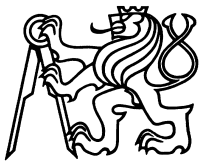

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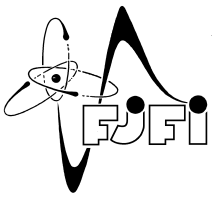

Search and state transfer by means of quantum walk

Vyhledávání a přenos stavu pomocí kvantové procházky

Master's Thesis

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- Zadání práce -

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Prohlášení

Prohlašuji, že jsem svou diplomovou práci vypracoval samostatně a použil jsem pouze podklady (literaturu, software, atd. . . .) uvedené v přiloženém seznamu.

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V Praze dne 5. 5. 2017 .....

Stanislav Skoupý

Název práce:

Vyhledávání a přenos stavu pomocí kvantové procházky

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Obor: Matematická fyzika

Druh práce: Diplomová práce

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Abstrakt: V této práci studujeme vyhledávací algoritmus a algoritmus pro přenos stavu docílený kvantovou procházkou. Je představeno obecné schéma vyhledávacího algoritmu a algoritmu pro přenos stavu. Je ukázáno, že úplného přenosu stavu pomocí kvantové procházky v diskrétním čase s mincí je docíleno na grafu hvězda, úplném bipartitním grafu a úplné grafu s jednou smyčkou na každém vrcholu v $O\left(\sqrt{N}\right)$ krocích. Úplný přenos stavu se také objeví na úplném grafu použitím Szegedyho kvantové procházky a kvantové procházky ve spojitém času. Nakonec dokážeme podmínku optimality vyhledávacího algoritmu pomocí Szegedyho kvantové procházky na regulárním grafu s využitím spektrálních vlastností příslušné stochastické matice.

Klíčová slova: kvantová procházka, vyhledávací algoritmus, přenos stavu

Title:

Search and state transfer by means of quantum walk

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Abstract: In this thesis we study the search algorithm and the state transfer algorithm by means of quantum walk. The general scheme of the search algorithm and the state transfer algorithm is introduced. It is shown that perfect state transfer is achieved for the star graph, the complete bipartite graph and the complete graph with self loop at each vertex using discrete time quantum walk with coins in $O\left(\sqrt{N}\right)$ steps. The perfect state transfer also occurs on the complete graph using the Szegedy's quantum walk and the continuous time quantum walk. At last the we prove the condition of optimality for the Szegedy's quantum walk search algorithm on the regular graphs using the spectral properties of the associated stochastic matrix.

Key words: quantum walk, search algorithm, state transfer

Contents

Introduction

In this thesis we study the search algorithm and state transfer algorithm by means of quantum. Quantum walks are important part of quantum computer science because it has been shown that they can be used as universal tool to implement quantum algorithms. We focus on the quantum walk search algorithm which can be used to speed up the search in unsorted database. Classic search algorithm need $O(N)$ steps in comparison to the quantum search $O\left(\sqrt{N}\right)$ steps. The state transfer algorithm can be use to communication across the quantum network.

In the first Chapter we study the Grover search algorithm and the Grover state transfer algorithm. The Grover search algorithm is not based on the quantum walk but the calculation of the success probability and the number of steps are very similar to the calculation used in the quantum walk search algorithm. In the second Chapter we describe the general scheme of the search algorithm and the state transfer algorithm by means of discrete time quantum walk with coins, Szegedy's discrete time quantum walk and continuous time quantum walk.

In the third Chapter we present the graph where the perfect state transfer is achieved in the sense that fidelity of the transfer goes to one. Using the discrete time quantum walk we show that the perfect state occurs at the star graph, the complete bipartite graph and the complete graph with self loop at each vertex. We obtain the perfect state transfer on the complete graph also using the Szegedy's walk state transfer algorithm and the continuous time quantum walk state transfer algorithm.

In the last Chapter we study the search algorithm on a random graphs. We review the work of Chakraborty *et al.* for the continuous time quantum walk on the random graph. They proved that the search algorithm is optimal for *almost all graphs*. In the second part of this Chapter we show that the Szegedy's quantum walk search algorithm is optimal for d-random regular graphs with the high probability.

Chapter 1

Grover search algorithm

In the first part of this chapter we describe the Grover search algorithm which was introduce in [1] by L. Grover. In the second part we modify the algorithm to achieve state transfer. This modification is general in a sense that we use the same modification in quantum walk search algorithm in both discrete and continuous time. The Grover's algorithm is quantum algorithm designed to search in unsorted database. The algorithm operate on quantum register of qubits.

Let us describe the Hilbert space of the quantum register and evolution operator of the algorithm. The basis of qubit register of length n is spanned states $|A_1A_2\dots A_n\rangle$ where $A_k \in \{0,1\}$. The dimension of the register Hilbert space is $N = 2^n$. To simplify the notation we label the states $|A_1A_2\dots A_n\rangle$ as $|j\rangle$ where $A_1A_2\dots A_n$ is binary representation of $j-1$, i.e. $j = \sum_{k=1}^{n} A_k 2^{k-1} + 1$. Then the Hilbert space is spanned by orthonormal basis $\{|j\rangle, j \in \{1,2,\dots,N\}\}$. The fact that algorithm works on quantum register is important for the physical implementation but it does not effect calculation of success probability. Hence, we suppose for following calculation in this chapter that N is any natural number and not just 2^n for some n.

The evolution operator of the search algorithm is composed of two operators which are Grover operator and quantum query. The Grover operator reads

$$\hat{G} = -\hat{I} + 2|\psi\rangle\langle\psi|, \tag{1.1}$$

where $|\psi\rangle$ is equal superposition of all basis states

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |j\rangle. \tag{1.2}$$

For a purpose of the search algorithm we suppose that there is a set of marked basis states which we want to find using the algorithm. Let us label the set and its elements as $\mathcal{M} = \{m_1, m_2, \dots, m_M\}$, where M is the size of $\mathcal{M}$. At each step of the algorithm we apply phase shift by π at the marked states and then the Grover operator. We implement the phase shift by π as quantum query which has a following form

$$\hat{Q} = \hat{I} - 2 \sum_{m_i \in \mathcal{M}} |m_i\rangle\langle m_i|. \tag{1.3}$$

Now we write the evolution operator of the algorithm as follows

$$\hat{U} = \hat{G}\hat{Q}. \tag{1.4}$$

After describing the Hilbert space and the evolution operator of the algorithm we give exact steps of the Grover search algorithm:

1. Initialize the system in equal superposition of basis states

$$|init\rangle = |\psi\rangle. \tag{1.5}$$

2. Apply the evolution operator $\hat{U}$ given by (1.4) T-times.

3. Measure the system.

We have to calculate the number of steps and the probability of success to complete the full definition of the algorithm.

We start the calculation by defining two orthonormal states which read

$$\begin{aligned} |\psi_m\rangle &= \frac{1}{\sqrt{M}} \sum_{m_i \in \mathcal{M}} |m_i\rangle \\ |\psi_1\rangle &= \frac{1}{\sqrt{N-M}} \sum_{j \notin \mathcal{M}} |j\rangle \end{aligned}. \tag{1.6}$$

It is easy to see that these two states span invariant subspace of evolution operator $\hat{U}$

$$\begin{aligned} \hat{U}|\psi_m\rangle &= \frac{N-2M}{N}|\psi_m\rangle - \frac{2\sqrt{M(N-M)}}{N}|\psi_1\rangle \\ \hat{U}|\psi_1\rangle &= \frac{2\sqrt{M(N-M)}}{N}|\psi_m\rangle + \frac{N-2M}{N}|\psi_1\rangle \end{aligned}. \tag{1.7}$$

The initial state of the algorithm also lies in this subspace

$$|init\rangle = \sqrt{\frac{M}{N}}|\psi_m\rangle + \sqrt{\frac{N-M}{N}}|\psi_1\rangle. \tag{1.8}$$

Hence, we analyse the evolution of the system only in this subspace which reduce the dimension and simplify the calculation. We introduce the effective evolution operator that is in the orthonormal basis (1.6) given by 2×2 matrix of the following form

$$U_{eff} = \begin{pmatrix} \frac{N-2M}{N} & \frac{2\sqrt{M(N-M)}}{N} \\ -\frac{2\sqrt{M(N-M)}}{N} & \frac{N-2M}{N} \end{pmatrix}. \tag{1.9}$$

Let us now calculate the spectrum of (1.9). $\hat{U}_{eff}$ has two conjugate eigenvalues

$$\lambda_\pm = e^{\pm i\omega}, \tag{1.10}$$

where eigenphase ω reads

$$\omega = \arccos\left(\frac{N-2M}{N}\right). \tag{1.11}$$

Corresponding eigenvectors are given by

$$|\lambda_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\psi_m\rangle \pm i|\psi_1\rangle\right). \tag{1.12}$$

The initial state in the eigenbasis has a following form

$$|init\rangle = \frac{\sqrt{N-M} + i\sqrt{M}}{\sqrt{2N}}|\lambda_+\rangle + \frac{\sqrt{N-M} - i\sqrt{M}}{\sqrt{2N}}|\lambda_-\rangle. \tag{1.13}$$

Now we calculate the state of the system after T steps as follows

$$\begin{aligned}|\phi(T)\rangle = \hat{U}^T|init\rangle &= \frac{\sqrt{N-M}+i\sqrt{M}}{\sqrt{2N}}e^{i\omega T}|\lambda_+\rangle + \frac{\sqrt{N-M}+i\sqrt{M}}{\sqrt{2N}}e^{-i\omega T}|\lambda_-\rangle \\ &= \frac{\sqrt{N-M}\cos(\omega T)+\sqrt{M}\sin(\omega T)}{\sqrt{N}}|\psi_m\rangle + \frac{\sqrt{M}\cos(\omega T)-\sqrt{N-M}\sin(\omega T)}{\sqrt{N}}|\psi_1\rangle\end{aligned}. \tag{1.14}$$

From (1.14) we calculate the probability of success which is given by

$$p(T) = \sum_{m_i\in\mathcal{M}} |\langle m_i|\phi(T)\rangle|^2 = \frac{\left|\sqrt{N-M}\cos(\omega T)+\sqrt{M}\sin(\omega T)\right|^2}{N}. \tag{1.15}$$

The expression has the highest value for condition

$$\omega T = \arccos\left(-\sqrt{\frac{N-M}{N}}\right). \tag{1.16}$$

Hence the number of steps is the closest integer to the number given by

$$T \approx \frac{\arccos\left(-\sqrt{\frac{N-M}{N}}\right)}{\arccos\left(\frac{N-2M}{N}\right)} \doteq \frac{\pi}{2\sqrt{M}}\sqrt{N} - \frac{1}{2} + O\left(\frac{1}{\sqrt{N}}\right) \tag{1.17}$$

where we use the Taylor expansion for large N. For T given by (1.17) the success probability (1.15) goes to 1 as follows

$$p = 1 - O\left(\frac{1}{N}\right). \tag{1.18}$$

Let us now modify the Grover search algorithm to achieve state transfer between two marked basis states, let us call them sender and receiver. We label the state corresponding to the sender as $|s\rangle$ and the state corresponding to the receiver as $|r\rangle$. We use the same evolution operator (1.4) with query

$$\hat{Q} = \hat{I} - 2|s\rangle\langle s| - 2|r\rangle\langle r|. \tag{1.19}$$

Difference between the search algorithm and the state transfer algorithm is the initial state. In the case of the state transfer algorithm we start with initial state $|s\rangle$. Thus the state transfer algorithm has a following steps:

1. Initialize the system in the state

$$|init\rangle = |s\rangle. \tag{1.20}$$

2. Apply the evolution operator $\hat{U}$ given by (1.4) T-times.

3. Measure the system.

We calculate the number of steps T to achieve the maximum fidelity of the state transfer to the target state $|r\rangle$. We start again by finding invariant subspace of the algorithm. It is easy to see that the invariant

subspace is spanned by the initial and target state and state $|\psi_1\rangle$ given by (1.6) for $M = 2$. The effective evolution operator in basis $\{|s\rangle, |r\rangle, |\psi_1\rangle\}$ is given by 3×3 matrix of the following form

$$U_{eff} = \begin{pmatrix} \frac{N-2}{N} & -\frac{2}{N} & \frac{2\sqrt{N-2}}{N} \\ -\frac{2}{N} & \frac{N-2}{N} & \frac{2\sqrt{N-2}}{N} \\ -\frac{2\sqrt{N-2}}{N} & -\frac{2\sqrt{N-2}}{N} & \frac{N-4}{N} \end{pmatrix}. \tag{1.21}$$

We diagonalize the effective evolution operator to calculate the number of steps T. One eigenvalue λ_0 is equal to 1 and corresponding eigenvector is

$$|\lambda_0\rangle = \frac{1}{\sqrt{2}} \left(|s\rangle - |r\rangle\right). \tag{1.22}$$

