Application of graph theory in quantum computer science

Summary of doctoral dissertation

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Abstract in English

In this dissertation we demonstrate that the continuous-time quantum walk models remain powerful for general graph structures. We consider two aspects of this problem.

First, it is known that the standard Continuous-Time Quantum Walk (CTQW), proposed by Childs and Goldstone, can propagate quickly on the infinite path graph. However, the Schrödinger equation requires that the Hamiltonian is symmetric, and thus only undirected graphs can be implemented. In this thesis we will address the question, whether it is possible to construct a continuous-time quantum walk on general directed graphs, preserving its propagation properties.

Secondly, the quantum spatial search defined through CTQW has been proven to work well on various undirected graphs. However, most of these graphs have very simple structures. The most advanced results concerned the Erdős-Rényi model of random graphs, which is the most popular but not realistic random graph model, and Barabási-Albert random graphs, for which full quadratic speed-up was not confirmed.

The dissertation consists of 7 chapters. In Chapter 1 we provided an introduction and motivation. In Chapter 2 we present a notation and preliminary concepts used in the dissertation.

In Chapters 3 and 4 we approach the first aspect. In Chapter 3 we propose a nonmoralizing global interaction quantum stochastic walk, which is well-definable on an arbitrary directed graph. We show that this model propagates rapidly on an infinite path graph. In order to achieve the propagation speed better than the classical one, we introduced a small amplitude transfer in the direction opposite to the direction of the existing arcs. In Chapter 4 we analyze the convergence properties of the introduced model. We also introduce two other quantum stochastic walk models called local and global interaction quantum stochastic walks. We show that each of these models has very different properties. In particular, local and nonmoralizing global models present the most intuitive behavior on directed graphs. Our analysis shows that it is indeed possible to introduce a fast continuous-time quantum walk which is well-definable on general directed graphs.

In Chapters 5 and 6 we study the second of the posed questions. In Chapter 5 we correct and improve state-of-the-art results on Erdős-Rényi graphs. We also demonstrate that the convergence is correct for all vertices, instead of only 'most of them'. Compared to the previous state-of-the-art results we show that Laplacian matrix is a much simpler operator to be taken into consideration compared to the adjacency matrix. In Chapter 6 we compare three different operators plausible for the quantum spatial search.

We show that the normalized Laplacian, under certain conditions, provides the full quadratic speed-up. We analyze two random graph models which output the graphs with complex structure with high probability. The analysis confirms that the proposed operator is indeed better than other commonly used operators. Finally, we propose the procedure which solves the problem of determining the optimal time for running the quantum search algorithm.

Finally, in Chapter 7 we review and conclude our results. The dissertation also consists of two Appendix sections, which provide the proofs for the results used in the dissertation.

List of publications

Publications and preprints relevant to the dissertation are highlighted with **bold**.

Published work

1. A. Glos, A. Krawiec, and Ł. Pawela, "Asymptotic entropy of the Gibbs state of complex networks," *Scientific Reports*, vol. 11, p. 311, 2021.
2. A. Glos, N. Nahimovs, K. Balakirev, and K. Khadiev, "Upperbounds on the probability of finding marked connected components using quantum walks," *Quantum Information Processing*, vol. 20, p. 6, 2021.
3. Z. Tabi, K. H. El-Safty, Z. Kallus, P. Hága, T. Kozsik, A. Glos, and Z. Zimborás, "Quantum optimization for the graph coloring problem with space-efficient embedding," in *2020 IEEE International Conference on Quantum Computing and Engineering (QCE)*, pp. 56–62, 2020.
4. A. Glos, "Spectral similarity for Barabási–Albert and Chung–Lu models," *Physica A: Statistical Mechanics and its Applications*, vol. 516, pp. 571–578, 2019.
5. A. Glos and J. A. Miszczak, "The role of quantum correlations in Cop and Robber game," *Quantum Studies: Mathematics and Foundations*, vol. 6, no. 1, pp. 15–26, 2019.
6. A. Glos and J. A. Miszczak, "Impact of the malicious input data modification on the efficiency of quantum spatial search," *Quantum Information Processing*, vol. 18, p. 343, 2019.
7. A. Glos and T. Januszek, "Impact of global and local interaction on quantum spatial search on Chimera graph," *International Journal of Quantum Information*, p. 1950040, 2019.
8. **A. Glos, J. Miszczak, and M. Ostaszewski, "QSWalk.jl: Julia package for quantum stochastic walks analysis,"** ***Computer Physics Communications*****, 2018.**
9. **K. Domino, A. Glos, M. Ostaszewski, P. Sadowski, and L. Pawela, "Properties of Quantum Stochastic Walks from the asymp-**

totic scaling exponent," *Quantum Information and Computation*, vol. 18, no. 3&4, pp. 0181–0199, 2018.

