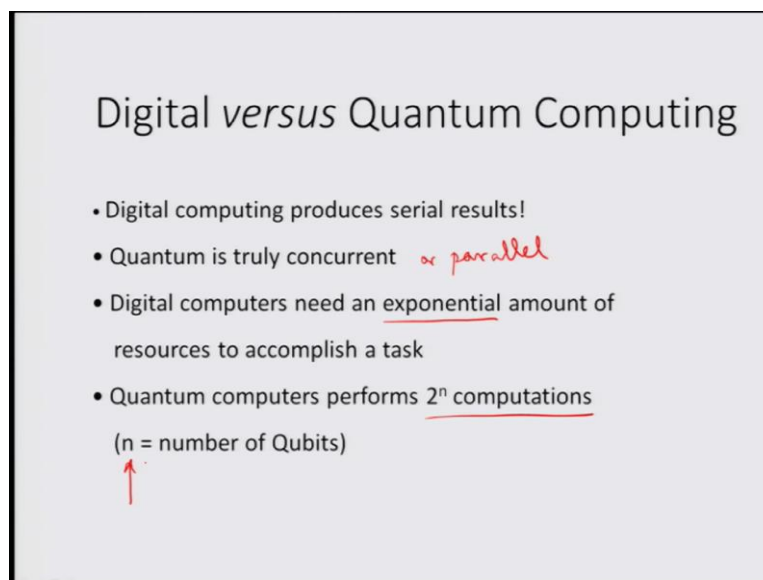


Implementation Aspects of Quantum Computing
Prof. Debabrata Goswami
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 40
Academic Development in Quantum Computing
Implementation- 1

We have been summarizing all the aspects of quantum computing implementations that we have been dealing with in this course in this week. What we are now trying to do is trying to see how all the different aspects that we have discussed in this course as a part of implementation, how does it work in conjunction to make sure that quantum computing becomes viability. It is an interdisciplinary field so it takes a lot of different areas, and therefore we are spending this last week in a lot of detailed discussions of the different aspects of subjects that we have covered.

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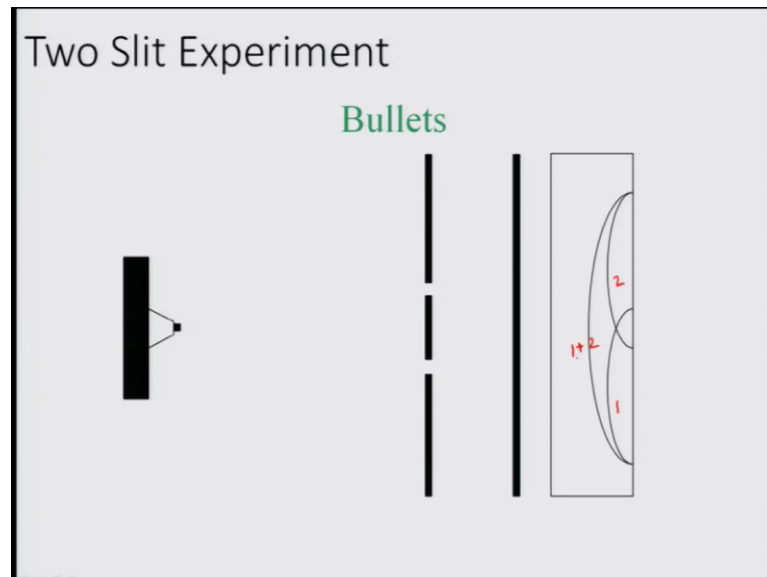
Digital *versus* Quantum Computing

- Digital computing produces serial results!
- Quantum is truly concurrent *or parallel*
- Digital computers need an exponential amount of resources to accomplish a task
- Quantum computers performs 2^n computations
(n = number of Qubits)
↑

So, in this lecture we will be looking into the digital versus quantum computing aspects from the principle of looking at the traveling salesman problem. What we have learned until now is the digital computing produces serial results; on the other hand quantum is truly concurrent or parallel. Digital computers need an exponential amount of resources

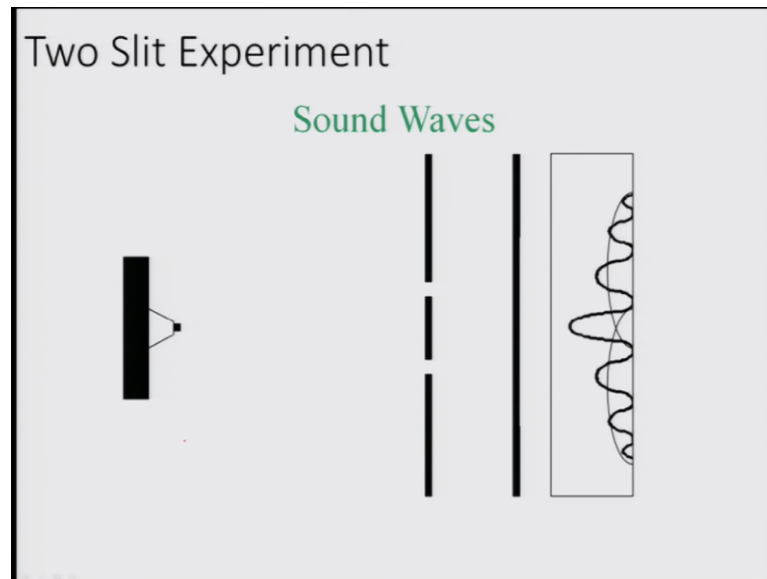
to accomplish a task, which can become polynomial in the quantum sense that is because quantum computers perform 2^n computations, where n is the number of qubits. So, these are the basic advantages we have taken when we went from digital to quantum.

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So, some of the very simple examples of the quantum nature has been told in terms of very basics of interference. For example, the 2 slit experiment, where if it is a classical case then for a single slit, the bullets will only come from one of the two places where the holes are.

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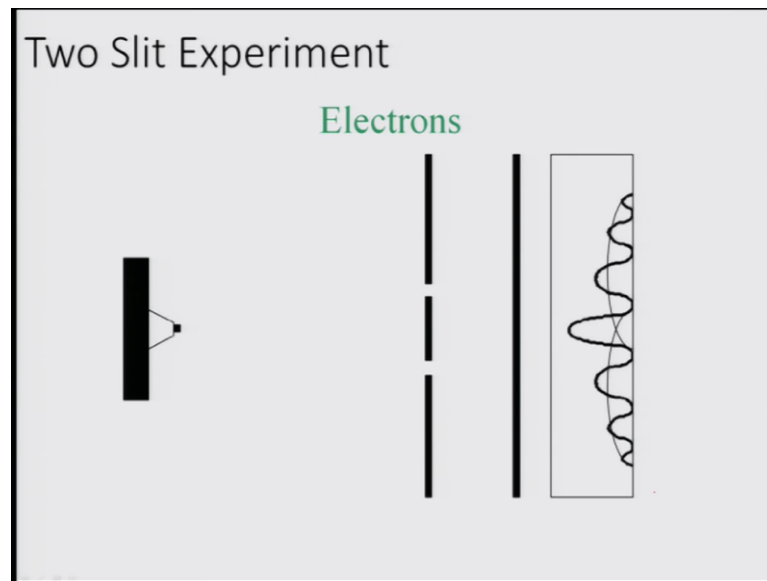


On the other hand when both of them are simultaneously present, then it produces interference for example, take a look at a wave for example, the sound waves their behavior is something which is very different from when only particles have being considered classical particles. So, to appreciate this let me show this once more.