The other two conjugate eigenvalues are given by

$$\lambda_\pm = e^{\pm i\omega}, \tag{1.23}$$

where ω has a following form

$$\omega = \arccos\left(\frac{N-4}{N}\right). \tag{1.24}$$

Eigenvalues $\lambda_\pm$ have eigenvectors

$$|\lambda_\pm\rangle = \frac{1}{2} \left(|s\rangle + |r\rangle\right) \pm \frac{i}{\sqrt{2}} |\psi_1\rangle. \tag{1.25}$$

The sender and the receiver states have in the eigenbasis of $\hat{U}_{eff}$ the form

$$\begin{aligned} |s\rangle &= \frac{1}{\sqrt{2}}|\lambda_0\rangle + \frac{1}{2} \left(|\lambda_+\rangle + |\lambda_-\rangle\right) \\ |r\rangle &= -\frac{1}{\sqrt{2}}|\lambda_0\rangle + \frac{1}{2} \left(|\lambda_+\rangle + |\lambda_-\rangle\right) \end{aligned}. \tag{1.26}$$

The state of the system after T steps reads

$$|\phi\left(T\right)\rangle = \hat{U}^T |init\rangle = \frac{1}{\sqrt{2}}|\lambda_0\rangle + \frac{e^{i\omega T}}{2} \left(|\lambda_+\rangle + e^{-2i\omega T}|\lambda_-\rangle\right) \tag{1.27}$$

We see that (1.27) rotate for $\omega T = \pi$ to the state $-|r\rangle$. Hence, we achieve the perfect state transfer if we set the number of steps T as the closest integer to $\frac{\pi}{\omega}$. Using Taylor expansion we estimate T as follows

$$T \approx \frac{\pi}{\arccos\left(\frac{N-4}{N}\right)} \doteq \frac{\pi}{2\sqrt{2}} \sqrt{N} + O\left(\frac{1}{\sqrt{N}}\right). \tag{1.28}$$

We also calculate the fidelity after T of steps of the state transfer. It reads

$$\mathcal{F}\left(T\right) = |\langle r|\phi\left(T\right)\rangle|^2 = \sin^4\left(\frac{\omega T}{2}\right). \tag{1.29}$$

Now if we substitute $T = \frac{\pi}{2\sqrt{2}} \sqrt{N}$ and (1.24) in (1.29) and we use Taylor expansion, we get the estimation of the maximum fidelity as follows

$$\mathcal{F}_{max}(N) = \sin^4\left(\arccos\left(\frac{N-4}{N}\right) \frac{\pi\sqrt{N}}{4\sqrt{2}}\right) \doteq 1 - O\left(\frac{1}{N^2}\right). \tag{1.30}$$

Hence, the perfect state transfer using modified Grover's algorithm is achieved.

Chapter 2

Quantum walk search and state transfer

In this Chapter we describe the three search algorithm on a graph which are based on different quantum walks. We start with discrete time quantum walk with coins, then we present Szegedy's walk algorithms and as the last type of walk we introduce continuous time quantum walk. Furthermore, we present how the quantum walk search algorithm is used for state transfer across the graph for all three cases.

2.1 Discrete quantum walk with coins

Our introduction of discrete time quantum walk algorithms is based on articles [2],[3],[4] and [5]. Before anything else we need to construct Hilbert space $\mathcal{H}_G$ of the graph and the evolution operator $\hat{U}$ of one step of the walk. Let $G = (V, E)$ be a graph, where V is the set of vertices and E is the set of edges. At first we assign to every vertex $v \in V$ the position state $|v\rangle_p$. If the system is in the state $|v\rangle_p$ then the particle is located at the vertex v. For implementation of the discrete time quantum walk we have to add to every vertex so called coin space which directs the evolution of the walk. The basis of the coin space of the vertex v is spanned by states $|w\rangle_c$ for all w where w is the neighbouring vertex of v in the graph, i.e. $\{v, w\} \in E$. Hence, the basis states of the walk Hilbert space have the form

$$|v, w\rangle := |v\rangle_p \otimes |w\rangle_c \tag{2.1}$$

and the whole basis reads

$$\{|v, w\rangle | \forall v, w \in V : \{v, w\} \in E\}. \tag{2.2}$$

Then we implement so called shift operator as follows

$$\hat{S}\,|v, w\rangle := |w, v\rangle. \tag{2.3}$$

Now we can say that if the system of the walk is in the state $|v, w\rangle$ then the particle is located at the vertex v and it will move to vertex w after application of the shift operator $\hat{S}$.

The evolution of the system is trivial if we use only the shift operator $\hat{S}$. The evolution operator $\hat{U}$ of the search algorithm consist of two operators, of the shift operator $\hat{S}$ and so called coin operator $\hat{C}$

$$\hat{U} := \hat{S}\,\hat{C}. \tag{2.4}$$

The main idea of the walk search algorithm is that we use different coin operators on the marked vertex coin space and on the coin spaces of other vertices. In the following chapters we use so called Grover

coin $\hat{G}$ on the vertices which are not marked and on the marked vertices we use only a phase shift by π or the Grover coin and the phase shift by π. The Grover coin reads

$$\hat{G}_v = -\hat{I} + 2|\psi_v\rangle\langle\psi_v| \tag{2.5}$$

where $|\psi_v\rangle$ is equal superposition of all directions of the coin space at the vertex v given by

$$|\psi_v\rangle = \frac{1}{\sqrt{d\,(v)}} \sum_{\substack{w \\ \{v,w\}\in E}} |v, w\rangle, \tag{2.6}$$

where $d\,(v)$ is the degree of the vertex v. The Grover coin is derived from the Grover operator (1.1). Let us have a set of marked vertices $\mathcal{M}$. The coin operator $\hat{C}$ has the form

$$\hat{C} = \sum_{v\in V} \hat{G}_v \hat{P}_v + \sum_{m\in\mathcal{M}} \left(\hat{C}_m - \hat{G}_m\right) \hat{P}_m \tag{2.7}$$

where $\hat{C}_m$ is the coin operator at the marked vertex m and $\hat{P}_v$ is projector on the coin subspace at the vertex v. The projector $\hat{P}_v$ reads

$$\hat{P}_v = \sum_{\substack{w \\ \{v,w\}\in E}} |v, w\rangle\langle v, w|. \tag{2.8}$$

We can now finally describe the general form of the discrete time quantum walk search algorithm. It is composed of following steps:

1. Initialize the system in the superposition of basis states

$$|init\rangle = \frac{1}{\sqrt{2|E|}} \sum_{v\in V} \sum_{\substack{w \\ \{v,w\}\in E}} |v, w\rangle. \tag{2.9}$$

2. Apply the evolution operator $\hat{U}$ given by (2.4) T-times.

3. Measure the system.

The complexity of algorithm T and the probability of succes p depend on the structure and the size of the graph. It was proved that the general quantum search algorithm cannot perform better then $\Omega\left(\sqrt{N}\right)$, where $N = |V|$ is the size of the graph [6]. Hence, we call the search algorithm on the graph G optimal if $T = O\left(\sqrt{N}\right)$ holds true.

The state transfer algorithm can be obtain from the search algorithm by simple modification. We have now two marked vertices, let us called them the sender and the receiver and we label these vertices by s and r respectively. Because we have two marked vertices we have to modify the coin operator, it is given by

$$\hat{C} = \sum_{v\in V} \hat{G}_v \hat{P}_v + \left(\hat{C}_s - \hat{G}_s\right) \hat{P}_s + \left(\hat{C}_r - \hat{G}_r\right) \hat{P}_r. \tag{2.10}$$

Then state transfer algorithm has the following steps:

1. Initialize the system in the superposition of all directions at the sender vertex

$$|init\rangle = \frac{1}{\sqrt{d\,(s)}} \sum_{\substack{w \\ \{s,w\}\in E}} |s, w\rangle. \tag{2.11}$$

2. Apply the evolution operator $\hat{U}$ given by (2.4) T-times.

3. Measure the system. The particle moves from the sender to the receiver with fidelity $\mathcal{F}$.

The complexity of algorithm T and the fidelity $\mathcal{F}$ depend again on the structure and the size of the graph. We say that the algorithm achieves the perfect state transfer if the fidelity is close to 1, i.e. the particle moves from the sender to the receiver.

2.2 Szegedy's walk

In this chapter we present different model of the quantum walks, so called Szegedy's walk. This model is a coinless discrete time quantum walk where the evolution operator is composed of reflection operators on the bipartite graph. We present two models of Szegedy's search algorithm. The first was introduced in [7] by Szegedy and it is based on modification of stochastic matrix P associated with graph G which also modifies the reflection operators. The second was presented in [8] by Santos who adds quantum quarry to the unperturbed Szegedy's walk.

We describe at first the Hilbert space of the walk and the reflection operators and then we present the evolution operator for both cases. Let us have the graph $G = (V, E)$ where we label the vertices from 1 to N, i.e. $V = \{1 \dots N\}$. We construct the new bipartite graph G' with $2N$ vertices from the original G by copying the original graph G, removing all edges in both graphs and adding new edges so that vertex v from original graph is connected to the vertex w' in the copy only if in the original graph vertices v and w were connected. The Hilbert space of Szegedy's walk is a tensor product of two N-dimensional Hilbert spaces and its basis is spanned by vectors of the following form

$$|j,k\rangle = |j\rangle \otimes |k\rangle,\ j,k \in \{1 \dots N\} \tag{2.12}$$

for $j,k \in \{1 \dots N\}$ where j denotes the position in the original graph and k denotes position in the copy. The reflection operators that compose the evolution operator are reflection around subspaces spanned by states $|\Phi_j\rangle$ and $|\Psi_k\rangle$. These operators read

$$\begin{aligned} \hat{\mathcal{R}}_A &= 2\sum_{j=1}^{N} |\Phi_j\rangle\langle\Phi_j| - I \\ \hat{\mathcal{R}}_B &= 2\sum_{k=1}^{N} |\Psi_k\rangle\langle\Psi_k| - I \end{aligned} \tag{2.13}$$

where $|\Phi_j\rangle$ and $|\Psi_k\rangle$ are given by

$$\begin{aligned} |\Phi_j\rangle &= |j\rangle \otimes \left(\sum_{k=1}^{N} \sqrt{P_{jk}}|k\rangle\right) \\ |\Psi_k\rangle &= \left(\sum_{j=1}^{N} \sqrt{P_{kj}}|j\rangle\right) \otimes |k\rangle \end{aligned}. \tag{2.14}$$

The numbers P_{jk} are elements of stochastic matrix associated to the graph G. The unperturbed evolution operator has the form

$$U = \hat{\mathcal{R}}_B \hat{\mathcal{R}}_A. \tag{2.15}$$

The search algorithm used in [7] uses reflection operators with modified stochastic matrix P' which elements are given by

$$P'_{jk} = \begin{cases} P_{jk} & j \notin \mathcal{M} \\ \delta_{jk} & j \in \mathcal{M} \end{cases} \tag{2.16}$$

where P_{jk} are elements of the original stochastic matrix of graph G, δ_{jk} is Kronecker delta and $\mathcal{M}$ is the set of marked vertices. The evolution operator $\hat{U}'$ of the search algorithm uses the reflection operator $\hat{\mathcal{R}}'_A$ and $\hat{\mathcal{R}}'_B$ around states $|\Phi'_j\rangle$ and $|\Psi'_j\rangle$ where we use P' instead of P.

Second approach uses operator composed of quantum quarries which reads

$$\hat{\mathcal{R}}_M = \left(\hat{I} - 2 \sum_{m \in \mathcal{M}} |m\rangle\langle m| \right) \otimes \hat{I} \tag{2.17}$$

and it is applyed before every step of unpertube walk. Thus we get the evolution operator $\hat{U}''$ according to [8] reads which reads

$$\hat{U}'' = \hat{\mathcal{R}}_B \hat{\mathcal{R}}_A \hat{\mathcal{R}}_M. \tag{2.18}$$

The Szegedy algorithms has the following steps:

1. Initialize the system in the superposition of all basis states corresponding to edges of the graph

$$|init\rangle = \frac{1}{\sqrt{N}} \sum_{j,k=1}^{N} \sqrt{P_{j,k}} |j,k\rangle. \tag{2.19}$$

2. Apply the evolution operator $\hat{U}'$ (or $\hat{U}''$ in the second case) T-times.

3. Measure the system.

The number of steps T and the probability of success depend on the structure and the size of the graph and also on the choice of the evolution operator.

Moving on to the state transfer algorithm, we have as before the sender and the receiver vertex. The algorithm goes as follows:

1. Initialize the system in the state corresponding to the sender vertex $|init\rangle = |\Phi'_s\rangle$ (or $|\Phi_s\rangle$ in the second case).

2. Apply the evolution operator $\hat{U}'$ (or $\hat{U}''$ in the second case) T-times.

3. Measure the system.

The number of steps T and the probability of success depend again on the structure and the size of the graph and also on the choice of the evolution operator.

