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Quantum Walks with Time-Dependent Hamiltonians
and their application to the spatial search problem on graph

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Abstract

In this thesis we study the properties of quantum walks with time dependent hamiltonian, focusing in particular on the application to the quantum search problem on graph. We compare the time independent and the time dependent approach for two graph topologies, the circular and the complete graph, which represent respectively the worst and best case scenario for the known quantum search. We also investigate the role of the function that regulates the time-dependance of the hamiltonian in the time scaling at which the solution is found. Lastly we exploit the consequences of the adiabatic theorem to study the localization properties of the time-dependent approach.

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Chapter 1

Preliminaries

In this chapter we present the basic theoretical knowledge necessary to understand this thesis. We begin by introducing graph theory, random walks and quantum walks. We then discuss the quantum search problem firstly introduced by Grover and the quantum walks implementation for the unstructured search by Childs and Goldstone. Then we present the adiabatic theorem and its application for computation with adiabatic evolution. Lastly we look at the differences between the quantum walks approach and the adiabatic evolution approach by Ronald and Cerf, which constitutes the basis from which our work is carried on.

1.1. Introduction to graph theory

A graph G is defined as a ordered pair (V, E), where V is a set of vertices and E is a set of edges, which represent the connection between any two pair of vertices. A vertex is usually indicated by the coursive letter v, and the corresponding edge connecting v to w is given by (v, w).

A graph can be characterized by many properties. Throughout our work we will only consider *simple graphs* characterized by being *undirected*, namely the edges E are symmetric, having no self loops such that $(v, v) \notin G$ and having no multiple equivalent edges. Additionally we require the graph to be *connected*, where each vertex can be reached by any other, following a path through the available edges.

It is then interesting to define the *vertex degree* d_j, that represents, given a vertex j, the number of edges that are incident to the vertex j (in the case of an undirected graph the degree does not dependend on the edges incident from or to the selected vertex).

If indeed any two vertices (i, j) are connected by an edge we define them as *adjacent*, and from this we can construct an analytical representation of a graph, given by an N-

dimensional square matrix called *adjacency matrix,* usually referred as A. The adjacency matrix is defined as following [1]:

$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in G \\ 0 & \text{otherwise} \end{cases} \tag{1.1}$$

which represents the connectivity of the graph.

Furthermore, we can introduce a diagonal matrix D that encodes the informations of the vertex degrees for a particular graph G. Calling the N vertices of the graph as $j = 1, 2..N$ the matrix D is defined as:

$$D = diag(d_1, ..., d_N) \tag{1.2}$$

where d_j is the degree of the vertex j. In this particular context a natural operative basis arises, in which one can associate to each ordered vertex of the graph a vector of the standard basis of the N-dimensional vector space.

In order to study the dynamics of the system we introduce a the *Laplacian matrix* L, also known as the *discrete Laplacian operator.* It is defined as

$$L = D - A \tag{1.3}$$

where D is the diagonal degrees matrix and A is the adjacenty matrix. The discrete Laplacian operator is the analog of the continous Laplace operator on discrete domain, and for the finite, undirected, simple and connected graphs that we're going to consider throughout our work, we can charactarize it by the following properties:

- L is symmetric given that both D and A are symmetric

- the sum of all elements over a rom/column equals to zero

- has a null eigenvalue which corresponds to the eigenvector $|\Psi_0\rangle = \frac{1}{\sqrt{N}}(1, 1, ..., 1)$

In the following paragraphs, we give a brief description of the graphs that will be consider througout the work.

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[1] If we had to define the adjacency matrix for a general graph the value of A_{ij} is not necessarily equal to one, but a general a_{ij} since it takes into account the possibilities of self loops and multiple equivalent edges. For the simple graphs consider in this thesis the given definition suffices.

1.1.1 Cycle Graph

A N-dimensional cycle graph $Cy(N)$ is a monodimensional structure with periodic boundary conditions $|N+1\rangle = |N\rangle$. The Laplacian is given by

$$L = 2\sum_{k=1}^{N} |k\rangle\langle k| - \sum_{k=1}^{N-1} |k\rangle\langle k+1| - \sum_{k=2}^{N} |k\rangle\langle k-1| - |N\rangle\langle 1| - |1\rangle\langle N| \qquad (1.4)$$