10. **A. Glos, A. Krawiec, R. Kukulski, and Z. Puchała, "Vertices cannot be hidden from quantum spatial search for almost all random graphs," *Quantum Information Processing*, vol. 17, no. 4, p. 81, 2018.**

11. **A. Glos and T. Wong, "Optimal quantum-walk search on Kronecker graphs with dominant or fixed regular initiators," *Physical Review A*, vol. 98, no. 6, p. 062334, 2018.**

12. **K. Domino, A. Glos, and M. Ostaszewski, "Superdiffusive Quantum Stochastic Walk definable on arbitrary directed graph," *Quantum Information & Computation*, vol. 17, no. 11-12, pp. 973–986, 2017.**

13. **A. Glos, J. A. Miszczak, and M. Ostaszewski, "Limiting properties of stochastic quantum walks on directed graphs," *Journal of Physics A: Mathematical and Theoretical*, vol. 51, no. 3, p. 035304, 2017.**

14. A. Glos and P. Sadowski, "Constructive quantum scaling of unitary matrices," *Quantum Information Processing*, vol. 15, no. 12, pp. 5145–5154, 2016.

15. D. Kurzyk and A. Glos, "Quantum inferring acausal structures and the Monty Hall problem," *Quantum Information Processing*, vol. 15, no. 12, pp. 4927–4937, 2016.

Preprints

1. **R. Kukulski and A. Glos, "Comment to 'Spatial search by quantum walk is optimal for almost all graphs'," *arXiv:2009.13309*, 2020.**

2. A. Glos, A. Krawiec, and Z. Zimborás, "Space-efficient binary optimization for variational computing," *arXiv:2009.07309*, 2020.

3. K. Domino and A. Glos, "Hiding higher order cross-correlations of multivariate data using Archimedean copulas," *arXiv:1803.07813*, 2018.

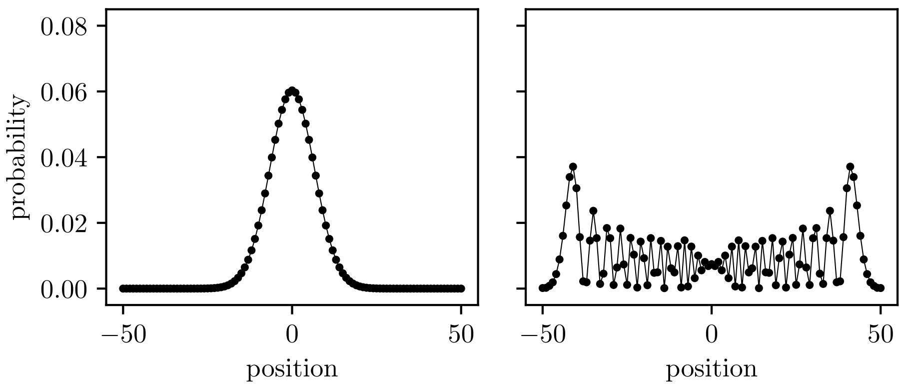
Extended summary

Recently, quantum computers have attracted a huge attention. This is because such devices can solve vital computational problems faster than their classical counterparts. What is more interesting, the speed-up is observable even in the complexity of algorithms. The best example is the Shor's algorithm [1] which solves the integer factorization problem in polynomial time in the terms of number length. It is notable to recall that any known classical algorithm that solves the same problem requires exponential time in a number of bits. Furthermore, the algorithm may threaten the current cryptographic protocols, as it can easily break RSA encryption.

The Shor's algorithm and other quantum algorithms [2,3] started an important and beautiful field called quantum computer science. The goal of this discipline is to construct the algorithms which are faster compared to the currently known algorithms for conventional computers. Despite numerous important theoretical algorithms [2, 4, 5], there are also the algorithms which have the potential practical application. One can point to the Grover's algorithm and its extensions [3,6], quantum annealing algorithms [7,8], variational optimization algorithms [9–12], and Quantum PageRank [13, 14].

Quantum algorithms can be divided into various classes according to the problem they solve or the computational model they are based on [15]. In this dissertation, we focus on a particularly important class called *quantum walks*, in which the amplitude transfer is done within some underlying graph structure [16–18]. It can be considered as an equivalent of random walk algorithms, where the probability mass transfer is not allowed when the states are not connected.

Quantum walks application comes in particular from its ballistic propagation. Let us consider a random walk on an infinite path with the probability localized at position 0. Then after time t, the probability distribution of finding the walker can be well approximated by Gauss distribution $N(0, \Theta(\sqrt{t}))$ [19]. Since the standard deviation grows proportionally to the square root of time, we say that the stochastic process obeys a normal diffusion. This is contrary to a quantum walk, where the standard deviation



(a) random walk

(b) quantum walk

Figure 1: Distribution of continuous-time random walk (left) vs continuous-time quantum walk (right) on a path graph with 101 nodes and after evolution time 22. The evolution starts in the middle of the graph.

grows like $\Theta(t^2)$ [20], i.e. we can observe the ballistic diffusion. Thus the propagation in a quantum walk may be much faster which may explain the speed-up appearing in quantum walk algorithms. The resulting distributions for both classical and quantum walks are presented in Fig. 1.