So, bullets are classical particles; let us consider the case where we are going to have 2 slits going on to a detector, but for understanding this let us start with one slit. So, when we have bullets passes through one here is the distribution. On the other hand if we have the bullet on the going through the other slit there is the distribution, only one of them are open if both of them are open then what will happen is will get a total distribution which is of this kind. So, $1 + 2$ and this 1 is one plus 2 .

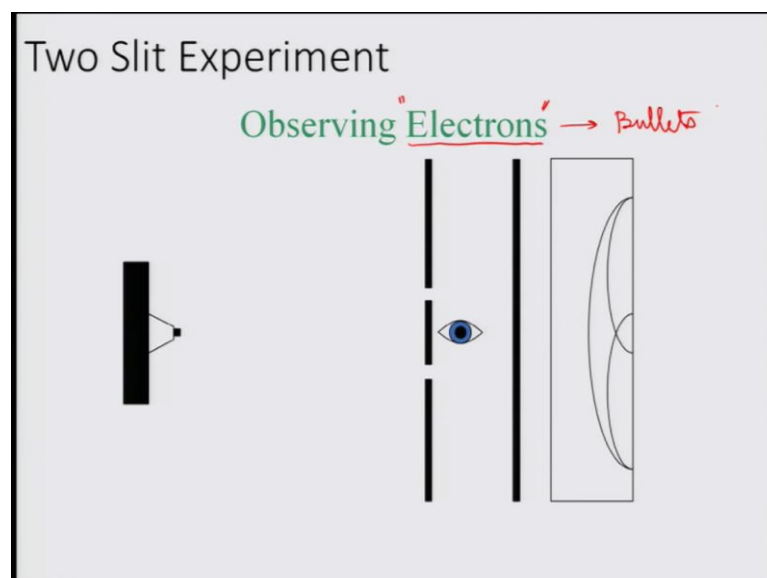
On the other hand when we do sound waves let say. then if we have the similar situation of one slit or the other slit the initial idea of having one each is fine, but when we have both the slits open they do not simply show the addition that we just showed you for the bullets instead it shows an oscillating pattern, which is the superposition which is distinct from the individuals that we talked about so that is the wave part or the interference nature of this.

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So, this same thing extend to the electrons, and just going to show this for completeness and so we know that electrons essentially although they are particles may be a light wave.

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But when we are observing electrons then we do see them as bullets; so they be a waste particles. So, that is the dilemma with quantum mechanics, which is what we are working

on when we go to fundamental particles which are quantum, then they have both the properties when we observe them that is when we make that classical, then they behave exactly like a particle analogues to the bullets that we talked about, but many of their other phenomena behave like wave like which is what when we talked about the sound wave. So, that is all the principles of quantum mechanics just summarized here.

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Basic Quantum Computation

- Qubit - can be 1, 0 or both 1 and 0
- $|x\rangle$ - number in Quantum Computer
- Superposition of states:

$$\sum_{i=0}^{2^N-1} a_i |s_i\rangle \quad \text{where:} \quad \sum_{i=0}^{2^N-1} |a_i|^2 = 1$$

So, in terms of quantum computation we have been utilizing the concept of superposition both 0 and 1 and the qubit representation has been in terms of the number of wave functions that we are using; so the superposition of states for instance would essentially have a concept of amplitude square of which leads to probability, these are all the concepts that we have taken as a result a summation of all the square of the amplitudes for the states would always be equal to 1 in order to make the probability loss to be sustained.

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Examples

$$\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

$$\frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle$$

So, we have been using these kinds of states: entangled states, superposition states.

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Representation

• n qubits: $2^n \times 1$ matrix represents the state:

• $|0\rangle$ would be represented by $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

• $|1\rangle$ would be represented by $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

• Equal superposition would be $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$

And we have been representing them either in vector term or in the matrix term.

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Changing States

- Unitary transformations change states
- Unitary matrix:
 - conjugate transpose = inverse

$$\overline{A}^T = A^{-1}$$

And whenever we want to change them we talk in terms of unitary transformations, which are essentially unitary matrices whose conjugate transpose is the inverse. Essentially ensuring their Hermitian nature of the system is preserved.

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Example

Hadamard Transform

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$
$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

So, we have shown many a times Hadamard transforms, where we can go from a

particular pure state to a mix state for instance.

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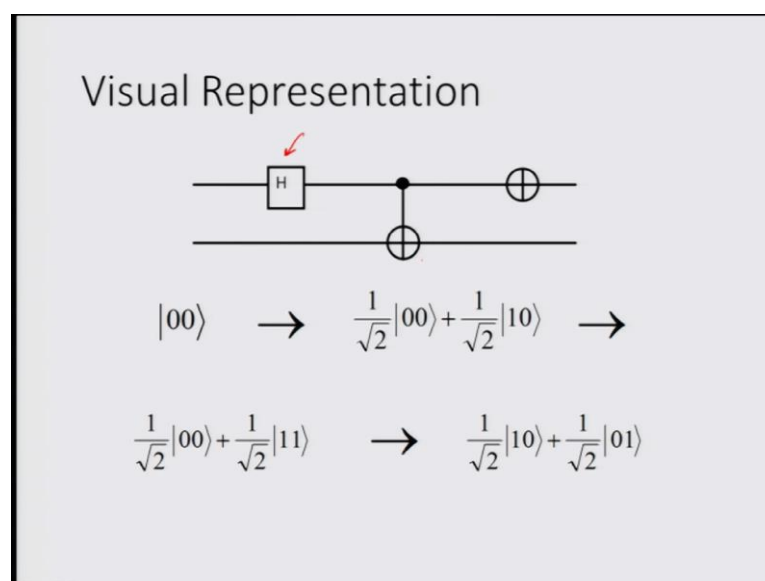
Example: CNot Gate

Not Gate:
$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} b \\ a \end{bmatrix}$$

CNot Gate:
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} a \\ b \\ d \\ c \end{bmatrix} \quad \begin{matrix} (00) \\ (01) \\ (10) \\ (11) \end{matrix}$$