2.3 Continuous time quantum walk

Last but not least, we describe the continuous time quantum walk search and state transfer algorithm. This section is based on articles [2] and [9]. The Hilbert space is simpler than for discrete time quantum

walks. The Hilbert space of graph G is spanned by states $\{|v\rangle, \forall v \in V\}$ which form the orthonormal basis. The evolution of the system is driven by the Schrödinger equation

$$i\hbar\partial_t|\phi(t)\rangle = \hat{H}|\phi(t)\rangle, \tag{2.20}$$

where $\hat{H}$ is Hamiltonian of the system. Since we use the Hamiltonian which is time independent we can express the evolution operator as follows

$$\hat{U}(t) = e^{-i\hat{H}t} \tag{2.21}$$

where we set $\hbar = 1$ from now on.

In the case of the search algorithm the Hamiltonian reads

$$\hat{H} = -\gamma\hat{A}_G - \sum_{m\in\mathcal{M}} |m\rangle\langle m| \tag{2.22}$$

where $\mathcal{M}$ is the set of the marked vertices, $\hat{A}_G$ is given by adjacency matrix A_G of the graph G and γ is a real number. The continuous time quantum walk search algorithm has the following steps:

1. Initialize the system in the superposition of basis states

$$|init\rangle = \frac{1}{\sqrt{|V|}}\sum_{v\in V}|v\rangle. \tag{2.23}$$

2. Let the system evolve with Hamiltonian (2.22) for time T.

3. Measure the system.

The probability of success p and the time T depend on the structure and the size of the graph G.

In the case of the state transfer algorithm the Hamiltonian reads

$$\hat{H} = -\gamma\hat{A}_G - |s\rangle\langle s| - |r\rangle\langle r| \tag{2.24}$$

where $|s\rangle$ is the sender vertex and $|r\rangle$ is the sender vertex. The state transfer algorithm has the following steps:

1. Initialize the system in the state $|init\rangle = |s\rangle$.

2. Let the system evolve with Hamiltonian (2.24) for time T.

3. Measure the system.

The fidelity of the state transfer $\mathcal{F}$ and the time T depend on the structure and the size of the graph G.

Chapter 3

Perfect state transfer

In this Chapter we present some examples of graphs where the perfect state transfer is achieved. We start with discrete time quantum walk state tranfer on the star graph, complete bipartite graph and complete graph with one additional self-loop at each vertex. Then we calculate the state transfer with Szegedy's walk on complete graph. The last expample is the continuous time quantum walk state transfer on the complete graph with self loops. We find subspace in the Hilbert space which is invariant with respect to the quantum walk and contains the initial and the target state. This helps us highly reduce the dimension of the problem. The results for the discrete time quantum walk state tranfer on the star graph and on the complete graph with one self loop and Szegedy's walk state transfer for complete graph are published in paper [10]. The result for complete bipartite graph is published in paper [11].

3.1 Star graph

At first we introduce the star graph and its Hilbert space, then we present invariant subspace and effective evolution operator and at last we show that the perfect state transfer is reached. The star graph consists of one central vertex and other vertices which are connected to the central vertex but not to each other. We label the central vertex as 0 and the vertices around from 1 to N. Hence, the corresponding position vectors are $|j\rangle_p$ where j goes form 0 to N. Because the outer vertices have only one neighbour their coin space is one dimensional, i.e. it is spanned by $|0\rangle_c$. The central vertex has N-dimensional coin space spanned by states $|j\rangle_c$ for j running from 1 to N. The general Hilbert space of the star graph is spanned by states $|0, j\rangle$ and $|j, 0\rangle$ for $\forall j \in \{1 \dots N\}$. The shift operator (2.3) can be written in this basis as

$$\hat{S} = \sum_{j=1}^{N} (|0, j\rangle\langle j, 0| + |j, 0\rangle\langle 0, j|) . \tag{3.1}$$

Let the sender and the receiver be outer vertices marked by vectors $|s, 0\rangle$ and $|r, 0\rangle$. Then the coin operator (2.10) reads

$$\hat{C} = \hat{G}_0\hat{P}_0 + \hat{I} - \hat{P}_0 - 2\hat{P}_s - 2\hat{P}_r, \tag{3.2}$$

where the $\hat{G}_0$ is the Grover coin (2.5) at the central vertex. The evolution operator has the form (2.4). Because the star graph is bipartite graph, the amplitude on the receiver vertex is non-zero only after even number of steps. To simplify our calculations we can use $\hat{U}^2$ instead of $\hat{U}$, i.e. we made 2 steps at once.

If we define now the following orthonormal states as

$$\begin{aligned} |s\rangle &:= |s,0\rangle \\ |r\rangle &:= |r,0\rangle \\ |\psi_1\rangle &:= \frac{1}{\sqrt{N-2}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} |j,0\rangle \end{aligned} \tag{3.3}$$

we see that they form invariant subspace with respect to $\hat{U}^2$

$$\begin{aligned} \hat{U}^2|s\rangle &= \frac{2-N}{N}|s\rangle - \frac{2}{N}|r\rangle - \frac{2\sqrt{N-2}}{N}|\psi_1\rangle \\ \hat{U}^2|r\rangle &= -\frac{2}{N}|s\rangle + \frac{N-2}{N}|r\rangle - \frac{2\sqrt{N-2}}{N}|\psi_1\rangle \\ \hat{U}^2|\psi_1\rangle &= \frac{2\sqrt{N-2}}{N}|s\rangle + \frac{2\sqrt{N-2}}{N}|r\rangle + \frac{\sqrt{N-4}}{N}|\psi_1\rangle \end{aligned} \quad . \tag{3.4}$$

We introduce the effective evolution operator of the transfer algorithm with initial state $|s\rangle$ and denote it as $\hat{U}_{eff}$. $\hat{U}_{eff}$ is in the basis $\{|s\rangle, |r\rangle, |z\rangle\}$ given by the following 3×3 matrix

$$U_{eff} = \begin{pmatrix} \frac{N-2}{N} & -\frac{2}{N} & \frac{2\sqrt{N-2}}{N} \\ -\frac{2}{N} & \frac{N-2}{N} & \frac{2\sqrt{N-2}}{N} \\ -\frac{2\sqrt{N-2}}{N} & -\frac{2\sqrt{N-2}}{N} & \frac{N-4}{N} \end{pmatrix}. \tag{3.5}$$

This is the same effective evolution operator as in the Grover state transfer algorithm (1.21). Because in the case of the star graph effective evolution operator correspond to two steps of the walk the number of steps is twice the number of steps of the Grover state transfer algorithm (1.28). Hence the number of steps is the closest even integer to the number

$$T \doteq \frac{\pi}{\sqrt{2}}\sqrt{N} + O\left(\frac{1}{\sqrt{N}}\right). \tag{3.6}$$

After (3.6) number of steps we reach the same fidelity as in the Grovers state transfer algorithm (1.30) and perfect state transfer is achieved on the star graph with discrete time quantum walk.

3.2 Complete bipartite graph

In the case of the complete bipartite we apply the same methods as in the star graph. The set of vertices of complete bipartite graph consists of 2 subsets, they are usually called *parts* of the graph. The vertices in one part are not connected between each other but they are connected to all vertices of the other part. Let us denote these parts as V_1 and V_2, where the part V_1 is the part that contains the sender vertex. The size of V_1 we denote by N and the size of V_2 by M. The position space of V_1 is spanned by states $|j\rangle_p$ where j goes from 1 to N and the position space of V_2 is spanned by states $|\beta\rangle_p$ where β goes from 1 to M. The coin space of vertices in V_1 is spanned by vectors $|\beta\rangle_c$ for $\beta \in \{1 \dots M\}$ and the coin space of vertices in V_2 is spanned by vectors $|j\rangle_c$ for $j \in \{1 \dots N\}$. The shift operator (2.3) reads

$$\hat{S} = \sum_{j=1}^{N}\sum_{\beta=1}^{M} \left(|\beta, j\rangle\langle j, \beta| + |j, \beta\rangle\langle\beta, j|\right). \tag{3.7}$$

There are two cases of positions of the marked vertices. The first case is that both the sender and the receiver are in the part V_1. The coin in this case is given by

$$\hat{C} = \sum_{\substack{j=1 \\ j\neq s,r}}^{N} \hat{G}_j \hat{P}_j - \hat{P}_s - \hat{P}_r + \sum_{\alpha=1}^{M} \hat{G}_\alpha \hat{P}_\alpha. \tag{3.8}$$

where $\hat{G}_j$ and $\hat{G}_\alpha$ are the Grover coins (2.5) and on the sender and receiver we use the phase shift by π. We again use U^2 instead of evolution operator U. If we set the invariant subspace of $\hat{U}^2$ to be spanned by the following basis states

$$\begin{aligned} |s\rangle &:= \frac{1}{\sqrt{M}} \sum_{\beta=1}^{M} |s,\beta\rangle \\ |r\rangle &:= \frac{1}{\sqrt{M}} \sum_{\beta=1}^{M} |r,\beta\rangle \\ |\psi\rangle &:= \frac{1}{\sqrt{(M)(N-2)}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} \sum_{\beta=1}^{M} |j,\beta\rangle \end{aligned} \tag{3.9}$$

we find out that the effective evolution operator has exactly the same form as the effective evolution operator of the star graph (3.5). Thus perfect state transfer is achieved after (3.6) steps in the case where both the sender and the receiver are in the same part.

In the second case, where the receiver is in the part V_2, the coin operator reads

$$\hat{C} = \sum_{\substack{j=1 \\ j\neq s}}^{N} \hat{G}_j \hat{P}_j - \hat{P}_s + \sum_{\substack{\alpha=1 \\ \alpha\neq s}}^{M} \hat{G}_\alpha \hat{P}_\alpha - \hat{P}_r. \tag{3.10}$$

To simplify the problem we find the invariant subspace in V_2 with respect to $\hat{U}^2$ and we move the initial state of the algorithm from part V_1 to V_2 by one application of $\hat{U}$. We can do that because the amplitude on receiver state is non-zero only after odd number of steps. Now we start with new initial state and we use $\hat{U}^2$ and define the effective evolution operator. The orthogonal vectors that span the invariant subspace have the form

$$\begin{aligned} |\alpha_1\rangle &:= |r, s\rangle \\ |\alpha_2\rangle &:= \frac{1}{\sqrt{N-1}} \sum_{\substack{j=1 \\ j\neq s}}^{N} |r, j\rangle \\ |\alpha_3\rangle &:= \frac{1}{\sqrt{M-1}} \sum_{\substack{\beta=1 \\ \beta\neq r}}^{M} |\beta, s\rangle \\ |\alpha_4\rangle &:= \frac{1}{\sqrt{(M-1)(N-1)}} \sum_{\substack{\beta=1 \\ \beta\neq r}}^{M} \sum_{\substack{j=1 \\ j\neq s}}^{N} |\beta, j\rangle \end{aligned} \tag{3.11}$$

The new initial state is given by

$$|init'\rangle = \hat{U}\left(\frac{1}{\sqrt{M}}\sum_{\beta=1}^{M}|s,\beta\rangle\right) = -\frac{1}{\sqrt{M}}\sum_{\beta=1}^{M}|\beta,s\rangle = -\frac{1}{\sqrt{M}}|\alpha_1\rangle - \sqrt{\frac{M-1}{M}}|\alpha_3\rangle \tag{3.12}$$

We also need to express the target state in the basis of invariant subspace. It reads

$$|r\rangle = \frac{1}{\sqrt{M}}\sum_{j=1}^{N}|r,j\rangle = \frac{1}{\sqrt{N}}|\alpha_1\rangle + \sqrt{\frac{N-1}{N}}|\alpha_2\rangle. \tag{3.13}$$

The effective evolution operator in basis (3.11) is given by the following 4×4 matrix

$$U_{eff} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{M-2}{M} & \frac{4\sqrt{(M-1)(N-1)}}{MN} & \frac{2\sqrt{M-1}(N-2)}{MN} \\ 0 & 0 & \frac{N-2}{N} & -\frac{2\sqrt{N-1}}{N} \\ 0 & -\frac{2\sqrt{M-1}}{M} & \frac{2(M-2)\sqrt{N-1}}{MN} & \frac{(M-2)(N-2)}{MN} \end{pmatrix}. \tag{3.14}$$

One eigenvector corresponding to eigenvalue $\lambda_{0,1} = 1$ can be seen right away, it is the vector $|\alpha_1\rangle$. There is a second eigenvector with eigenvalue $\lambda_{0,2} = 1$ and it has the following form

$$|\lambda_0\rangle = \sqrt{\frac{M-1}{M+N-1}}|\alpha_2\rangle + \sqrt{\frac{N-1}{M+N-1}}|\alpha_2\rangle - \frac{1}{\sqrt{M+N-1}}|\alpha_4\rangle. \tag{3.15}$$