A pictorial representation of a cycle graph is given in Fig with the corrisponding laplacian matrix.
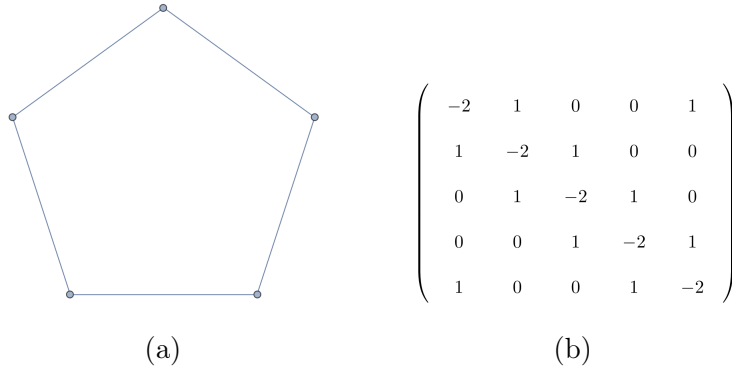

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 1 & -2 \end{pmatrix}$$

(a)   (b)

Figure 1.1: Pictorial representation of a cycle graph with 5 nodes (a), and the matricial representation for the Laplacian of Cy(5)

1.1.2 Complete Graph

A graph with N vertices is said to be complete if every node is adjacent to all the other N-1 nodes, thus representing a finite bidimensional structure. Its Laplacian matrix is given by:

$$L = (N-1)\sum_{j=1}^{N} |j\rangle\langle j| - \sum_{k\neq j} |j\rangle\langle k| \qquad (1.5)$$

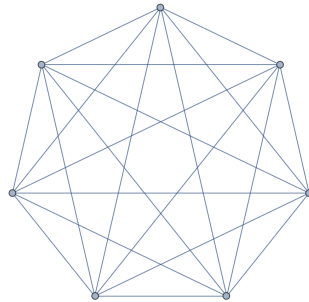A pictorial representation of a complete graph is given in figure. We will refere to this kind of graph with $C(N)$.

Figure 1.2: Pictorial representation of a complete graph with N=7

1.2.   Quantum Walks

The continous time quantum walk (CTQW) is the direct analougue of the classical continous time random walk (CTRW). We begin by considering the classical one, expanding later on the quantum mechanical counterpart.

Let j be a note of a graph G and the initial node, such date the initial state of the system is $|j\rangle$. Then, we denote the transition probability of the walker to go from node j to a node k in a time t with $p_{k,j}(t)$. The state after time t is given by $|j;t\rangle$, such that the overlap with node k is $\langle k|j;t\rangle = p_{j,k}(t)$.

The dynamics resulting in the state $|j;t\rangle$ follows from transition rates per unit time between two nodes. In particular these transition rates are the components of the so-called *transfer matrix T*, namely $T_{ij} = \langle k|T|j\rangle$. If we assume a Markovian process, the following master equation defines the CTRW evolution:

$$\frac{d}{dt}p_{k,j}(t) = \sum_l T_{kl}p_{l,j}(t) \tag{1.6}$$

In the simplest case, where the transitions rates for all edges are equal, the transfer matrix is closely related to the Laplacian matrix through :

$$T = -\gamma L \tag{1.7}$$

where γ is the transition rate. The solution of eq. (1.6), along with the normalization constrains $\sum_{k=1}^{N} p_{k,j}(t) = 1 \ \forall t$, is given by

$$p_{ij}(t) = \langle k|e^{Tt}|j\rangle = \langle k|e^{-\gamma At}|j\rangle \tag{1.8}$$

Turning to quantum mechanics the evolution of any physical system obeys the Schroedinger equation, and QWs represent no exception. The dynamics of the CTQW is governed by a specific Hamiltonian H, such that the Schroedinger equation for the transition *amplitudes* $\alpha_{i,j}(t)$ is given by

$$\frac{d}{dt}\alpha_{i,j}(t) = -i \sum_l H_{k,l}\alpha_{l,j}(t) \tag{1.9}$$

where H is the Hamiltonian of the systemm, and for semplicity we assume $\hbar = 1$. The formal solution of such differential equation is similarly to the CTRW given by

$$\alpha_{l,j}(t) = \langle k|e^{-iHt}|j\rangle \tag{1.10}$$

where e^{-iHt} is the quantum mechanical time-evolution operator. We immediately notice the similar structure of equations (1.6) and (1.10), with the only difference apart from the imaginary unit that the first is a differential equation for transition probabilities

while the latter allows to compute transition amplitudes. The similarity is further pushed bu Farhi and Gutmann in 1998 [1], when they proposed to identify the Hamiltonian H of the system with the negative of the classical transfer matrix T, which as we've seen previously is the Laplacian of the graph [2]:

$$H = -T = L \tag{1.11}$$

Therefore the Laplacian matrix completely determines the evolution of the quantum system as well as the classical scenario.