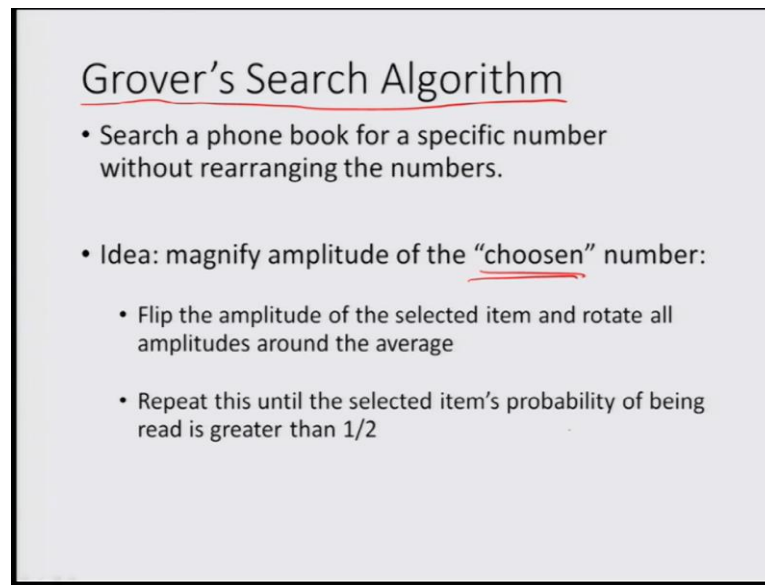
We also have talked about other simpler gates, for example the CNot Gate, the Not Gate; CNot is the 2 qubit gate Not gate can be single qubit gate and so on and so forth.

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There are visual representations, which essentially tell us about the circuits the wires the representation of the gates and how they interact the Hadamard, CNot and so on and so forth.

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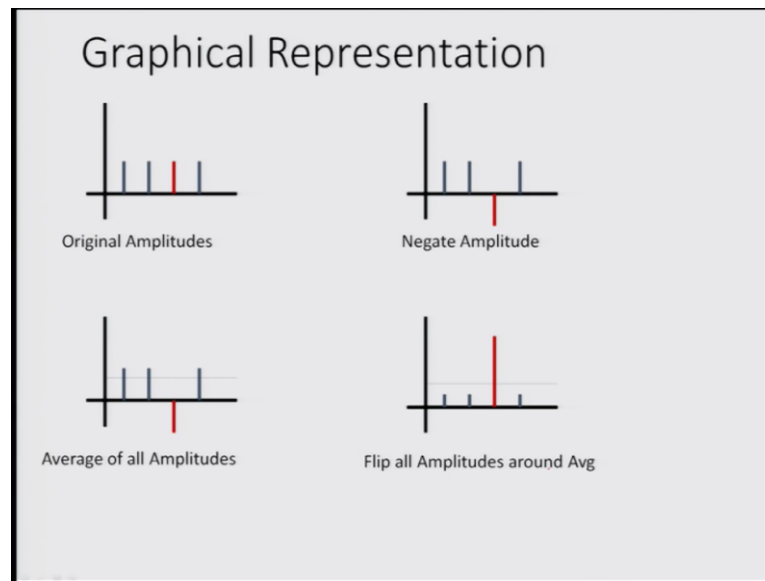
Grover's Search Algorithm

- Search a phone book for a specific number without rearranging the numbers.
- Idea: magnify amplitude of the "chosen" number:
 - Flip the amplitude of the selected item and rotate all amplitudes around the average
 - Repeat this until the selected item's probability of being read is greater than $1/2$

In order to do something more interesting, we would like to use one of the algorithms which help us in getting forward with ideas of computation and one of the major ones as we have discussed is the Grover's search algorithm, which is in polynomial time whereas, the one in Shor's algorithm is in exponential time; however, the Grover's algorithm has the advantage of wider applicability because it is looking for research.

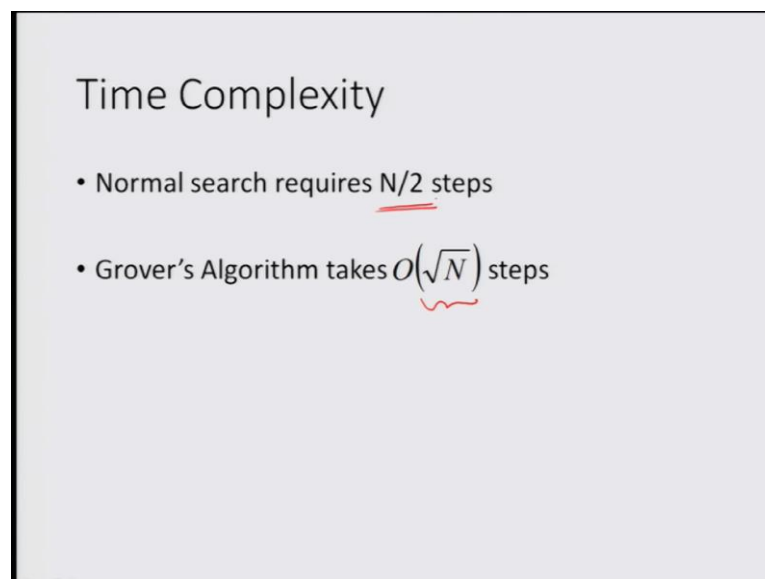
So, it is analogy is always given with respect to searching in unsorted set of data for example a phone book, to find a specific number without rearranging. So, the ideas always have been to magnify the amplitude of the chosen number, and always we use the concept that there is an oracle which knows the solution. So, you flip the amplitudes of the selected items and rotate all the amplitudes around the average and repeat this until the selected items probability of being read is greater than half so that it can be observed.

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So, in terms of graphical representation, this is what we have done earlier at once we get a marked system basically can go through the flip and then average them and then flip all the amplitudes around the average to get the mark state amplified.