The conjugate eigenvalues have the form of $\lambda_\pm = e^{\pm i\omega}$ where eigenphase ω is given by

$$\omega = \arccos\left(\frac{MN-2M-2N+2}{MN}\right). \tag{3.16}$$

The corresponding eigenvectors can be written as

$$\begin{aligned} |\lambda_\pm\rangle = {} & \frac{M-1\mp i\sqrt{(M-1)(N-1)(M+N-1)}}{\sqrt{2}\sqrt{(M-1)(M+N-1)(M+N-2)}}|\alpha_2\rangle + \\ & + \frac{M\sqrt{N-2+\frac{M}{M+N-1}}}{\sqrt{2}\left(N-1\mp i\sqrt{(M-1)(N-1)(M+N-1)}\right)}|\alpha_3\rangle + \sqrt{\frac{M+N-2}{2(M+N-1)}}|\alpha_4\rangle \end{aligned} \tag{3.17}$$

If we express the receiver and the initial states in the eigenbasis of (3.14) we can calculate the general fidelity of the state transfer after t application of (3.14). The expression of the receiver and the initial state in eigenbasis of $\hat{U}_{eff}$ are rather long and they are only useful to calculate the fidelity. We write just the fidelity after $2t+1$ number of steps. It reads

$$\begin{aligned} \mathcal{F}(2t+1) &= \left|\left\langle r\left|\left(\hat{U}_{eff}\right)^t\right|init'\right\rangle\right|^2 = \\ &= \frac{\left|MN-(M-1)(N-1)\cos(\omega t)+\sqrt{(M-1)(N-1)(M+N-1)}\sin(\omega t)\right|^2}{MN(M+N-1)^2}. \end{aligned} \tag{3.18}$$

We find that (3.18) reach the maximum for

$$\omega t = \arccos\left(-\sqrt{\frac{(M-1)(N-1)}{MN}}\right). \tag{3.19}$$

We calculate the number of steps of the walk from (3.19) and from (3.16) as follows

$$T = 2t + 1 \approx \frac{2 \arccos\left(-\sqrt{\frac{(M-1)(N-1)}{MN}}\right)}{\arccos\left(\frac{MN-2M-2N+2}{MN}\right)} + 1 \tag{3.20}$$

More precisely we chose the odd integer which is the closet to the number (3.20). If we substitute the condition (3.19) in (3.18) we get the expression for the maximum fidelity as follows

$$\mathcal{F}_{max}(N, M) = \left(\frac{\sqrt{NM} + \sqrt{(N-1)(M-1)}}{N + M - 1}\right)^2. \tag{3.21}$$

From that we see that the perfect state transfer is achieved only if $N = M$. Substituting this condition in (3.20) and with help of Taylor expansion we get the same number of steps as in the star graph

$$T \doteq \frac{\pi}{\sqrt{2}}\sqrt{N} + O\left(\frac{1}{\sqrt{N}}\right). \tag{3.22}$$

In this case we can estimate the maximum fidelity again with help of Taylor expansion from (3.18) as follows

$$\mathcal{F}_{max}(N) \doteq 1 - O\left(\frac{1}{N}\right). \tag{3.23}$$

The perfect state transfer with the sender and the receiver in different parts of bipartite graph occurs after $T = \frac{\pi}{\sqrt{2}}\sqrt{N}$ steps when both parts have the same size. In figure 3.1 we see how the maximum fidelity depends on the size of both parts. The time evolution of fidelity is displayed in figure 3.2 for the bipartite graph where the both parts have 200 vertices.

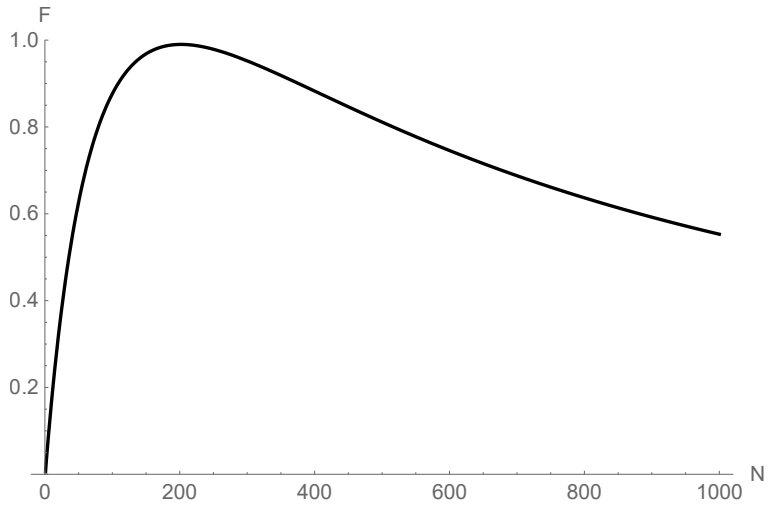

Figure 3.1: The maximum of fidelity $\mathcal{F}_{max}$ depending on the size of V_1 given by (3.21). The part with the receiver vertex V_2 has 200 vertices. The perfect state transfer is reached for $|V_1| = 200$.

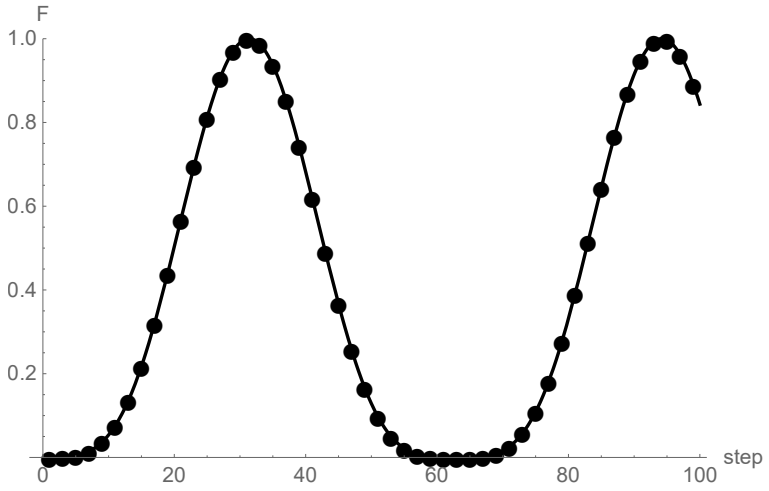

Figure 3.2: The time evolution of the fidelity $\mathcal{F}$ of the state transfer from the sender vertex to the receiver vertex during 100 steps on the bipartite graph with 200 vertices in each part. The dots correspond to the numerical simulation and the line is given by (3.18). The fidelity is plotted only at the odd positions, because it is zero at the even positions. The maximum is reached after 30 steps which agrees with (3.22)

3.3 Complete graph with self loop

We consider the state transfer on the complete graph with one self loop because it was shown in [12] that the search algorithm on the same graph finds the marked vertex with probability close to 1. Additional self loops slow down the search and also lower the probability of success. We start again with description of the graph and its Hilbert space before we show that the perfect state transfer works. We label the vertices of the complete graph from 1 to N. Then the position space is spanned by vectors $|j\rangle_p$ where j goes from 1 to N. The coin space at each vertex is spanned by $|j\rangle_c$ where j runs from 1 to N. In this case the Hilbert space can be written as a tensor product of the position space and the coin space

$$\mathcal{H}_G = \mathcal{H}_p^N \otimes \mathcal{H}_c^N. \tag{3.24}$$

We use the same shift operator (2.3). It can be now rewritten as

$$\hat{S} = \sum_{j,k=1}^{N} |j,k\rangle\langle k,j|. \tag{3.25}$$

But the coin operator of the marked vertices is now different from the coin operator of the star graph and the complete bipartite graph. Now we use at the marked vertices the Grover coin with additional phase shift by π instead of just phase shift alone. The coin operator reads

$$\hat{C} = \sum_{j=1}^{N} \hat{G}_j\hat{P}_j - 2\hat{G}_s\hat{P}_s - 2\hat{G}_r\hat{P}_r. \tag{3.26}$$

The evolution operator is given by (2.4). Because it was proven in [12] that two steps of the walk are equivalent to one step of the Grover algorithm we use again $\hat{U}^2$ instead of the evolution operator

to simplify the calculation. Let us now have subspace spanned by following orthonormal vectors

$$
\begin{aligned}
|s\rangle &:= \frac{1}{\sqrt{N}} \sum_{k=1}^{N} |s,k\rangle \\
|r\rangle &:= \frac{1}{\sqrt{N}} \sum_{k=1}^{N} |r,k\rangle \\
|\psi_1'\rangle &:= \frac{1}{\sqrt{2(N-2)}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} (|j,s\rangle + |j,r\rangle) \\
|\psi_2'\rangle &:= \frac{1}{N-2} \sum_{\substack{j,k=1 \\ j,k\neq s,r}}^{N} |j,k\rangle \\
|\psi_3'\rangle &:= \sqrt{\frac{2}{N(N-2)}} \sum_{k=1}^{N} |s,k\rangle - \sqrt{\frac{N}{2(N-2)}}(|s,s\rangle + |s,r\rangle) \\
|\psi_4'\rangle &:= \sqrt{\frac{2}{N(N-2)}} \sum_{k=1}^{N} |r,k\rangle - \sqrt{\frac{N}{2(N-2)}}(|r,s\rangle + |r,r\rangle)
\end{aligned}
\tag{3.27}
$$

where we see that $|s\rangle$ is the initial state of the walk and $|r\rangle$ is the receiver state. This subspace is invariant with respect to the $\hat{U}^2$, but can be further reduce to dimension 5. Because the invariant subspace contains one eigenvector $|\varphi\rangle$ of $\hat{U}^2$ which is orthogonal to the sender and the receiver state, the orthogonal complement in this subspace is also invariant subspace of $\hat{U}^2$ and it contains the sender and the receiver. We set this orthogonal complement as our new invariant subspace. The eigenvector $|\varphi\rangle$ is given by

$$
|\varphi\rangle = \frac{1}{\sqrt{N}}|\psi_1'\rangle + \sqrt{\frac{N-2}{2N}}|\psi_2'\rangle + \frac{1}{2}|\psi_3'\rangle + \frac{1}{2}|\psi_4'\rangle. \tag{3.28}
$$

The basis of reduced invariant subspace is spanned by $|s\rangle$, $|r\rangle$ and three other vectors which have the form

$$
\begin{aligned}
|\psi_1\rangle &= \sqrt{\frac{N-2}{N}}|\psi_1'\rangle - \sqrt{\frac{2}{N}}|\psi_2'\rangle = \frac{1}{\sqrt{2N}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} (|j,s\rangle + |j,r\rangle) - \frac{\sqrt{2}}{(N-2)\sqrt{N}} \sum_{\substack{j,k=1 \\ j,k\neq s,r}}^{N} |j,k\rangle \\
|\psi_2\rangle &= \frac{1}{\sqrt{2}}|\psi_3'\rangle - \frac{1}{\sqrt{2}}|\psi_4'\rangle = \frac{1}{\sqrt{N(N-2)}} \sum_{\substack{k=1 \\ k\neq s,r}}^{N} (|s,k\rangle - |r,k\rangle) + \sqrt{\frac{N-2}{4N}} (|r,r\rangle + |r,s\rangle - |s,r\rangle - |s,s\rangle) \\
|\psi_3\rangle &= \frac{1}{\sqrt{N}}|\psi_1'\rangle + \sqrt{\frac{N-2}{2N}}|\psi_2'\rangle - \frac{1}{2}|\psi_3'\rangle - -\frac{1}{2}|\psi_4'\rangle \\
&= \frac{1}{\sqrt{2N(N-2)}} \left(\sum_{\substack{j,k=1 \\ j,k\neq s,r}}^{N} |j,k\rangle + \sum_{\substack{j=1 \\ j\neq s,r}}^{N} (|j,s\rangle + |j,r\rangle) - \sum_{\substack{k=1 \\ k\neq s,r}}^{N} (|s,k\rangle + |r,k\rangle) \right) \\
&+ \sqrt{\frac{N-2}{8N}} (|r,r\rangle + |r,s\rangle + |s,r\rangle + |s,s\rangle)
\end{aligned}
\tag{3.29}
$$