Despite the fact that the very first quantum walk is almost 20 years old, there are two important questions regarding the generality of the results in the terms of graph structure. Many quantum closed-system walk models, proposed so far, were definable on relatively general graph structures [18,21, 22]. However, it was shown under general and reasonable assumptions that by using the closed-system quantum evolution one cannot define a quantum walk on a general directed graph [23]. This results from the quasi-periodicity of the closed-system evolution, i.e. there exists an arbitrarily large time evolution t after which the system evolves to the state close to the initial state. This in turn implies that a closed-system quantum walk can only be well-defined for graphs, where, for arbitrary two nodes, there is a path connecting them.

Since close-system quantum walks are not sufficient to model the evolution on general directed graphs, interactions with the environment are necessary. However, currently known open quantum walk models do not yield the ballistic propagation [24–26]. In particular, for the continuous-time open quantum walk [24], the classical evolution destroys its coherence, and the proposed model lacks the ballistic propagation. It has been an open question whether there exists a quantum walk model which preserves the directed graph structure and whose propagation is better than the propagation observed in random walks. This may be important, for the directed graph model, for example in the case of the evolution for classical heuristic optimization algorithms like simulated annealing or tabu search.

There is a similar lack of generality for quantum spatial search algorithms. The quantum search algorithms are defined as the graph-restricted evolution, which aims at finding a marked node. Note that there are known examples of discrete quantum walks, yielding even a quadratic speed-up over an arbitrary Markov-chain walk [21, 27]. However, general and simple results are still missing for continuous-time quantum walks.

The first continuous-time quantum spatial search algorithm [18] has been deeply investigated for the special classes of graphs like complete graphs [18], grid graphs [18], binary trees [28], simplex of complete graphs [29], and others [30–32]. Based on these results, the special properties of quantum walks were presented. While the obtained results were an important step toward the development of quantum search algorithms, all of the graphs considered were almost regular (meaning all vertices have very similar degrees) and we can split the vertices into several classes (so-called vertex-transitivity), within which the vertices are indistinguishable.

The first approach in generalizing the above results was made for Erdős-Rényi graphs [33–37]. While these graphs are not regular, the deviations between the highest and the smallest degrees are sufficiently small to provide very tight results on the efficiency of quantum search on these graphs. Then three more general results were provided. The first one showed a quadratic speed-up compared to a general Markov-chain search [38], at the cost of larger Hilbert space. Additionally, in [39] quite general conditions for (optimal) quantum search for original continuous-time spatial search were presented. However, the application of these results required the full eigen-decomposition of the graph-based Hamiltonian, which in general is a hard computational task. In fact, this task is much more demanding compared to the quantum or even the classical search itself. Finally, in [40] the authors determined the efficiency of the quantum spatial search for complex graphs. However, while the speed-up over the classical search was shown, it remains an open question whether the quadratic speed-up over the Markov search is achievable.

Dissertation overview In the scope of the dissertation we demonstrate that the continuous-time quantum walk models remain powerful for general graph structure. The analysis was done by approaching two problems:

1. Does a time-independent continuous-time quantum walk model which

is definable for general directed graphs and which maintains fast propagation exist?

2. Is the original continuous-time quantum walk based spatial search [18] powerful enough to offer the speed-up for heterogeneous graphs?

Note that for both problems the context of 'general graph structure' changes. For the first problem, we focus on directed graphs, while for the second problem – on undirected graphs with significant deviation between the degrees of vertices. Currently, most of the results for quantum search considers almost regular graphs. Therefore, we consider heterogeneous graphs as a reasonable next step for investigation.

The first problem is approached using the formalism of quantum stochastic walks [41]. The model is a generalization of both continuous-time quantum walk [18] and continuous-time random walk. For the second problem, we analyze the CTQW-based spatial search [18] on random heterogeneous graphs and complex Barabási-Albert graphs [42]. The latter is a paradigmatic random graph model which simulates Internet network evolution.

The dissertation is organized as follows. In Chapter 2 we present a notation and preliminary information used in the dissertation. In Chapter 3 we analyze a quantum walk model presented in [41], in the context of the propagation. We improve the model into *nonmoralizing quantum stochastic walk* which is well-defined on any directed graphs. In order to achieve better than classical diffusion, we allowed a small amplitude transfer in the direction opposite to the direction of the existing arcs. In Chapter 4 we present convergence properties of the introduced model and compare it to other well-known quantum stochastic walk models. We confirm that the structure of the directed graph is indeed preserved. In Chapter 5 we improve the results for Erdős-Rényi presented in [33], in order to clarify the approach to the analysis of CTQW-based spatial search to random graphs. In Chapter 6 we present the analysis of the spatial search algorithm for heterogeneous and complex graphs. Finally, in Chapter 7 we justify the correctness of our hypothesis in the context of the results presented in the dissertation.

The results presented in Chapters 3 and 4 are based on the results from [43–45]. The results presented in chapters 5 and 6 are based on the results from [36, 37, 46, 47].

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