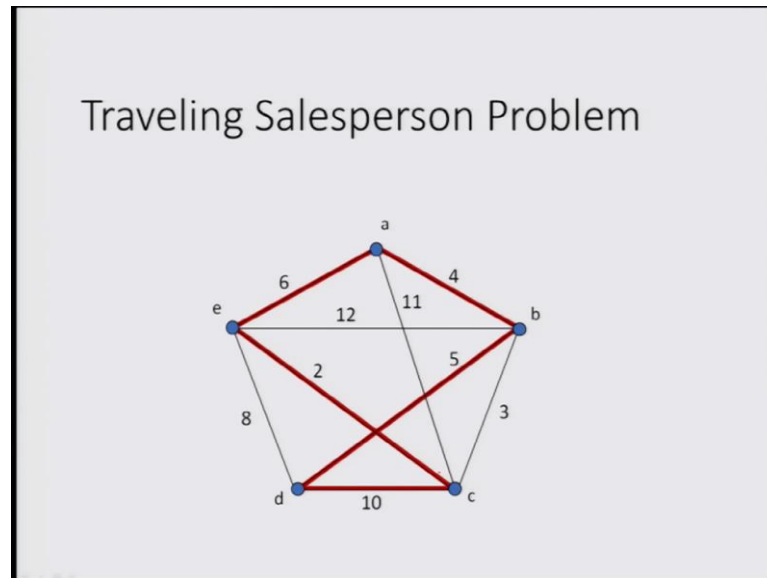
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The time complexity as i mentioned it is in terms of square root of N whereas; in terms

of a normal classical surge the minimum number on an average that you require is an N by 2. So, there is a large in hands men when we go to Grover's algorithm.

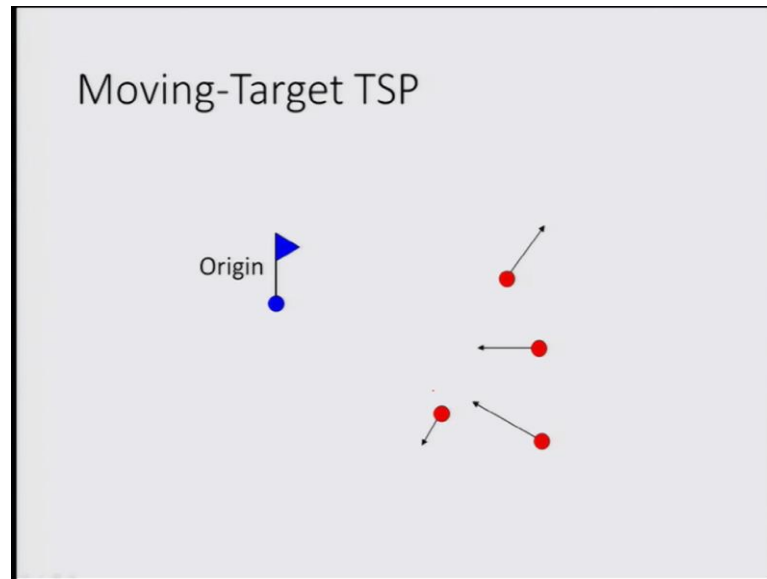
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Now, we would like to actually extend this problem to the traveling salesmen problem, that is because the principle of a traveling salesmen problem is that they require going through the different paths with different levels and the difficulty is that it is not possible to go through the search in this particular case, in a simple polynomial structure as it is possible for a classical computer. So, here is an example of a traveling salesman problem, where the a b c d e are the vertices or the points into which these traveling salesman is suppose to go that individual can take different paths and that is roughly the basic idea behind this problem to start with and they can have different weightage factors depending on how many times a particular path is being traveled versus the other.

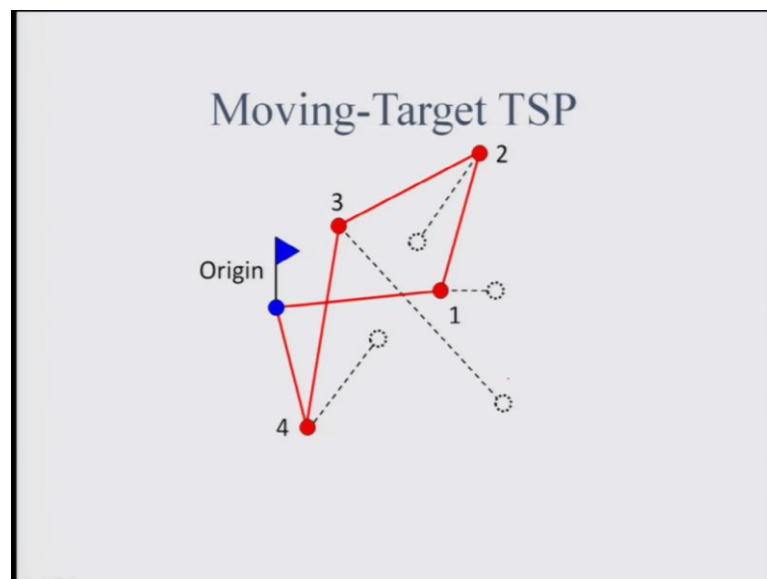
So, here is an example of a path which is being shown here; where this particular path route can be taken to go to all the 5 points that we have discussed.

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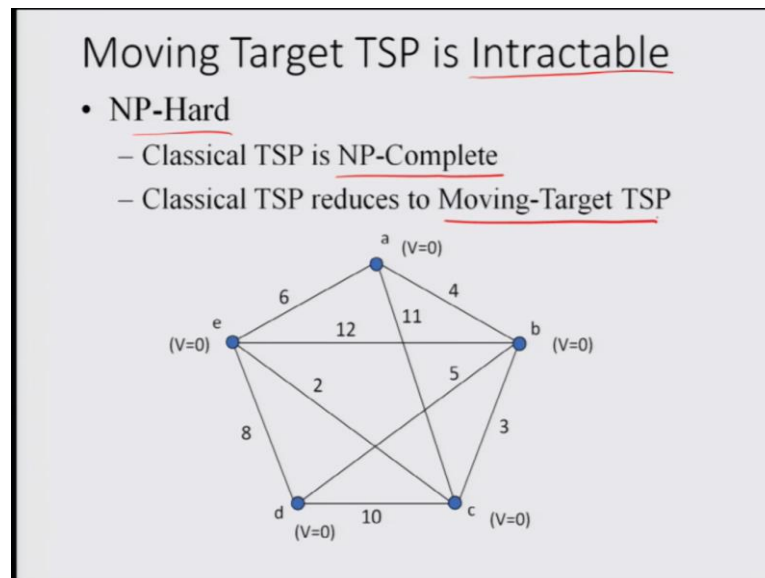
So, this is sort of like a moving target traveling salesman that we just discussed that the target itself is moving, so that you can do a traveling salesman moving target point to be problem. So, we have this origin from where it starts and we have the particles or the points move with respect to the origin. So, these two are moving away whereas, the other 2 are moving closer to the origin and while this happens as you can see here.

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We define this problem as the moving target traveling salesman problem and depending on how they move we have this initial and the different positions as we have defined here. So, this is the basic idea behind this moving target traveling salesman problem.

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So, it is a very difficult problem because it is an intractable problem, it is non determinate polynomial hard; because the classical traveling salesman problem which is generally without the moving target is a NP complete problem whereas, the classical TSP can be reduced to a moving target traveling salesman problem TSP, under this regime where it is a NP hard problems.