1.3.   Grover's Quantum Search

In 1997 Lov K. Grover addressed the search problem through a quantum mechanical algorithm [4]. The search problem itself can be formulated in the following way: given an unsorted database containing N items, with only one satisfing a given condition, that one item has to be retrieved. Once an item is examined, it's possible to determine whether it represents the solution or not in just one step. Classically, the most efficient algorithm has to check each and every item in the database individually. If the item checked satisfies the condition the process stops, otherwise it will continue to examine the remaining items until the solution is find. On average, the algorithm will have to check $0.5N$ items before finding the desired one.

On the other hand, Grover's quantum mechanical approach takes advantage of the *superposition* of states in a quantum system, and by having the input and output in such superposition can find the desired objects in $O(\sqrt{N})$ *quantum mechanical steps*, instead of $O(N)$ classical steps. As we shall see later, this quantum mechanicals steps consists of an elementary unitary operation.

Let's look at the algorithm to the quantum search problem more in detail, in particular setting the stage for the search algorithm in terms of an *oracle*, which plays a central role in Grover's search and throughout the entire thesis. Additionally, this allows us to present a very general description of the search procedure, and a geometric way to visualize its action [6].

Suppose we want to search through a search space of N elements, and let's consider the indices of such elements - instead of the actual elements - which clearly are numbers from 0 to $N - 1$. In order to easily store the index in n bits we consider $N = 2^n$, and assume that the particular search problem has M solutions, with $1 \leq M \leq N$. We can now easily represent one instance of the search, i.e. checking if the item satisfies a particular condition, with a function $f(x)$, where x is the index integer ranging from 0 to $N - 1$. The function is such that if x represents the solution to the search problem

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[2] Please note that in this particular scenario the transition amplitude γ is set to one.

$f(x) = 1$, and $f(x) = 0$ if not a solution.

1.4. Search by Quantum Walks

The search problem first introduced by Grover can be reformulated in terms of search based on a continous-time quantum walk on a graph [2].

In order to do so we need to modify the quantum walk hamiltonian of eq. (1.11) so that the vertex $|w\rangle$ is somewhat special. Therefore, an *oracle hamiltonian* is introduced:

$$H_w = -|w\rangle\langle w| \tag{1.12}$$

that has energy zero for all but the vertex $|w\rangle$ for which it has enenergy -1. Therefore the Grover problem becomes finding the ground state of this hamiltonian.

To implement the search we consider the Hamiltonian

$$H = \gamma L + H_w = \gamma L - |w\rangle\langle w| \tag{1.13}$$

where L is the laplacian of the graph G, that as we've seen in section? governs the evolution of the quantum walk.

The quantum search routine works as following:

- we consider the balanced superposition of all possible states, namely

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_j |j\rangle \tag{1.14}$$

- we run the quantum walk for a time t_f and find the corrisponding evolved state using the hamiltonian H

$$|\psi(t_f)\rangle = U(t_f)|s\rangle = \exp\left\{ -\frac{i}{\hbar} H t_f \right\}|s\rangle \tag{1.15}$$

(Note that this evolution is valid only for time-independent hamiltonians.)

- we then measure the state onto the target $|w\rangle$ and find the corrisponding probability

$$p = |\langle w|\psi(t_f)\rangle|^2 \tag{1.16}$$

The objective is to find the optimal value of γ so that the success probability $|\langle w|\psi(t_f)\rangle|^2$ is as close as possible to 1 for the smallest t_f.

We can turn our attention on trying to understand why we should expect this algorithm to give a success probability for some values of γ, t_f. To motivate this we need

to frame the problem in terms of Hamiltonian spectrum. In particular we look at the two extremes, namely $\gamma \to \infty$ and $\gamma \to 0$.

- as $\gamma \to \infty$ the contribution of H_w is somewhat negligible, to the point that the ground state of H is $|s\rangle$[3]

- on the other hand, if $\gamma \to 0$ the contribution of the Laplacian to the overall Hamiltonian H disappears and thus the ground state of H is close to $|w\rangle$

We expect that for some intermediate γ the ground state will transition from $|w\rangle$ to $|s\rangle$ and thus could have substantial overlap on both for a certain value of γ. Additionally, if the first excited states have substantial overlap at such values of γ, then the Hamiltonian will drive transitions between two states, thus rotating the state from $|s\rangle$ to one with substantial overlap with $|w\rangle$, giving the success probability that we previously talked about. In particular this transition will happen in a time that dependes on the Hamiltonian eigenvalues separation between the first and ground state, namely $1/(E_1 - E_0)$.

