computing is they are the ones which end up producing the gates.

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So, here is a an example of how the simple idea of frequency chirping, which is basically linearly changing the frequency across the pulse can be put to a use; this is connected to the idea that chirp is a term which has been around for a very long time, it has been adapted from the concept that birds make the frequency modulating sound and that is how the chirping of birds have been associated with this principle of chirp pulses. So, they have these principle ideas where the chirp parameters can be defined in terms of the change of the frequency as it undergoes within the pulse. So, they can be interacting and their interaction with the molecular system can be understood in as a function of their parameter.



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So, one of the places where this has become very interesting is the idea of using such pulses in the gas phase for controlling the fragmentation process, which may have different applications, but in terms of our particular goal we will present how this is done.

However, this particular technology itself as a lot of bear in to the controlled environment principles that we have always been talking about in terms of quantum computing ideas and applications, where in this case the beam chamber is generated through a supersonic jet expansion in a very low pressure environment, which is effectively generated by use of turbo pumps and diffusion pumps and any other pumping techniques, so that the their zone over which the molecules expand are under the condition that they have a laminar flow and the laser can in fact, interact across under that condition with a well known mark number and the proper temperature associated with these molecules.

These interactions may lead to the fragmentation of these molecules and those fragments are then measured through a time of light mass spectrometer and measured through a multi channel plate the signal, which gives rise to the fragments that we are finally looking at. In this particular case a laser operating at a 1000 hertz was used with ample intensity to be able to undergo break down of the molecules that were being looked at.



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Now, what was notice very interestingly is the fragmentation pathway for a simple enough molecule n-propyl-benzene dependent on the way the frequency of frequency content of the laser that was used for this fragmentation was and that resulted in different fragmentation ratios, that was dependent on the frequency content of the laser pulse.

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So, if there was no chirp associated with a laser, as it has been shown here transform limited with each of the chirp parameter is 0, this is the transform limit or the regular Gaussian beam, this is the distribution of the ions which has seen.

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However, the mass spectra of the n propyl benzene changes as the frequency chirp is changed between positive and negative frequencies and as they are mapped in a more systematic manner.

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What is able to be seen is there is a laser induced control of the fragmentation of the n propyl benzene, because of the applied chirp parameter and this is interesting because that would mean that these fragments can essentially relate to the applied field conditioning and that can in turn act as the understanding parameter for some bit of information. This is similar to the ideas which were originally propounded by Bergsman and others; where they had used the fragmentation principle to finally, read off how certain states were more populated than the others in terms of the interaction of the cesium grade berg state with respect to the applied field which had some information on it.

So, given the fact that the information content on this particular case can be related to the frequency content of these pulses, they can also interact to show how this information is being translated into the fragment ratios which have been seen here. So, in particular for example, C 6 H 5 plus has and as a very strong positioning at and a positive value whereas, the C 6 H 5 plus as a very strong positioning at a negative value and so these two for instance can serve as markers for that whereas, the beta 0 which is essentially now has the maximum coming for the C 7 H 7 at the beta 0 position. So, they all have different characteristics associated with the fragmentation property, based on the character of the frequency which has been used.

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This is because the fragmentation path keeps on changing as a result of the applied chirp and so they undergo different directions of getting into the different fragments as we have been showing here.

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The same is true for the polarization dependence of the various fragments of the fragment ions seals of these n-propyl benzene; however, one thing is to be noted in case of the polarization dependence is the fact that the variation of the different fragment ions

with respect to the polarization angle essentially peak at given particular values and that is independent of the fragment character.

So, all the fragments for instance peak at specific values of the polarization, which sort of provides the polarization parameter as an intensity parameter; whereas, in terms of the frequency component the chirp of the pulse we found that certain fragments are specific in specifically inclined towards certain frequency components. So, the polarization component can be more like a intensity in this particular kind of a control knob whereas, the other frequency sweep parameter in this case is very subject to the character of the fragment that we are looking at.

So, having multiple control knobs like this are very important for controlling quantum objects because that is the way how these gates and knobs can be connected and be utilized for information processing of quantum objects.



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So, this is the idea behind adding the polarization and the chirp simultaneously on a particular experiment as we have discussed here and it is possible to therefore, use both the control knobs which are independent of each other: one acting as an intensity switch and the other one acting more like a frequency switch for looking at these different fragments.

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So, this multi parameter control with laser polarization and pulse chirp essentially are useful, because they are mutually exclusive one acting only on the intensity part and the other acting on the character of the fragment that are being looked at.

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Another important aspect we looked at in term in this connection was also to look at how the chemical dynamics of a system may be affected as a result of laser frequency changing instantaneously within the laser, as we have been talking about in terms of frequency sweeper changes and what we found at here also the parameter of frequency sweep did create a major change between the resulting products depending on how it is interacting.

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So, in order to establish this we essentially used a very symmetric experiment, we used a very rudimentary process where a dimer of a molecule was being broken up into the monomers and so in terms of measurements, it was very clear that there was a peak due to the dimer and there was a peak due to the monomer and the distinction between the two could be easily understood as the experiment was being done.

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So, under the same conditions of the gas phase experiments as we have defined discussed in the earlier case, these systems could be looked at by using the frequency modulation of the laser pulse as it is undergoing interaction with this system and what we find is that given our pulse width of the laser the fragments are very specifically distributed to the dimer and the monomer, which let us our experiment to work well.

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If the intensity of the laser goes too high and it becomes complicated in terms of interpreting the results because other fragments start appearing, but if it is done in such a way only the two fragments the monomer and the dimer appear and it is easy to do these experiments.

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So, we basically set up the experimental condition in such a way that we were able to look at only the two major components that are of interest in this particular kind of work.

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And what we found is that the result of what we found was that the affect of the chirp on the parent ion yield was very symmetric as expected with respect to the second harmonic generation of the system, essentially showing that the process was only intensity dependent.

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However, when the relative yield of the monomer was being looked at, it was found that the negative chirp had a huge impact on the formation of the enhanced formation of the monomer as compared to the case when it was positively chopped pulses were used. So, that is how one of the very important parameters were applied in this particular case to make sure that we understand that the chirp parameters are being applied properly to be able to study this process with care.



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So, overall it was possible to understand that the relative ion yield of the monomers was favored when negative chirp was used versus the positive chirp, but the yield of the dimer essentially remained consistent with the application of this particular process.

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So, the spatial control with pulse laser opens up possibility of spatial temporal control; polarization can also play an important role in spatial control; control knobs which were used by a spatial modulation, temporal reputation, exploiting temporal shaping and polarization and for the traditional molecular control the control knobs that we explode were frequency chirp, there is a polarization and the control of dimerization versus is breakdown was also being looked down. So, these sort of set the space for how quantum computing and use of quantum objects for doing computation can be utilized.

Another area of development of quantum computing in our particular approach has been the idea of spatial modulation, in these particular cases we were mostly using temporal modulation, the spatial modulation part works extremely well if one can use a tweezer or a way to hold on to a particle as we have shown in terms of ion traps as possible to relatively move objects and so this is the same principle that we have used in the case of liquids by using optical traps and to discuss that part I will be going into the next lecture.

So, we will end this lecture with this principle that we have managed to show the different kinds of qubits and optical interactions that we have done until now in terms of quantum computing in this respect. So, we will see you in the next lecture.