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The slide is titled "NP-Complete" and is underlined. It lists two versions of the problem:

- Contained in NP:
 1. Decision version: \exists path with time $< T$?
 - Non-deterministically travel all paths. If one exists with time $< T$, return TRUE. Else, return FALSE
 2. Optimization version: what is min-time path?
 - Upper-bound T with initial random path. Then, binary search the range by testing $T/2$, $T/4$, etc. to find optimal the minimum-time path

So, by giving some velocity to each of them we can get this. So, the non determinant polynomial complete set means that it is contained in non determinant polynomial kind of principles, and the decision version is based on the tree path with time which is less than the time that it takes, non deterministically travel all the paths if one exists with time less than our time T , return true else return false.

So, this is one option this is contained in both of them are contained in our the non determinant polynomial version; the other version is the optimization version, which is the what is the minimum time path that is taken where the upper bound up time with initial random path then binary search the range by testing T by $2T$ by 4 etcetera to find the optimal minimum time path. So, this is a NP complete problem in to which we are trying to see how the search is going to work or not.

So, in the classical sense it is a very difficult problem because whenever this is necessary it needs to be able to visit each and every element of the path which means that each of these would take that many time travel paths and that is why it is a very a non determinate polynomial kind of a complete path that is necessary to be taken classically.

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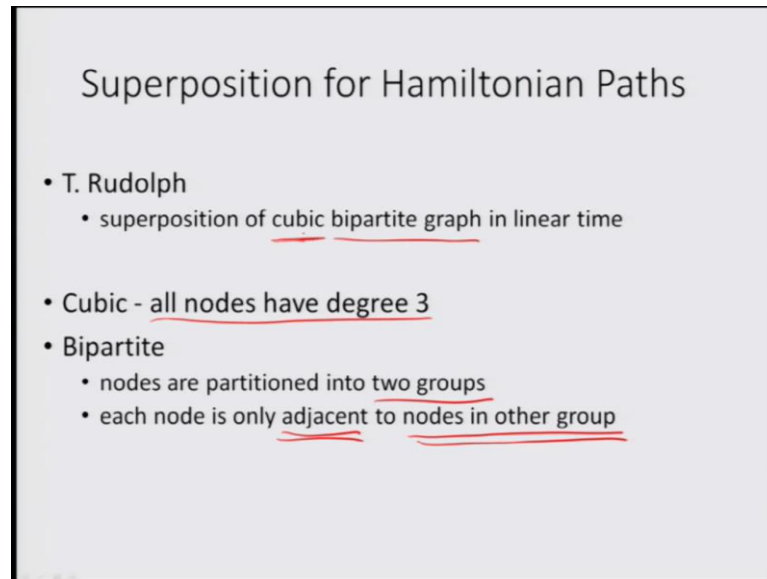
Quantum Computing Solution

- Step 1 - Traverse every possible path
- Step 2 - Search through paths superposition to find a shortest path

In the quantum computing case; however, it is possible to traverse every possible path, why using some tricks of quantum computing that will be shown and then once that is possible, then we can have a search through all the paths superposition to find the shortest route.

So, this key element of superposition which exists in the quantum computing way of looking into this problem enables to take advantage of superposition of the different paths once they are all possible to be traversed.

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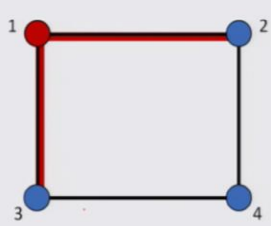
Superposition for Hamiltonian Paths

- T. Rudolph
 - superposition of cubic bipartite graph in linear time
- Cubic - all nodes have degree 3
- Bipartite
 - nodes are partitioned into two groups
 - each node is only adjacent to nodes in other group

His was a problem which was initially (Refer Time: 13:52) out by Rudolph by utilization of superposition of cubic bipartite graph in linear time, in terms of cubic means the all the nodes have degree 3, bipartite means the nodes are partitioned into 2 groups each node is only adjacent to nodes in other group. So, this is the advantage of making this particular approach where it was possible to come up with a cubic bipartite graph in linear time by utilizing this principle.

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Example



$|1000\rangle|1000\rangle|0000\rangle|0000\rangle|0000\rangle$

$|1000\rangle|1\rangle$

$|1100\rangle|1\rangle|2\rangle + |1010\rangle|1\rangle|3\rangle$


$|0100\rangle|1\rangle|2\rangle|1\rangle + |1101\rangle|1\rangle|2\rangle|4\rangle + |0010\rangle|1\rangle|3\rangle|1\rangle + |1011\rangle|1\rangle|3\rangle|4\rangle$

$|0000\rangle|1\rangle|2\rangle|1\rangle|2\rangle + |0110\rangle|1\rangle|2\rangle|1\rangle|3\rangle + |1001\rangle|1\rangle|2\rangle|4\rangle|2\rangle + |1111\rangle|1\rangle|2\rangle|4\rangle|3\rangle +$
 $|0110\rangle|1\rangle|3\rangle|1\rangle|2\rangle + |0000\rangle|1\rangle|3\rangle|1\rangle|3\rangle + |1111\rangle|1\rangle|3\rangle|4\rangle|2\rangle + |1001\rangle|1\rangle|3\rangle|4\rangle|3\rangle$

So, here is an example of this problem, we take this same condition of a bipartite cubic graph in which we will be using the 4 qubits, such that they are going to come in a set, so that they can interact with the first part and then can get superimposed into the 2 different sets; one set is between 1 end 2 and 1 end 3 and the other one would then be put up with the other 2 sets and so the superposition grows as we have shown here.

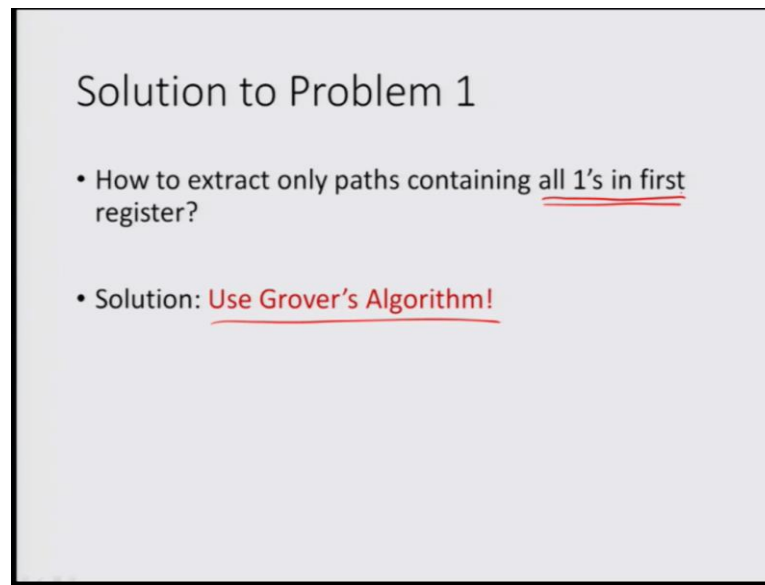
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Potential Problems

- Problem 1:
 - Extract the Hamiltonian paths
- Problem 2:
 - Find cycles, not paths
- Problem 3:
 - Only works for cubic graphs 

Now, the potential problem in these cases is that the extracting the Hamiltonian path and the second problem would be finding the cycle but not the path, and the actual fact of these kind of a graph theoretical approach is that only works for cubic graphs.