The effective evolution operator in this basis is given by following 5×5 matrix

$$U_{eff} = \begin{pmatrix} \frac{(N-2)(N-4)}{N^2} & -\frac{2(N-4)}{N^2} & \frac{4\sqrt{2}(N-2)}{N^2} & -\frac{2\sqrt{N-2}}{N} & \frac{2\sqrt{2}\sqrt{N-2}(N-4)}{N^2} \\ -\frac{2(N-4)}{N^2} & \frac{(N-2)(N-4)}{N^2} & \frac{4\sqrt{2}(N-2)}{N^2} & \frac{2\sqrt{N-2}}{N} & \frac{2\sqrt{2}\sqrt{N-2}(N-4)}{N^2} \\ \frac{4\sqrt{2}(N-2)}{N^2} & \frac{4\sqrt{2}(N-2)}{N^2} & \frac{(N-4)^2}{N^2} & 0 & -\frac{4\sqrt{N-2}(N-4)}{N^2} \\ \frac{2\sqrt{N-2}}{N} & -\frac{2\sqrt{N-2}}{N} & 0 & \frac{N-4}{N} & 0 \\ -\frac{2\sqrt{2}\sqrt{N-2}(N-4)}{N^2} & -\frac{2\sqrt{2}\sqrt{N-2}(N-4)}{N^2} & \frac{4\sqrt{N-2}(N-4)}{N^2} & 0 & \frac{N^2-16N+32}{N^2} \end{pmatrix}. \tag{3.30}$$

The spectrum of $\hat{U}_{eff}$ is composed of $\lambda_0 = 1$ and two pairs of conjugate eigenvalues of the following form

$$\begin{aligned} \lambda_{1,\pm} &= e^{\pm i\omega} \\ \lambda_{2,\pm} &= e^{\pm 2i\omega} \end{aligned} \tag{3.31}$$

where the eigenphase ω is given by (1.24). The corresponding eigenvectors reads

$$\begin{aligned} |\lambda_0\rangle &= \frac{1}{2}|s\rangle + \frac{1}{2}|r\rangle + \frac{1}{\sqrt{2}}|\psi_1\rangle \\ |\lambda_{1,\pm}\rangle &= \frac{1}{2}|s\rangle - \frac{1}{2}|r\rangle \mp \frac{i}{\sqrt{2}}|\psi_2\rangle \\ |\lambda_{2,\pm}\rangle &= \frac{1}{2\sqrt{2}}|s\rangle + \frac{1}{2\sqrt{2}}|r\rangle - \frac{1}{2}|\psi_1\rangle \pm \frac{i}{\sqrt{2}}|\psi_3\rangle \end{aligned} . \tag{3.32}$$

The sender and the receiver states can be rewritten in eigenbasis of $\hat{U}_{eff}$ as

$$\begin{aligned} |s\rangle &= \frac{1}{2}|\lambda_0\rangle + \frac{1}{2}\left(|\lambda_{1,+}\rangle + |\lambda_{1,-}\rangle\right) + \frac{1}{2\sqrt{2}}\left(|\lambda_{2,+}\rangle + |\lambda_{2,-}\rangle\right) \\ |r\rangle &= \frac{1}{2}|\lambda_0\rangle - \frac{1}{2}\left(|\lambda_{1,+}\rangle + |\varphi_{1,-}\rangle\right) + \frac{1}{2\sqrt{2}}\left(|\lambda_{2,+}\rangle + |\lambda_{2,-}\rangle\right) \end{aligned} . \tag{3.33}$$

The state of the walk after $2t$ steps can be now expressed as

$$\hat{U}^{2t}|s\rangle = \left(\hat{U}_{eff}\right)^t |s\rangle = \frac{1}{2}|\lambda_0\rangle + \frac{e^{i\omega t}}{2}\left(|\lambda_{1,+}\rangle + e^{-2i\omega t}|\lambda_{1,-}\rangle\right) + \frac{e^{2i\omega t}}{2\sqrt{2}}\left(|\lambda_{2,+}\rangle + e^{-4i\omega t}|\lambda_{2,-}\rangle\right). \tag{3.34}$$

We see that for $\omega t = \pi$ the state of the walk (3.34) is equal to $|r\rangle$. We get the same condition for the number of steps as for the star graph. The number of steps T is the same as for the star graph (3.6). The evolution of fidelity is given by

$$\mathcal{F}(T = 2t) = \left|\left\langle r \middle| \left(\hat{U}_{eff}\right)^t \middle| s \right\rangle\right|^2 = \cos^2(\omega t)\sin^4\left(\frac{\omega t}{2}\right) \tag{3.35}$$

and the maximum fidelity after $T = \frac{\pi}{\sqrt{2}}\sqrt{N}$ has the same form as (1.30). Hence, the perfect state transfer is reached.

3.4 Szegedy's quantum walk on the complete graph

In this section we examine the state transfer algorithm on the complete graph using Santos model of Szegedy's quantum walk. For G to be complete graph the elements of the stochastic matrix has the following form

$$p_{jk} = \frac{1 - \delta_{jk}}{N - 1}. \tag{3.36}$$

The vectors (2.14) now read

$$|\Phi_j\rangle = \frac{1}{\sqrt{N-1}} \sum_{\substack{k=1 \\ k\neq j}}^{N} |j,k\rangle$$
$$|\Psi_k\rangle = \frac{1}{\sqrt{N-1}} \sum_{\substack{j=1 \\ j\neq k}}^{N} |j,k\rangle \quad . \tag{3.37}$$

We show using evolution operator (2.18) that it takes $O\left(\sqrt{N}\right)$ steps for the large size graph to transfer the initial state

$$|s\rangle = |\Phi_s\rangle = \frac{1}{\sqrt{N-1}} \sum_{\substack{k=1 \\ k\neq s}}^{N} |s,k\rangle \tag{3.38}$$

to the final state

$$|r\rangle = |\Phi_r\rangle = \frac{1}{\sqrt{N-1}} \sum_{\substack{k=1 \\ k\neq r}}^{N} |r,k\rangle \tag{3.39}$$

with high probability. We find that the invariant subspace is spanned by the states $|s\rangle$ and $|r\rangle$ and further five orthonormal states which have the following form

$$|\psi_1\rangle = \frac{1}{\sqrt{(N-2)(N-3)}} \sum_{\substack{j,k=1 \\ j,k\neq s,r \\ j\neq k}}^{N} |j,k\rangle$$
$$|\psi_2\rangle = \frac{1}{\sqrt{(N-1)(N-2)}} \sum_{\substack{k=1 \\ k\neq s,r}}^{N} |s,k\rangle - \sqrt{\frac{N-2}{N-1}}|s,r\rangle$$
$$|\psi_3\rangle = \frac{1}{\sqrt{(N-1)(N-2)}} \sum_{\substack{k=1 \\ k\neq s,r}}^{N} |r,k\rangle - \sqrt{\frac{N-2}{N-1}}|r,s\rangle\,. \tag{3.40}$$
$$|\psi_4\rangle = \frac{1}{\sqrt{N-2}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} |j,s\rangle$$
$$|\psi_5\rangle = \frac{1}{\sqrt{N-2}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} |j,r\rangle$$

The effective evolution operator in this basis has the form of following 7×7 matrix

$$U_{eff} = \begin{pmatrix} \frac{N-3}{N-1} & -\frac{2(N-2)}{(N-1)^2} & \frac{2\sqrt{N-2}(N-3)^{3/2}}{(N-1)^{5/2}} & 0 & \frac{2\sqrt{N-2}}{(N-1)^2} & \frac{4(N-2)^{3/2}}{(N-1)^{5/2}} & \frac{2\sqrt{N-2}(N-3)}{(N-1)^{5/2}} \\ -\frac{2(N-2)}{(N-1)^2} & \frac{N-3}{N-1} & \frac{2\sqrt{N-2}(N-3)^{3/2}}{(N-1)^{5/2}} & \frac{2\sqrt{N-2}}{(N-1)^2} & 0 & \frac{2\sqrt{N-2}(N-3)}{(N-1)^{5/2}} & \frac{4(N-2)^{3/2}}{(N-1)^{5/2}} \\ -2\sqrt{\frac{(N-2)(N-3)}{(N-1)^3}} & -2\sqrt{\frac{(N-2)(N-3)}{(N-1)^3}} & \frac{(N-5)^2}{(N-1)^2} & \frac{2\sqrt{N-3}}{(N-1)^{3/2}} & \frac{2\sqrt{N-3}}{(N-1)^{3/2}} & \frac{2\sqrt{N-3}(N-5)}{(N-1)^2} & \frac{2\sqrt{N-3}(N-5)}{(N-1)^2} \\ 0 & -\frac{2\sqrt{N-2}}{(N-1)^2} & -\frac{2(N+1)\sqrt{N-3}}{(N-1)^{5/2}} & -\frac{N-3}{N-1} & \frac{2}{(N-1)^2} & -\frac{4}{(N-1)^{5/2}} & \frac{2N(N-3)}{(N-1)^{5/2}} \\ -\frac{2\sqrt{N-2}}{(N-1)^2} & 0 & -\frac{2(N+1)\sqrt{N-3}}{(N-1)^{5/2}} & \frac{2}{(N-1)^2} & -\frac{N-3}{N-1} & \frac{2N(N-3)}{(N-1)^{5/2}} & -\frac{4}{(N-1)^{5/2}} \\ 0 & -2\sqrt{\frac{N-2}{(N-1)^3}} & \frac{2(N-3)^{3/2}}{(N-1)^2} & 0 & -\frac{2(N-2)}{(N-1)^{3/2}} & -\frac{(N-3)^2}{(N-1)^2} & \frac{2(N-3)}{(N-1)^2} \\ -2\sqrt{\frac{N-2}{(N-1)^3}} & 0 & \frac{2(N-3)^{3/2}}{(N-1)^2} & -\frac{2(N-2)}{(N-1)^{3/2}} & 0 & \frac{2(N-3)}{(N-1)^2} & -\frac{(N-3)^2}{(N-1)^2} \end{pmatrix} \tag{3.41}$$

The spectrum of (3.41) is composed of one eigenvalues $\lambda_0 = 1$ and 3 pairs of conjugate eigenvalues given by

$$\begin{aligned} \lambda_{1,\pm} &= e^{\pm i\omega_1} \\ \lambda_{2,\pm} &= e^{\pm i\omega_2} \\ \lambda_{2,\pm} &= e^{\pm i\omega_3} \end{aligned} \tag{3.42}$$

where eigephases read

$$\begin{aligned} \omega_1 &= \arccos\left(\frac{4-N+\Delta}{(N-1)^2}\right) \\ \omega_2 &= \arccos\left(\frac{4-N-\Delta}{(N-1)^2}\right) \\ \omega_3 &= \arccos\left(\frac{N(4-N)-5}{(N-1)^2}\right) \end{aligned} \tag{3.43}$$

with Δ of the following form

$$\Delta = \sqrt{N^4 - 10N^3 + 35N^2 - 50N + 33}. \tag{3.44}$$

The calculation of eigenvectors is quite difficult and we present only eigenvectors that are important for the estimation of the number of steps. The eigenvector corresponding to λ_0 reads

$$\begin{aligned} |\lambda_0\rangle &= \sqrt{\frac{N(N-3)+2}{2(N(N-3)+3)}}\left(|s\rangle - |r\rangle\right) + \sqrt{\frac{1}{2(N(N-3)+3)}}\left(|\psi_4\rangle - |\psi_5\rangle\right) \\ &\doteq \frac{1}{\sqrt{2}}\left(|s\rangle - |r\rangle\right) + O\left(\frac{1}{\sqrt{N}}\right) \end{aligned}. \tag{3.45}$$

We see that $|\lambda_0\rangle$ gets for large N close to the form of eigenvector of the Grover state transfer algorithm (1.22). Another two important eigenvectors are $|\lambda_{1,\pm}\rangle$ which correspond to eigenvalues $\lambda_{1,\pm}$. The vectors $|\lambda_{1,\pm}\rangle$ for large N have the form

$$|\lambda_{1,\pm}\rangle = \frac{1}{2}\left(|s\rangle + |r\rangle\right) \pm \frac{1}{\sqrt{2}}|\psi_1\rangle + O\left(\frac{1}{\sqrt{N}}\right). \tag{3.46}$$

The rest of the eigenstates can be neglected because their overlaps with the initial and the final state goes to zero as $O(\frac{1}{\sqrt{N}})$. The eigenvectors $|\lambda_{1,\pm}\rangle$ also resemble the eigenstates of the Grover state transfer

algorithm (3.17). Hence, we see for $N \to \infty$ that evolution of Szegedy's walk is close to effective evolution of the Grover state transfer algorithm. The eigenphase ω_1 is different then the eigenphase (1.24) in the Grover state transfer algorithm but the condition $T\omega_1 = \pi$ for the limit of large N is sufficient for the perfect state transfer. The number of steps T is the closest integer to π/ω_1, i.e. we get the estimation of the following form

$$T \approx \frac{\pi}{\arccos\left(\frac{4-N+\Delta}{(N-1)^2}\right)} \doteq \frac{\pi}{2\sqrt{2}}\sqrt{N} + O\left(\frac{1}{\sqrt{N}}\right). \tag{3.47}$$

We estimate the fidelity with the same precision as follows

$$\mathcal{F}(t) = \left|\left\langle r \left| \left(\hat{U}_{eff}\right)^t \right| s \right\rangle\right|^2 \approx \sin^4\left(\frac{t\omega_1}{2}\right). \tag{3.48}$$

We show that the Szegedy's walk performs the perfect state transfer for sufficiently large N after $\frac{\pi}{2\sqrt{2}}\sqrt{N}$ steps. The time evolution of the fidelity is presented in figure 3.3 for the complete graph with 40 vertices.