This is a good description of the algorithm if the dimension of the graph is sufficiently high. However, if we consider a d-dimensional lattice with d independent of N we still see that for a critical value of γ the state switches from the ground state to the first excited state, but for $d < 4$ the $|w\rangle$ state does not have substantial overlap on the ground and fist excited state, thus the algorithm does not work.

Comments on the oracle H_w: The oracle introduce in this fashion is exactly the continous-time version of the reflection R_w in Grover's algorithm [8] because by itself it only evolves the marked vertex $|w\rangle$ by a phase

$$e^{-i|w\rangle\langle w|t}|w\rangle = e^{-it}|w\rangle \tag{1.17}$$

while leaving the other vertices unchanced, thus making this the continous-time version of a yes/no oracle.

1.4.1 Search on Complete Graph

We now look at the complete graph which can be thought of having dimension proportional to N and represents the simples example of the quantum walk search application [2].

We begin by noticing that adding a multiple of the identity matrix to the Laplacian only contributes a global unobservable phase. We add $-NI$ so that:

$$L - NI = N|s\rangle\langle s| \tag{1.18}$$

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[3]Note that regardless of the graph topology considered, $|s\rangle$ is the ground state of the Laplacian, with $L|s\rangle = 0$.

This gives us the following Hamiltonian:

$$H = -\gamma N|s\rangle\langle s| - |w\rangle\langle w| \tag{1.19}$$

In particular we know that this hamiltonian acts non-trivially in a two dimensional subspace spanned by $|s\rangle$ and $|w\rangle$, thus making it stright-forward to compute its spectrum. If we use the $\{|w\rangle, |r\rangle\}$ basis, the hamiltonian can be expressed in the following way:

$$H = \frac{-1}{N}\begin{pmatrix} N+1 & \sqrt{N-1} \\ \sqrt{N-1} & N-1 \end{pmatrix} \tag{1.20}$$

Applying the time-evolution operator to the initial state $|s\rangle$, the system at time t will be

$$|\psi(t)\rangle = e^{it}\begin{pmatrix} \frac{1}{\sqrt{N}}\cos(\frac{t}{\sqrt{N}}) + i\sin(\frac{t}{\sqrt{N}}) \\ \sqrt{\frac{N-1}{N}}\cos(\frac{t}{\sqrt{N}}) \end{pmatrix} \tag{1.21}$$

and for $t = \pi\sqrt{N}/2$ the system reaches a success probability of 1, namely

$$p = \left|\langle w|\psi(t)\rangle\right|^2_{t=\pi\sqrt{N}/2} = \left|\langle w|ie^{it}w\rangle\right|^2 = 1 \tag{1.22}$$

recalling that in the 2-dimensional subspace $w = (0,1)$. Thus the walk rotates the state from $|s\rangle$ to $|w\rangle$ in $O(\sqrt{N})$.

1.5. Search by Adiabatic Evolution

We now address the computation by adiabatic evolution firstly introduced by Farhi et al., that takes advantage of the adiabatic theorem to find the solution of a computational problem [3]. We begin by looking at the *adiabatic theorem* and its implication. Then, an overview of the adiabatic implementation of the algorithm for solving the unstructured search problem is given which has a time scaling of $O(N)$. Lastly, we see how applying the adiabatic theorem *locally* can lead to a time of order $O(\sqrt{N})$ which is optimal.

1.5.1 Adiabatic Theorem

A quantum system evolves according to the Schroedinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle \tag{1.23}$$

and defining the instantaneous eigenstates and eigenvalues of H(t) by

$$H(t)|l;t\rangle = E_l(t)|l;t\rangle \tag{1.24}$$

such that $E_0(t) \geq E_1(t) \geq ... \geq E_{N-1}(t)$.