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Solution to Problem 1

- How to extract only paths containing all 1's in first register?
- Solution: Use Grover's Algorithm!

So, in terms of solution to the first problem of extracting the Hamiltonian path; only the paths containing all ones in the first register is the question which we. So, in that case we can use the Grover's algorithm, so the first part where we are only going to focus on only the ones in the first register we can utilize the Grover's algorithm.

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Solution to Problem 2

- Use black box for Hamiltonian paths to solve for Hamiltonian cycles?
- Solution:

The diagram illustrates the solution to Problem 2 through three stages of graph construction. In the first stage, a graph with 4 nodes (one on the left, three on the right) and 3 edges is shown. In the second stage, the graph is expanded to 5 nodes (one on the left, four on the right) with 6 edges. In the third stage, the graph is further expanded to 6 nodes (two on the left, four on the right) with 9 edges. The nodes on the right are grouped by a green oval in each stage.

For the second part we can use the black box for Hamiltonian paths to solve for Hamiltonian cycles, and that corresponds to the graph theoretic approach of Hamiltonian paths.

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Solution to Problem 3

- Problem 3: non-cubic graphs
- Solution:
 - Make all nodes have the same degree
 - Degree must be a power of 2
 - Algorithm when all nodes have degree 2^i

And finally, for non cubic graphs, we can make all nodes have the same degree; where in

the degree must be a power of 2 and the algorithm when all nodes have degree 2 to the power i.

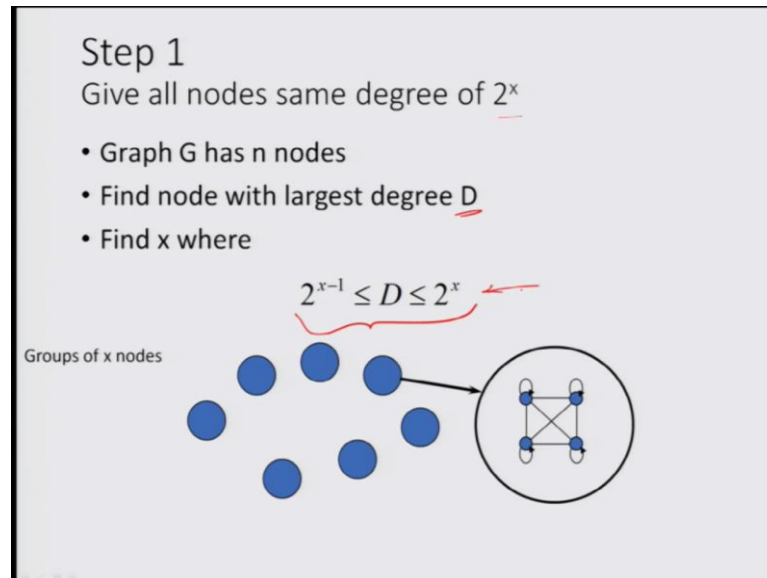
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Step 1
Give all nodes same degree of 2^x

- Graph G has n nodes
- Find node with largest degree D
- Find x where

$$2^{x-1} \leq D \leq 2^x$$

Groups of x nodes

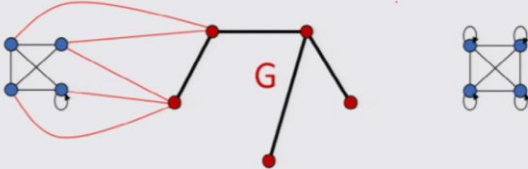


So, in steps one we can give all nodes same degree of 2^x the graph G has n nodes, we find the nodes with the largest degree D and we find a value x where the node degree lies in between the 2 possibilities. So, this is essentially how it looks, we have situation which is of this particular kind in this format; where in we are making the groups of x nodes of the path which can be then mapped into this set and we can try to find out how these nodes can be contain within this set.

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Step 1 (continued)

- Go through the graph G node by node, and go through the new nodes set by set:

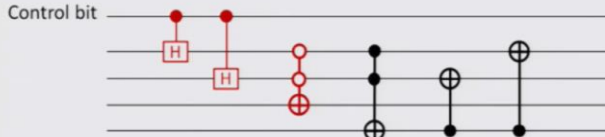


So, we go through the graph G node by node and go through the new nodes set by set and what we get is a set where we can put them together in this kind of a path, and link them by using this particular principle.

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Algorithm

- Quantum transition for nodes with 2^x degree:



$$|0000\rangle \quad \frac{1}{2}|0000\rangle + \frac{1}{2}|1000\rangle$$

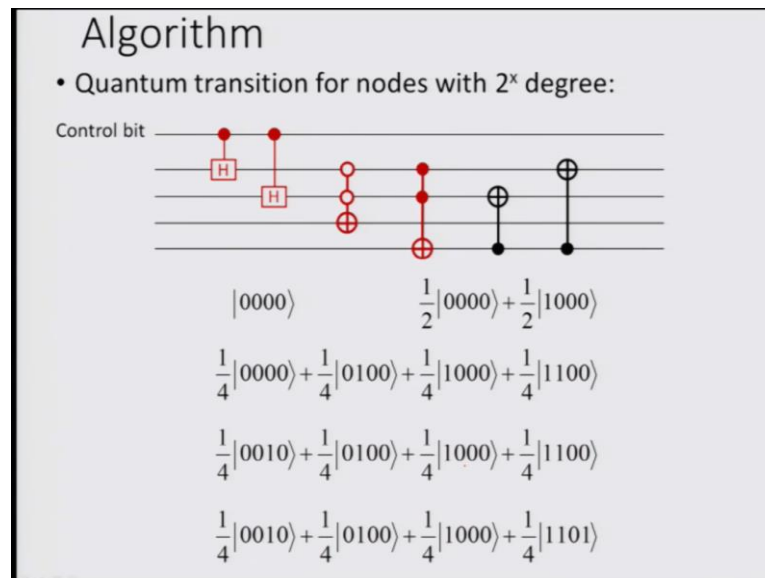
$$\frac{1}{4}|0000\rangle + \frac{1}{4}|0100\rangle + \frac{1}{4}|1000\rangle + \frac{1}{4}|1100\rangle$$

$$\frac{1}{4}|0010\rangle + \frac{1}{4}|0100\rangle + \frac{1}{4}|1000\rangle + \frac{1}{4}|1100\rangle$$