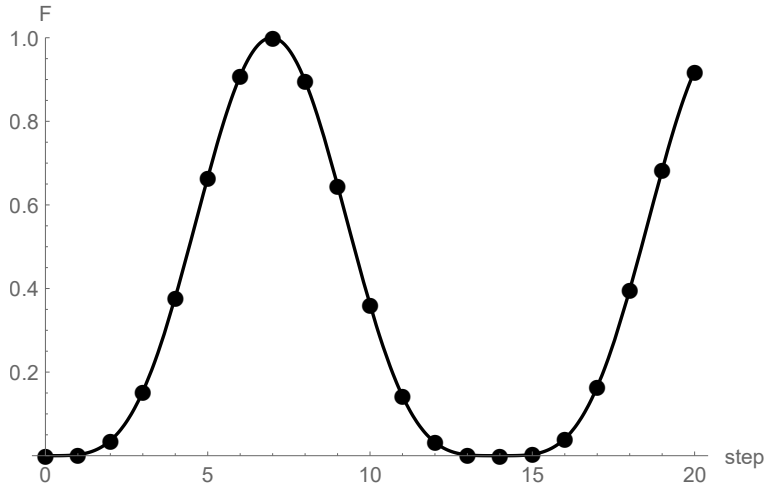

Figure 3.3: The time evolution of the fidelity $\mathcal{F}$ of the state transfer in Szegedy's quantum walk model during 20 steps. The corresponding complete graph has 40 vertices. The dots correspond to the numerical simulation and the line is given by (3.48). The maximum is reached after 7 steps which agrees with (3.47).

3.5 Continuous time quantum walk on complete graph with self loops

Since we calculate the state transfer on the complete graph with two different types of discrete time quantum walk we do the same same for continuous time walk. The Hilbert space is spanned by vector $\{|j\rangle; j \in \{1, 2, \ldots, N\}\}$. We consider the complete graph with L self loops at each vertex. The adjacency matrix, which defines the Hamiltonian of the system (2.24), reads

$$A_{N,L} = \begin{pmatrix} L & 1 & 1 & \ldots & 1 \\ 1 & L & 1 & \ldots & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & \ldots & 1 & L & 1 \\ 1 & \ldots & 1 & 1 & L \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & \ldots & 1 \\ 1 & 0 & 1 & \ldots & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & \ldots & 1 & 0 & 1 \\ 1 & \ldots & 1 & 1 & 0 \end{pmatrix} + L \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \ldots & 0 & 1 & 0 \\ 0 & \ldots & 0 & 0 & 1 \end{pmatrix} \tag{3.49}$$

where the dimension of the matrices are $N \times N$ and L is the number of self loops at each vertex. Because the Hamiltonians $\hat{H}$ and $\hat{H} + \alpha\hat{I}$ generate the same evolution for any real α it follows from (3.49) that number of loops does not matter. We set the graph to have one self loop at each vertex. We also set $\gamma = \frac{1}{N}$ in (2.24).

It is easy to see that subspace spanned by states $|s\rangle$,$|r\rangle$ and

$$|\psi_1\rangle = \frac{1}{\sqrt{N-2}} \sum_{\substack{j=1 \\ j\neq s,r}}^{N} |j\rangle \tag{3.50}$$

is invariant with respect to the Hamiltonian (2.24). Since the initial and the target states lies in this subspace we find the invariant subspace of the state transfer algorithm. We introduce the effective Hamiltonian which is given in basis $\{|s\rangle, |r\rangle, |\psi_1\rangle\}$ by 3×3 matrix

$$H_{eff} = -\begin{pmatrix} 1+\frac{1}{N} & \frac{1}{N} & \frac{\sqrt{N-2}}{N} \\ \frac{1}{N} & 1+\frac{1}{N} & \frac{\sqrt{N-2}}{N} \\ \frac{\sqrt{N-2}}{N} & \frac{\sqrt{N-2}}{N} & \frac{N-2}{N} \end{pmatrix}. \tag{3.51}$$

Let us now calculate the running time of the algorithm by diagonalizing the effective Hamiltonian. Spectrum of $\hat{H}_{eff}$ is composed of three eigenvalues which are given by

$$\begin{aligned} \lambda_1 &= -1 \\ \lambda_2 &= -1 - \sqrt{\frac{2}{N}}. \\ \lambda_3 &= -1 + \sqrt{\frac{2}{N}} \end{aligned} \tag{3.52}$$

Their corresponding eigenvectors reads

$$\begin{aligned} |\lambda_1\rangle &= \frac{1}{\sqrt{2}}(|s\rangle - |r\rangle) \\ |\lambda_2\rangle &= \frac{\sqrt{\sqrt{N}+\sqrt{2}}}{2N^{\frac{1}{4}}}(|s\rangle + |r\rangle) + \frac{\sqrt{\sqrt{N}-\sqrt{2}}}{\sqrt{2}N^{\frac{1}{4}}}|\psi_1\rangle. \\ |\lambda_3\rangle &= \frac{\sqrt{\sqrt{N}-\sqrt{2}}}{2N^{\frac{1}{4}}}(|s\rangle + |r\rangle) - \frac{\sqrt{\sqrt{N}+\sqrt{2}}}{\sqrt{2}N^{\frac{1}{4}}}|\psi_1\rangle \end{aligned} \tag{3.53}$$

The initial state and the target state have in the eigenbasis of $\hat{H}_{eff}$ the following form

$$\begin{aligned} |s\rangle &= \frac{1}{\sqrt{2}}|\lambda_1\rangle + \frac{\sqrt{\sqrt{N}+\sqrt{2}}}{2N^{\frac{1}{4}}}|\lambda_2\rangle + \frac{\sqrt{\sqrt{N}-\sqrt{2}}}{\sqrt{2}N^{\frac{1}{4}}}|\lambda_3\rangle \\ |r\rangle &= -\frac{1}{\sqrt{2}}|\lambda_1\rangle + \frac{\sqrt{\sqrt{N}+\sqrt{2}}}{2N^{\frac{1}{4}}}|\lambda_2\rangle + \frac{\sqrt{\sqrt{N}-\sqrt{2}}}{\sqrt{2}N^{\frac{1}{4}}}|\lambda_3\rangle \end{aligned} . \tag{3.54}$$

Now we calculate the evolution of fidelity as follows

$$\mathcal{F}(T) = \left|\left\langle r \left| e^{-i\hat{H}T} \right| s \right\rangle\right|^2 = \frac{N\left(\cos\left(\sqrt{\frac{2}{N}}T\right) - 1\right)^2 + 2\sin^2\left(\sqrt{\frac{2}{N}}T\right)}{4N}. \tag{3.55}$$

For $T\sqrt{\frac{2}{N}} = \pi$ fidelity (3.55) reaches the maximum and goes to 1. Hence the perfect state transfer is achieved for time $T = \frac{\pi}{\sqrt{2}}\sqrt{N}$.

Chapter 4

Quantum search on regular graphs

In first part of this Chapter we review the results from S. Chakraborty *et al.* [9] for continuous time quantum walk search. They found a sufficient condition for the search algorithm to be optimal and they used it to show that the search algorithm is optimal for *almost all graphs*. We use their results as motivation, because in the second part of this Chapter we focus on the Szegedy's search algorithm on the regular graph. We find the condition for the Szegedy's search algorithm on the regular graph to find marked vertex after $O\left(\sqrt{N}\right)$ steps with probability $\frac{\sigma}{4} - O\left(\frac{1}{N}\right)$ where σ is the gap between the largest and the second largest eigenvalue of the associated stochastic matrix.

4.1 Continuous time quantum walk on random graphs

In this section we describe the results of [9] in further detail. We start by presenting condition for the continuous time quantum walk search to achieve optimality, i.e. to find the marked vertex in $O\left(\sqrt{N}\right)$ time. Then we show with the help of this condition that the optimal search is reached for *almost all graphs*.

Using the Hamiltonian (2.22) and initial state $|init\rangle = |\psi\rangle = \sum_{j=1}^{N} |j\rangle$ Chakraborty *et al.* proved the following condition for optimality of the search:

Lemma 1. *Let $\hat{H}_1$ be a Hamiltonian with eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_k$ (satisfying $\lambda_1 = 1$ and $|\lambda_i| \leq c < 1$ for all $i > 1$) and eigenvectors $|v_1\rangle = |\psi\rangle$, $|v_2\rangle$, …, $|v_k\rangle$ and let $\hat{H}_2 = |m\rangle\langle m|$ with $|\langle m|\psi\rangle| = \epsilon$. For an appropriate choice of $r = O(1)$, applying the Hamiltonian $(1 + r)\hat{H}_1 + \hat{H}_2$ to the starting state $|v_1\rangle = |\psi\rangle$ for time $\Theta\left(\frac{1}{\epsilon}\right)$ results in a state $|f\rangle$ with $|\langle m|f\rangle|^2 \geq \frac{1-c}{1+c} - O(1)$.*

Let $\lambda_1^A \geq \lambda_2^A \geq \ldots \geq \lambda_N^A$ be eigenvalues of the adjacency matrix A_G. Then the first Hamiltonian $\hat{H}_1$ in Lemma 1 corresponds to the adjacency matrix $\hat{H}_1 = \gamma \hat{A}_G$ where γ is chosen to be $\frac{1}{\lambda_1^A}$. The optimal search is achieved when $\frac{\lambda_2^A}{\lambda_1^A} \leq c < 1$ and when $|\psi\rangle$ is eigenvector of $\hat{A}_G$, since $|\langle m|\psi\rangle| = \frac{1}{\sqrt{N}}$ implies that the search time is $\Theta\left(\sqrt{N}\right)$.

Since equal superposition of all basis states $|\psi\rangle$ is an eigenvector of all d-regular graph with largest eigenvalue d they directly fulfil one condition of the Lemma 1. It has been shown in [13] that the second largest eigenvalue of d-random regular graph is $O\left(d^{\frac{3}{4}}\right)$ for $d \geq 3$ with high probability where d-random regular graph is a graph uniformly picked up from the set of all d-regular graphs. Hence d-random graphs fulfil $\frac{\lambda_2^A}{\lambda_1^A} = O\left(d^{-\frac{1}{4}}\right) < 1$ with high probability and the optimal search is achieved according to Lemma 1.

Another model of random graphs is Erdös-Renyi random graph which is a graph $G(N, P)$ with N vertices where every edge between any two vertices has probability P to be in this graph. Some property

of the graph holds for *almost all graphs* if the probability for graph $G(N, P)$ having this property goes to 1 for N going to infinity. Chakraborty *et al.* found using results in [14] and [15] that as long as the probability is higher than $\frac{\log^{3/4}(N)}{N}$ there is a spectral gap between the largest and the second largest eigenvalue of the adjacency matrix and $\frac{\lambda_2^A}{\lambda_1^A}$ is bounded by a constant. They also found that the equal superposition of all basis states converges to the eigenvector of the largest eigenvalue for $P \geq \frac{\log^{3/2}(N)}{N}$. Thus the optimal search is achieved according to the Lemma 1 for *almost all graphs*.

4.2 Szegedy's quantum walk search on regular graphs

In this section we consider the Szegedy's quantum walk search algorithm on the regular graph using the evolution operator $\hat{U}'$. At first we write the results for the regular graph which were already proven by Szegedy in [7]. He found relation between the spectrum of the symmetric stochastic matrix and the spectrum of the evolution operator of the walk and the relation between spectral gap of the symmetric stochastic matrix and the upper bound of the number of steps of the search algorithm. Since this theorem does not give the exact number of steps of the algorithm we later prove theorem for regular graphs which gives better estimations on the number of steps and a different estimation of the probability of success.

At first let us look on the theorem proved by Szegedy. The theorem reads for one marked vertex

Theorem 2. *Let P be a symmetric stochastic matrix of graph G with one marked vertex. Let σ be the eigenvalue gap of P. Then after randomly picked number of steps $T \in \left[1, \frac{1000}{\sqrt{\sigma}}\sqrt{N}\right]$ the probability to find the marked vertex is at least $\frac{1}{1000}$.*

The inconveniences of this theorem are that the number of steps is picked randomly from the large interval and the lower bound of success probability is quite low. Also the only graph that is connected and has a symmetric stochastic matrix is the regular graph, so the theorem only holds for regular graphs. The limitation of the regular graphs comes from the fact that we can calculate directly the spectrum of the evolution operator only from the spectrum of the symmetric stochastic matrix.