The adiabatic theorem states that if the gap between the two lowest energy levels, $E_1(t) - E_0(t) > 0$, is stritcly greater than zero then for $T \to \infty$ the probability of being in the ground state is equal to one, namely

$$\lim_{T \to \infty} |\langle l = 0; t = T | \psi(T) \rangle| = 1 \tag{1.25}$$

This means that if the system is chosen to evolve at a slow enough rate, the instantaneous hamiltonian will remain in the ground state throught the evolution. It is useful to consider a smooth one-parameter hamiltonian $H(s)$ such that $s = t/T$, with $t \in [0, T]$ so that $s \in [0, 1]$. Let's now define the energy minimum gap by

$$g_{min} = \min_{0 \leq s \leq 1} (E_1(s) - E_0(s)) \tag{1.26}$$

In addition we can find a time lower bound T^* such that for $T \gg T^*$ the probability is arbitrarily close to 1, in detail

$$T \gg \frac{\varepsilon}{g_{min}^2} \tag{1.27}$$

where

$$\varepsilon = \max_{0 \leq s \leq 1} \left| \left\langle l = 1; s \left| \frac{dH(s)}{dt} \right| l = 0; s \right\rangle \right| \tag{1.28}$$

Let's now discuss how to take advantage of the adiabatic theorem introducing the usual way in which the adiabatic evolution is implemented. It is often presented a problem hamiltonian H_P whose ground state is not so straight forward to find; on the other hand we can prepare the system in abeginning hamiltonian H_B whose ground state is known. The problem hamiltonian encodes the solution of the problem, while the beginning hamiltonian is a tool for easily preparing the state to be evolved. The adiabatic implementation then consists, assuming that the ground state of H_P is unique, in having a time dependent hamiltonian $H(s)$ such that

$$H(s) = (1 - s)H_B + sH_P \tag{1.29}$$

In this way we can prepare for $s = 0$ the system in H_B and let it evolve so that for $s = 1$ it reaches H_P. Thanks to the adiabatic theorem, if it's made to evolve sufficiently slowly we will find ourself in the ground state of the problem hamiltonian, which is exactly the solution.

1.5.2   Global adiabatic evolution

Let's now apply what just seen to the unsorted search problem [7]. As done in Section? we consider an unsorted database of N elements such that $N = 2^n$, so that the elements in this particular basis can be written as $|i\rangle$, with $i = 0, ..., N - 1$. The marked state can

be then denoted as $|w\rangle$, and we begin by considering the initial state as the superposition of all the elements $|i\rangle$:

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N-1} |i\rangle \tag{1.30}$$

With this in mind we design two particular Hamiltonians H_0 and H_w such that $|\psi_0\rangle$ is the ground state of the first while $|w\rangle$ is the ground state of the latter:

$$H_0 = I - |\psi_0\rangle\langle\psi_0| \tag{1.31}$$
$$H_w = I - |w\rangle\langle w| \tag{1.32}$$

The time-dependent Hamiltonian follows from the adiabatic implementation discussed in Section?, where H_0 is the beginning hamiltonian while H_w is the problem hamiltonian. It thus consists in a linear interpolation between H_0 and H_w:

$$H(t) = (1-s)H_0 + sH_w \tag{1.33}$$

where $s = t/T$ is the linear interpolating schedule.

The search routine runs as usual, beginning with preparing the system in the state $|\psi(0)\rangle = |\psi_0\rangle$ and then applying the Hamiltonian $H(t)$ for a time T. We're interested in finding the time-dependent condition such that the system evolves sufficiently slowly, allowing us to find the solution $|w\rangle$ with high probability. First, we determine the quantity $\langle \frac{dH}{dt}\rangle$:

$$\langle\frac{dH}{dt}\rangle_{0,1} = \frac{ds}{dt}\langle\frac{dH}{ds}\rangle_{0,1} = \frac{1}{T}\langle\frac{dH}{ds}\rangle_{0,1} \tag{1.34}$$

We then find the eigenvalues of the Hamiltonian and determine the separation g between the ground state and first excited one, namely E_1 and E_0, as a function of the interpolating schedule s:

$$g = \sqrt{1 - 4\frac{N-1}{N}s(1-s)} \tag{1.35}$$

We're interested in the minimum gap $g_{\min}$ which is found for $s = 1/2$. Additionally we find that $\left|\langle\frac{dH}{ds}\rangle_{0,1}\right| \leq 1$, therefore Eq? becomes:

$$\frac{\left|\langle\frac{dH}{ds}\rangle_{0,1}\right|}{g_{\min}^2} \leq \varepsilon \tag{1.36}$$

1.5.3   Local adiabatic evolution

1.6.   Impossibility of Adiabatic Quantum Walks

In this section we show that an *adiabatic quantum walks* based search algorithm cannot be implemented with the usual Grover's oracle and requires a more sophisticated

structure. This section, based on a paper by Wong et al. [8], sets the basis on which our work takes place.

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