So, the algorithm which requires this quantum transition for nodes with 2 to the power x

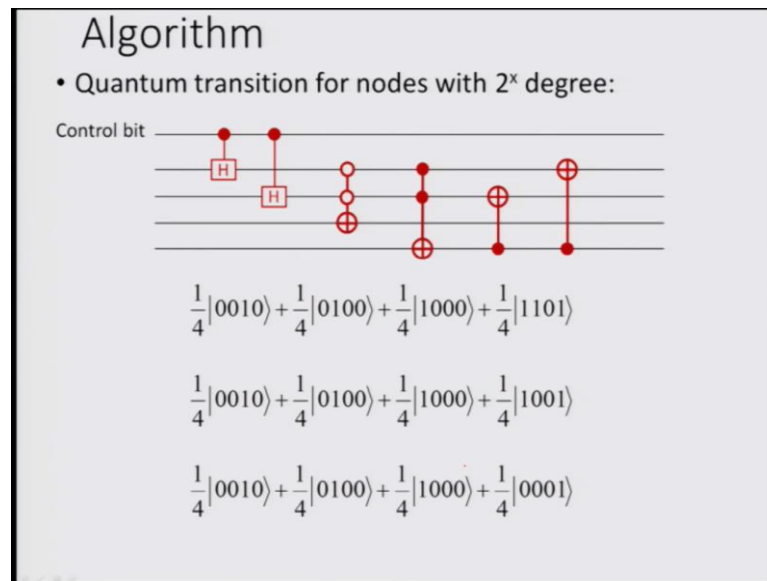
degree, would be having of this format where we have the control bit coming. If it is all zeros then it essentially just as a mixing of 2 states whereas, if goes through the other sets then it will be going through this particular set of operations.

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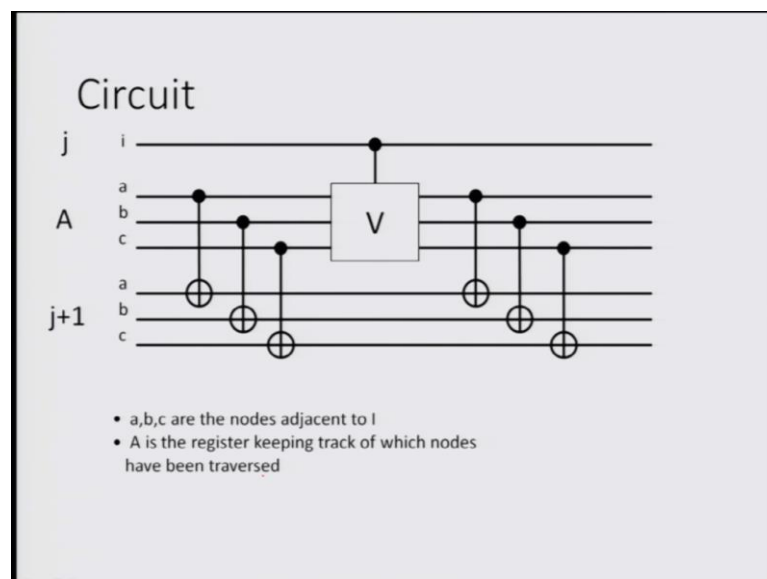
So, the first operation when the control bit comes, it is going through a Hadamard. So, that is how the first Hadamard works, the next one essentially takes another Hadamard of the 2 and then we are putting in a control naught on top of that.

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So, the final one is another set of the control naught and here we are then going back to the set, where we start the other control naught set. And then finally, we get to the sets that we are interested in.

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So, here is the circuit that we get here, it goes through that many elements that we are

going by and it is in iterative (Refer Time: 18:55) a b c are the nodes adjacent to the input, a is the register keeping track of which nodes have been transversed and in this way all the nodes are being covered.

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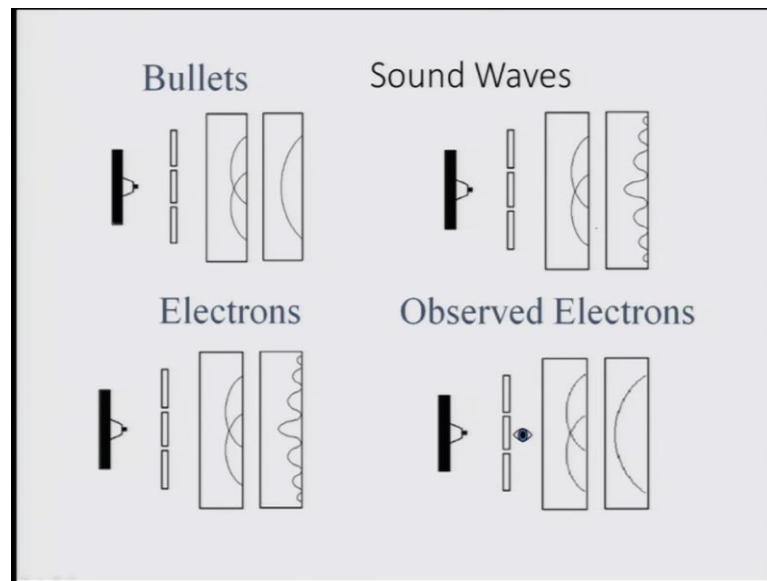
Finding the Minimum

- Measure the lengths register (M)
- Create superposition again
- Now search for all paths $< M$
- On average, do this $\log(k)$ times
 - k is the number of items in the superposition



Once that is done, the minimum is being found by measuring the lengths register M we create a superposition again. Now we search for all paths such that it is less than M on an average we have to do this log of k times and k is the number of items in the superposition. So, this is how it looks we go through iteration one, then in the second time make the flip and so the point about the average keeps on moving. And then finally, we are able to go through this entire step. So, we can do this on an average log of k times so that we can get the number of items in this super position.

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So, what we have understood here is the same principle that we did at the very beginning where we said that we started off with the idea of particles and electrons which have quantum system have the properties of wave like the sound waves, but when observed they behave like particles like the bullets that is what we did.