Before we write the spectrum of the evolution operator we introduce concept of *idle* and *busy* subspaces also used by Szegedy. Lets have two subspaces $\mathcal{A}$ and $\mathcal{B}$ of the Hilbert space of the walk which are spanned by the states $\{|\Phi_1\rangle, \ldots, |\Phi_N\rangle\}$ and $\{|\Psi_1\rangle, \ldots, |\Psi_N\rangle\}$ respectively. We call the subspace $\mathcal{A}^\perp \cap \mathcal{B}^\perp$ *idle* subspace since the evolution operator (2.15) acts as identity on this subspace. The *busy* subspace is the orthogonal complement of the *idle* subspace, i.e $(\mathcal{A}^\perp \cap \mathcal{B}^\perp)^\perp$. Since the spectrum of the evolution operator is trivial in the *idle* subspace we are only interested in the spectrum in the *busy* space.

Now we describe the spectrum of the evolution operator. The spectrum was already found by Szegedy in [7]. The spectrum of the evolution operator (2.15) on the *busy* space is derived from the spectrum of matrix D which is given by $D = \sqrt{P \circ P^T}$ where $\circ$ is the element-wise product, i.e. $D_{jk} = \sqrt{P_{jk}P_{jk}^T} = \sqrt{P_{jk}P_{kj}}$. All states that lies in the subspace $\mathcal{A} \cap \mathcal{B}$ are eigenvectors of the evolution operator with eigenvalue 1. To describe the rest of the spectrum we define two linear mapping $\mathcal{L}_\mathcal{A}$, $\mathcal{L}_\mathcal{B}$ which map $\mathbb{C}^N$ onto the subspace $\mathcal{A}$ and $\mathcal{B}$ respectively and read

$$\begin{aligned} \mathcal{L}_\mathcal{A}\left(\overrightarrow{x}\right) &= \sum_{j=1}^{N} x_j |\Phi_j\rangle \\ \mathcal{L}_\mathcal{B}\left(\overrightarrow{x}\right) &= \sum_{k=1}^{N} x_k |\Psi_k\rangle \end{aligned} . \tag{4.1}$$

The eigenvectors of the evolution operator which correspond to eigenvalue -1 are given by $|u^0_{\mathcal{A}}\rangle = \mathcal{L}_{\mathcal{A}}\left(\overrightarrow{u}^0\right)$ and $|u^0_{\mathcal{B}}\rangle = \mathcal{L}_{\mathcal{B}}\left(\overrightarrow{u}^0\right)$ where $\overrightarrow{u}^0$ is the eigenvector of the matrix D with eigenvalue 0. We get two conjugate eigenvalues $\lambda^\nu_\pm$ of the evolution operator for every eigenvalue ν of the matrix D for which $1 > \nu > 0$ holds true. The eigenvalues $\lambda^\nu_\pm$ are given by

$$\lambda^\nu_\pm = 2\nu^2 - 1 \pm i2\nu\sqrt{1-\nu^2}. \tag{4.2}$$

The eigenphase ω^ν which corresponds to eigenvalues $\lambda^\nu_\pm = e^{\pm i\omega^\nu}$ is given by $\omega^\nu = \arccos\left(2\nu^2 - 1\right)$. The eigenvectors of $\lambda^\nu_\pm$ have the following form

$$|\lambda^\nu_\pm\rangle = \frac{1}{\sqrt{2}\sqrt{1-\nu^2}}\left(|u^\nu_{\mathcal{A}}\rangle + \left(-\nu \mp i\sqrt{1-\nu^2}\right)|u^\nu_{\mathcal{B}}\rangle\right) \tag{4.3}$$

where $\overrightarrow{u}^\nu$ is the eigenvector of D with eigenvalue ν, $|u^\nu_{\mathcal{A}}\rangle = \mathcal{L}_{\mathcal{A}}\left(\overrightarrow{u}^\nu\right)$ and $|u^\nu_{\mathcal{B}}\rangle = \mathcal{L}_{\mathcal{B}}\left(\overrightarrow{u}^\nu\right)$.

We are focusing on the regular graphs because the stochastic matrix is symmetric and hence $D = P$, i.e. we get direct connection between the spectrum of the stochastic matrix and the evolution operator. Also it holds for regular graph that $P = \frac{1}{d}A_G$ where d is degree of vertices and A_G is the adjacency matrix of the graph. Thus we obtain the eigenvalues of the stochastic matrix of the d-regular graph just by dividing the eigenvalues of the adjacency matrix by d.

Let us now look at the matrix D' derived from the modified stochastic matrix P' for the search algorithm. For the symmetric stochastic matrix P which has the form

$$P = \begin{pmatrix} P_1 & \overrightarrow{P}_2 \\ \overrightarrow{P}_2^T & 0 \end{pmatrix} \tag{4.4}$$

we get the matrix P' which reads

$$P' = \begin{pmatrix} P_1 & P_2 \\ 0 & 1 \end{pmatrix} \tag{4.5}$$

where we consider only one marked vertex in the graph and we arrange the marked vertex at the last position without lost of generality. Then the matrix D' reads

$$D' = \begin{pmatrix} P_1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.6}$$

The largest eigenvalue of the matrix D' is 1, the second largest eigenvalue μ of D' is the largest eigenvalue of P_1 which is $(N-1)\times(N-1)$ symmetric matrix. The following Lemma proven by Szegedy in [7] gives an estimation of the size of μ. The lemma reads:

Lemma 3. *The largest eigenvalue μ of P_1 lies in the interval $\left[1 - \frac{1}{N-1}, 1 - \frac{\sigma}{2N}\right]$ where σ is the gap between the first and the second largest eigenvalue of the original stochastic matrix P.*

We use Lemma 3 further in the text to prove estimation of the probability of the success, so we repeat briefly the proof given by Szegedy.

The lower bound on the largest eigenvalue comes from the fact that for symmetric matrix with non-negative elements the largest eigenvalue is equal to the norm of the matrix. We get

$$\mu = \|P_1\| = \sup\left\{\|P_1\overrightarrow{x}'\| : \overrightarrow{x}' \in \mathbb{C}^{N-1} \wedge \|\overrightarrow{x}'\| = 1\right\} \geq \|P_1\overrightarrow{y}'\| = 1 - \frac{1}{N-1} \tag{4.7}$$

where is $\overrightarrow{y}'$ is normalized equal superposition of all basis vectors in dimension $N-1$.

Finding the upper bound of μ is more difficult. The eigenvector of the largest eigenvalue of the symmetric matrix with non-negative elements has also non-negative coordinates. Let us denote this eigenvector of P_1 as $\overrightarrow{a}'$, i.e. $P_1\overrightarrow{a}' = \mu\overrightarrow{a}'$. We define N dimensional expansion vector of $\overrightarrow{a}'$ and label it as $\overrightarrow{a}$. The first $N-1$ coordinates of $\overrightarrow{a}$ are the coordinates of $\overrightarrow{a}'$ and last one is zero. We rewrite the vector $\overrightarrow{a}$ in the eigenbasis of the original stochastic matrix P as follows

$$\overrightarrow{a} = \alpha\overrightarrow{y} + \sum_{k=2}^{N} \alpha_k \overrightarrow{u}^k \tag{4.8}$$

where $\overrightarrow{y}$ is normalized equal superposition of all basis vectors in dimension N and also $P\overrightarrow{y} = \overrightarrow{y}$, $\overrightarrow{u}^k$ are other normalized eigenvectors of P. Since $\|\overrightarrow{a}\| = 1$ holds true we have $\alpha^2 + \sum_k \alpha_k^2 = 1$. We estimate the size of α as follows

$$\alpha = \left(\overrightarrow{a}|\overrightarrow{y}\right) = \sqrt{\frac{N-1}{N}}\left(\overrightarrow{a}'|\overrightarrow{y}'\right) \leq \sqrt{1-\frac{1}{N}} \tag{4.9}$$

where $(\cdot|\cdot)$ is the scalar product in $\mathbb{C}^N$ and $\mathbb{C}^{N-1}$. From (4.9) we get $\sum_{k=2}^{N}\alpha_k^2 = 1-\alpha^2 \geq \frac{1}{N}$. Suppose ν_k is the eigenvalue associated with $\overrightarrow{u}^k$ then we get $P\overrightarrow{a} = \alpha\overrightarrow{y} + \sum_{k=2}^{N}\alpha_k\nu_k\overrightarrow{u}^k$. Since $\nu_k \leq 1-\sigma$ we have the following estimation

$$\begin{aligned} \|P\overrightarrow{a}\|^2 &= \alpha^2 + \sum_k \alpha_k^2\nu_k^2 \leq \alpha^2 + (1-\sigma)^2\sum_k \alpha_k^2\nu_k^2 \leq \\ &\leq \alpha^2 + (1-\sigma)\sum_k \alpha_k^2\nu_k^2 \leq \alpha^2 + \sum_k \alpha_k^2\nu_k^2 - \sigma\sum_k \alpha_k^2\nu_k^2 \leq 1 - \frac{\sigma}{N}. \end{aligned} \tag{4.10}$$

At last from

$$\|P\overrightarrow{a}\|^2 \geq \|D\overrightarrow{a}\|^2 = \|P_1\overrightarrow{a}'\|^2 = \mu^2 \tag{4.11}$$

and from (4.10) we receive the upper bound $\mu^2 \leq 1-\frac{\sigma}{N} \Rightarrow \mu \leq 1-\frac{\sigma}{2N}$.

Having proven the Lemma 3 we move on to the search algorithm itself and we summarize our results in the following theorem:

Theorem 4. *Let P be a symmetric stochastic matrix of the d-regular graph G with one marked vertex. Let σ be the eigenvalue gap of P that fulfils $\frac{1}{\sigma\sqrt{N}} \ll 1$. Then after number of steps $T \in \left[\frac{\pi}{8\sqrt{2}}\sqrt{N}, \frac{\pi}{8\sqrt{\sigma}}\sqrt{N}\right]$ the probability to find the marked vertex is at least $\frac{\sigma}{4} - O\left(\frac{1}{N}\right)$.*

We prove the Theorem 4 by showing that it is possible to approximate the evolution of the walk in the *busy* subspace by evolution only in the two dimensional subspace spanned by states $|\lambda_\pm^\mu\rangle$.

The two eigenstates $|\lambda_\pm^\mu\rangle$ of the evolution operator $\hat{U}'$ have the form

$$|\lambda_\pm^\mu\rangle = \frac{1}{\sqrt{2}\sqrt{1-\mu^2}}\left(|a_{\mathcal{A}}\rangle + \left(-\mu \mp i\sqrt{1-\mu^2}\right)|a_{\mathcal{B}}\rangle\right) \tag{4.12}$$

and they correspond to the eigenvector $\overrightarrow{a}$ with the eigenvalue μ that is defines in the proof of the Lemma 3. The state $|a_{\mathcal{A}}\rangle$ and $|a_{\mathcal{B}}\rangle$ in (4.12) are constructed using linear map (4.1) because we have $\mathcal{L}_{\mathcal{A}}\left(\overrightarrow{a}\right) = \mathcal{L}_{\mathcal{A}'}\left(\overrightarrow{a}\right)$ and $\mathcal{L}_{\mathcal{B}}\left(\overrightarrow{a}\right) = \mathcal{L}_{\mathcal{B}'}\left(\overrightarrow{a}\right)$ thanks to $a_N = 0$. The initial and the target states are given by

$$\begin{aligned} |init\rangle &= \frac{1}{\sqrt{N}}\sum_{j=1}^{N}|\Phi_i\rangle \\ |target\rangle &= |\Phi_N\rangle \end{aligned}. \tag{4.13}$$

Now we calculate the scalar product between the states (4.12) and the initial and the target state. At first we calculate

$$\begin{aligned} c := \langle a_{\mathcal{A}}|init\rangle = \langle a_{\mathcal{B}}|init\rangle &= \frac{1}{\sqrt{N}} \sum_{j,k=1}^{N} a_j \sqrt{P_{jk}P_{jk}} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N-1} a_j \sum_{k=1}^{N} P_{jk} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N-1} a_j = \left(\overrightarrow{a}|\overrightarrow{y}\right) \\ \langle a_{\mathcal{A}}|target\rangle &= \sum_{k=1}^{N} a_N \sqrt{P_{Nk}P_{Nk}} = 0 \\ f := \langle a_{\mathcal{B}}|target\rangle &= \sum_{j=1}^{N-1} a_j \sqrt{P_{jN}P_{jN}} = \sum_{j=1}^{N-1} a_j P_{jN} = \left(\overrightarrow{a}|\overrightarrow{P_2}\right) \end{aligned} \tag{4.14}$$

where $\overrightarrow{y}$ is the normalized equal superposition of all basis vectors in $\mathbb{C}^N$. Using the fact that $P\overrightarrow{y} = \overrightarrow{y}$ we rewrite f as follows

$$\begin{aligned} \left(\overrightarrow{a}|\overrightarrow{y}\right) = \left(\overrightarrow{y}|\overrightarrow{a}\right) = \left(\overrightarrow{y}|P\overrightarrow{a}\right) = \left(\overrightarrow{y}|D'\overrightarrow{a}\right) + \frac{1}{\sqrt{N}}\left(\overrightarrow{a}|\overrightarrow{P_2}\right) = \mu\left(\overrightarrow{y}|\overrightarrow{a}\right) + \frac{1}{\sqrt{N}}\left(\overrightarrow{a}|\overrightarrow{P_2}\right) \\ f = \left(\overrightarrow{a}|\overrightarrow{P_2}\right) = \sqrt{N}(1-\mu)\left(\overrightarrow{a}|\overrightarrow{y}\right) \end{aligned}. \tag{4.15}$$

Then we get

$$\begin{aligned} c_\pm := \langle\lambda_\pm^\mu|init\rangle &= \frac{c}{\sqrt{2}\sqrt{1-\mu^2}}\left(1-\mu \mp i\sqrt{1-\mu^2}\right) \\ f_\pm := \langle\lambda_\pm^\mu|target\rangle &= \frac{f}{\sqrt{2}\sqrt{1-\mu^2}}\left(-\mu \mp i\sqrt{1-\mu^2}\right) \end{aligned}. \tag{4.16}$$

Now we rewrite the initial and the target states

$$\begin{aligned} |init\rangle &= c_+|\lambda_+^\mu\rangle + c_-|\lambda_-^\mu\rangle + k_1|r_1\rangle \\ |target\rangle &= f_+|\lambda_+^\mu\rangle + f_-|\lambda_-^\mu\rangle + k_2|r_2\rangle \end{aligned} \tag{4.17}$$

where the states $|r_j\rangle$ are orthogonal to $|\lambda_\pm^\mu\rangle$ and normalized to 1. From $|||init\rangle|| = 1$ and $|||target\rangle|| = 1$ we get the conditions for k_1 and k_2 that read

$$\begin{aligned} |k_1|^2 &= 1 - 2|c_\pm|^2 = 1 - \left(\overrightarrow{a}|\overrightarrow{y}\right)^2 \frac{2(1-\mu)}{1-\mu^2} = \frac{1+\mu-2\left(\overrightarrow{a}|\overrightarrow{y}\right)^2}{1+\mu} \\ |k_2|^2 &= 1 - \left(\overrightarrow{a}|\overrightarrow{y}\right)^2 \frac{N(1-\mu)}{1+\mu} \end{aligned} \tag{4.18}$$

The accuracy of the approximation of the evolution with the initial state $|init\rangle$ in the subspace spanned by $|\lambda_\pm^\mu\rangle$ is growing with $|k_1|$ getting smaller. We show by finding the lower bound of the scalar product $\left(\overrightarrow{a}|\overrightarrow{y}\right)$ that $|k_1| \ll 1$.

We use the perturbation theory on the vector $\overrightarrow{a}$ to find the lower bound of $\left(\overrightarrow{a}|\overrightarrow{y}\right)$. Suppose that $\overrightarrow{a}$ is expressed as follows

$$\overrightarrow{a} = \overrightarrow{y} + \sum_j \varepsilon^j \overrightarrow{z}^j \tag{4.19}$$

where ε is a real number and $\overrightarrow{z}^j$ are not yet specified vectors in $\mathbb{C}^N$. The vector $\overrightarrow{a}$ is the eigenvector of a matrix given by

$$\begin{pmatrix} P_1 & 0 \\ 0 & 0 \end{pmatrix} = \left(\begin{pmatrix} P_1 & \overrightarrow{P}_2 \\ \overrightarrow{P}_2^T & 0 \end{pmatrix} + \frac{1}{d} \begin{pmatrix} 0 & -d\overrightarrow{P}_2 \\ -d\overrightarrow{P}_2^T & 0 \end{pmatrix} \right) = (P + \varepsilon V) \tag{4.20}$$

with eigenvalue $\mu = 1 + \sum_j \varepsilon^j \beta_j$. From $\|\overrightarrow{a}\|^2 = 1$ we receive the following expression

$$1 = \|\overrightarrow{a}\|^2 = 1 + \varepsilon 2\left(\overrightarrow{z}^1 | \overrightarrow{y}\right) + \varepsilon^2 \left[2\left(\overrightarrow{z}^2 | \overrightarrow{y}\right) + \left(\overrightarrow{z}^1 | \overrightarrow{z}^1\right)\right] + O\left(\varepsilon^3\right) \tag{4.21}$$

which fixes $\left(\overrightarrow{z}^1 | \overrightarrow{y}\right) = 0$ and $\left(\overrightarrow{z}^2 | \overrightarrow{y}\right) = -\frac{1}{2}\left(\overrightarrow{z}^1 | \overrightarrow{z}^1\right)$. The vector $\overrightarrow{z}^1$ is given by

$$\overrightarrow{z}^1 = \sum_{k=2}^{N} \frac{\left(\overrightarrow{u}^k | V\overrightarrow{y}\right)}{1 - \nu_k} \overrightarrow{u}^k. \tag{4.22}$$

Now we use approximation only to the second order. Thus the scalar product reads

$$\left(\overrightarrow{a} | \overrightarrow{y}\right) = 1 - \frac{1}{2d^2}\left(\overrightarrow{z}^1 | \overrightarrow{z}^1\right). \tag{4.23}$$

Since we have $1 - \nu_k \geq \sigma$ we approximate $\left(\overrightarrow{z}^1 | \overrightarrow{z}^1\right)$ as follows

$$\begin{aligned} \left(\overrightarrow{z}^1 | \overrightarrow{z}^1\right) &= \sum_{k=2}^{N} \frac{\left(\overrightarrow{u}^k | V\overrightarrow{y}\right)^2}{(1-\nu_k)^2} \leq \frac{1}{\sigma^2} \sum_{k=2}^{N} \left(\overrightarrow{u}^k | V\overrightarrow{y}\right)^2 = \|V\overrightarrow{y}\|^2 - \left(\overrightarrow{y} | V\overrightarrow{y}\right)^2 \\ \|V\overrightarrow{y}\|^2 &= \frac{d^2}{N} + \frac{d}{N} \\ \left(\overrightarrow{y} | V\overrightarrow{y}\right)^2 &= \frac{4d^2}{N^2} \\ \left(\overrightarrow{z}^1 | \overrightarrow{z}^1\right) &\leq \frac{d^2}{\sigma^2 N}\left(1 + \frac{1}{d} - \frac{4}{N}\right) \end{aligned} \quad . \tag{4.24}$$

Now we give the lower bound on the scalar product which reads

$$\left(\overrightarrow{a} | \overrightarrow{y}\right) \geq 1 - \frac{1}{2\sigma^2 N}\left(1 + \frac{1}{d} - \frac{4}{N}\right). \tag{4.25}$$

Moving back to the estimation of $|k_1|$ in (4.18) we obtain

$$\begin{aligned} |k_1|^2 &= \frac{1 + \mu - 2\left(\overrightarrow{a} | \overrightarrow{y}\right)^2}{1 + \mu} \leq \frac{-\frac{\sigma}{2N} + \frac{2}{\sigma^2 N}\left(1 + \frac{1}{d}\right) + O(\frac{1}{N^2})}{2 - \frac{1}{N-1}} = \frac{1}{2\sigma^2 N}\left(2 + \frac{2}{d} - \frac{\sigma^3}{2}\right) + O\left(\frac{1}{N^2}\right) \\ |k_1| &\leq \frac{1}{\sigma\sqrt{2N}} \sqrt{2 + \frac{2}{d} - \frac{\sigma^3}{2}} + O\left(\frac{1}{N}\right) \end{aligned} \tag{4.26}$$

which gives with the initial condition $\frac{1}{\sigma\sqrt{N}} \ll 1$ required result that $|k_1| \ll 1$. Hence we neglect the part of the initial state corresponding to $|r_1\rangle$ in the calculation of the success probability. The probability to

find the marked vertex after t steps is given by

$$\begin{aligned}
p(t) &= |\langle target|\left(\hat{U}'\right)^t|init\rangle|^2 \approx |c_+ f_+ e^{i\omega^\mu t} + c_- f_- e^{-i\omega^\mu t}|^2 = \\
&= \frac{c^2 f^2}{4(1-\mu^2)^2}\left|\left(1-\mu-i\sqrt{1-\mu^2}\right)\left(-\mu-i\sqrt{1-\mu^2}\right)e^{i\omega^\mu t} + \left(1-\mu+i\sqrt{1-\mu^2}\right)\left(-\mu+i\sqrt{1-\mu^2}\right)e^{-i\omega^\mu t}\right|^2 = \\
&= \frac{c^2 f^2}{4(1-\mu^2)^2}\left|\left(2\lambda^2-\mu-1\right)\left(e^{i\omega^\mu t}+e^{i\omega^\mu t}\right) + i\,(2\mu-1)\,\sqrt{1-\mu}\left(e^{i\omega^\mu t}+e^{i\omega^\mu t}\right)\right|^2 = \\
&= \frac{c^2 f^2}{(1-\mu^2)^2}\left|\left(2\mu^2-\mu-1\right)\cos(\omega^\mu t) - (2\mu-1)\,\sqrt{1-\mu^2}\sin(\omega t)\right|^2 = \\
&= \frac{c^2 f^2}{(1+\mu)^2(\mu-1)}\left(1+\mu\left(4\mu^2-3\right)\cos(2\omega^\mu t) - \left(4\mu^2-1\right)\sqrt{1-\mu^2}\sin(2\omega^\mu t)\right)
\end{aligned} \tag{4.27}$$

The probability reaches maximum for the following condition

$$2\omega^\mu t = \arccos\left(-\sqrt{\frac{-4\mu^3+3\mu+1}{2}}\right) \approx \frac{\pi}{2} + O\left(\frac{1}{\sqrt{N}}\right) \tag{4.28}$$

where we use Lemma 3 and Taylor expansion. From (4.28) we get the number of steps that is given by

$$T = \frac{\pi}{4\omega} = \frac{\pi}{4\arccos\left(2\mu^2-1\right)} \approx \frac{\pi}{8\sqrt{2}\sqrt{1-\mu}} + O\left(\sqrt{1-\mu}\right) \tag{4.29}$$

and hence the number of steps lies in the interval $\left[\frac{\pi}{8\sqrt{2}}\sqrt{N}, \frac{\pi}{8\sqrt{\sigma}}\sqrt{N}\right]$. Substituting (4.28) in (4.27) we get the maximal probability which reads

$$\begin{aligned}
p &\approx c^2 f^2 \frac{(2\mu-1)^2}{1-\mu^2} = \left(\overrightarrow{a}\,|\,\overrightarrow{y}\right)^4 \frac{N(1-\mu)(2\mu-1)^2}{(1+\mu)} \geq \\
&\geq \left(1-\frac{2}{\sigma^2 N}\left(1+\frac{1}{d}\right)+O\left(\frac{1}{N^2}\right)\right)\frac{\frac{\sigma}{2}\left(1-\frac{2}{N-1}\right)^2}{2-\frac{\sigma}{2N}} = \frac{\sigma}{4} - O\left(\frac{1}{N}\right)
\end{aligned}. \tag{4.30}$$

This completes the proof of Theorem 4.

In the first section of this Chapter we use results from [13] to show that the continuous time quantum walk search is optimal for the d-random regular graphs with the high probability. The second largest eigenvalue of the stochastic matrix of the d-random regular graph is according to [13] $O\left(d^{-\frac{1}{4}}\right)$ for $d \geq 3$. The condition $\frac{1}{\sigma\sqrt{N}} \ll 1$ is fulfilled for sufficiently large N and the Szegedy's search algorithm is optimal for the d-random regular graph with high probability.

Conclusion

We study in this thesis the quantum walks search algorithm and the quantum walk state transfer algorithm. In the first Chapter we discuss the Grover search algorithm and the Grover state transfer algorithm. We show that the Grover search algorithm is optimal and that the Grover state transfer algorithm achieves the perfect state transfer after $O\left(\sqrt{N}\right)$ steps.

In the second chapter we present the general scheme of the quantum walks search algorithm for the cases of the discrete time quantum walk with coins, the Szegedy's quantum walk and the continuous time quantum walk. We demonstrate how to get the quantum walk state transfer algorithm by modifying the quantum walk search algorithm. In the third Chapter we show the case of the graphs where the perfect state transfer occurs. Using the discrete time quantum walk perfect state transfer is achieved on the star graph, the complete bipartite graph and the complete graph with one self loop at each vertex in $O\left(\sqrt{N}\right)$ steps. The perfect state transfer is also achieved for the complete bipartite graph using the Szegedy's walk for N going to infinity. The continuous time quantum walk achieves the perfect state transfer on the complete graph with self loops at the time $O\left(\sqrt{N}\right)$.

In the last Chapter we focus on the search algorithm on the regular graphs. Using the Szegedy's results for the spectrum of the evolution operator we find and prove new condition for the search algorithm to be optimal. We show that the search algorithm is optimal for the d-random regular graphs for $d \geq 3$ with the high probability.

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