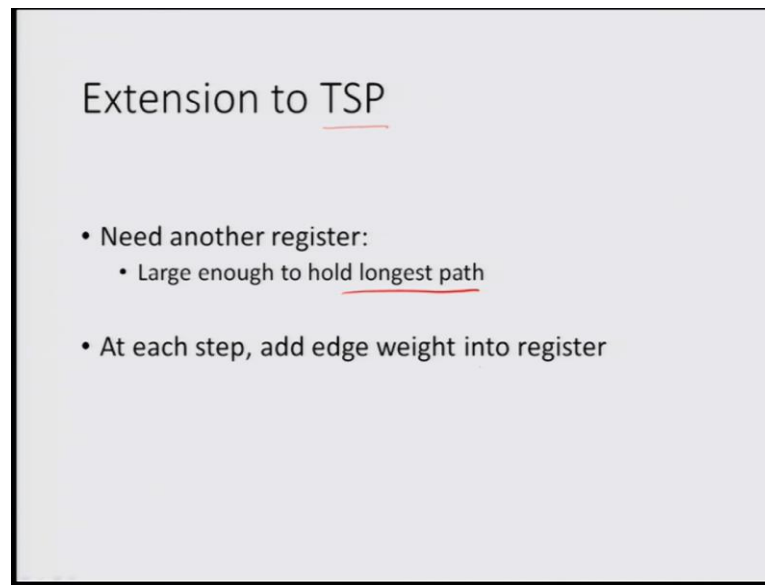
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Observations

- Algorithm works for all graphs
- May double # of nodes
- Takes $O(n)$ steps
- Search first register for all 1's
- Added nodes do not affect solution

So, the algorithm works well for all graphs, it may double number of nodes, but it takes order n steps; when we search the first register for all 1's and the added nodes do not affect the solution. So, these are the key observations for this operation.

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Extension to TSP

- Need another register:
 - Large enough to hold longest path
- At each step, add edge weight into register

Now, this can be extended to the overall traveling salesman problem where we need another register large enough to hold the longest path and at each step add edge weight into the register.

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Iteration


- All paths of length n & their weights
- Run algorithm for Hamiltonian cycles
 - Look for all 1's in the first register
- Superposition of all Hamiltonian cycles
- Grover's algorithm on sum register finds min

All the paths of length n and their weights would run an algorithm for Hamiltonian cycles, and we will look for ones in the first register, superposition of all the Hamiltonian cycles and then the Grover's algorithm on some register finds the minimum.

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Extension to Moving-Target TSP

- Moving Target TSP
 - Each node has a velocity
 - Find the minimum-weight round trip



The diagram shows two blue nodes, each with two velocity vectors. The left node has vectors labeled v_{2x} and v_{2y} . The right node has vectors labeled v_{1x} and v_{1y} . A red dot is positioned between the two nodes, representing a target node.

So, now after having seen this how it works on regular TSP, it can be then extended to

the moving target TSP. In this moving target TSP each node has a velocity; we find the minimum weight a round trip for each of them.

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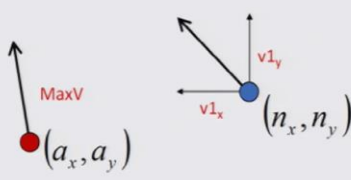
Moving-Target TSP Solution

- Add a time register
- Track the total time elapsed so far
- Each step: calculate time to reach next node

$$v_x t + n_x = v_x t + a_x$$
$$v_y t + n_y = v_y t + a_y$$
$$v_x^2 + v_y^2 = MaxV^2$$

Unknowns:

v_x	v_y	t
-------	-------	-----



So, we add a time register; track the total time elapsed so far for each of these motions, each step would calculate the time to reach the next node as the motion occurs and the unknowns for us are the velocity along this direction V_x V_y and the time.

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Determining the Optimal Path

- Add time to reach next node to total sum
- Find the minimum, similar to TSP
- Added time complexity is linear

So, in order to determine the optimal path, need to add time to reach the next node to the total sum; need to find the minimum which is similar to the TSP problem that we just did before and we need we have an added time complexity is which is linear the added time complexity. In this case is linear because of the velocity component.

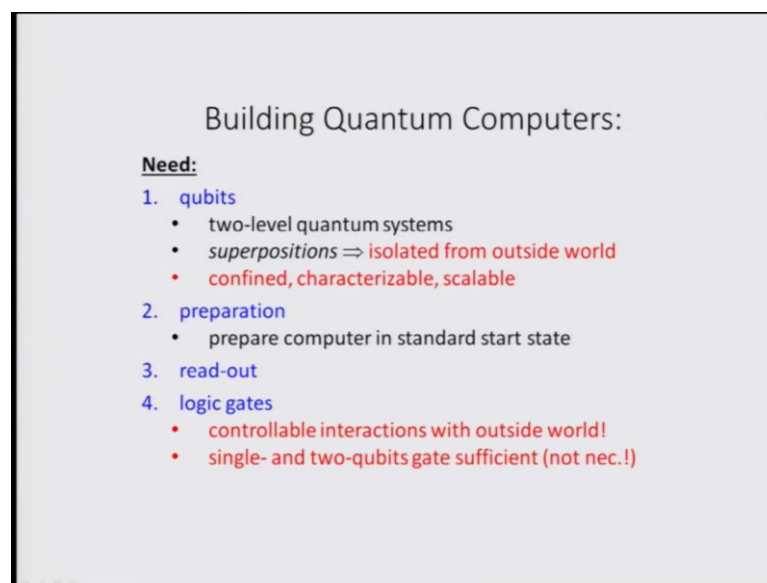
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Summary

- Extended Hamiltonian path algorithm for cubic bipartite graphs [Rudolph's]
- For TSP and Moving-Target TSP, paths superposition can be obtained in linear time
- Grover's search algorithm works in time SQRT of # of objects in superposition
- 2ⁿ different paths: total time is O(2^{n/2})

So, in summary what we have shown in this particular approach of Rudolph is that the; have extended the Hamiltonian path algorithm for cubic bi parted graphs, for traveling salesman problem and for moving target traveling salesman problem, paths superposition can be obtained in linear time. The Grover search algorithm works in square root of number of objects in superposition and there are 2^n different paths. So, the total time is order $2^{n/2}$ which is still in polynomial time.

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Building Quantum Computers:

Need:

1. qubits
 - two-level quantum systems
 - *superpositions* \Rightarrow *isolated from outside world*
 - *confined, characterizable, scalable*
2. preparation
 - prepare computer in standard start state
3. read-out
4. logic gates
 - *controllable interactions with outside world!*
 - *single- and two-qubits gate sufficient (not nec.!)*

And therefore, this has a benefit over the way how algorithms can be applied to non determinate polynomials and their principles.

We will also look at another kind of problem in this context which is related to traveling salesman problem in a slightly different way. But generally at this point this idea the fact that we can search an appropriate path for the different trajectories which are involved in traveling salesman are very important for making progress in terms of algorithm development as well as application of these algorithm developments to problems which are quite difficult to be taken care in terms of classical computing.

So, all the non determinate polynomial problems have been targeted and attempted through quantum computing by using these kinds of principles. So, may be if time

permits I would actually do one more of this kind of problem in the next class.

Thank you.