Disorder and entropy rate in discrete time quantum walks

PhD theses

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Introduction

Walks are elementary processes that consist of a sequence of atomic steps. If the sequence of steps is random, we call the process *random walk*. In general, random walks follow the Liouville equation, thus can be fully described and understood in terms of classical mechanics. Random walks are basic mathematical tools, used to model a rich variety of physical systems. The path of a single dye molecule in water (diffusion), the fluctuation of stocks, the spreading of diseases, and surfing on the internet are amongst the typical examples of such systems. In computational sciences it was also found beneficial to employ random walks, e.g. as an approach to describe probabilistic Turing machines.

Quantum walks are quantum mechanical extensions of classical random walks. As random walks are suitable tools used in statistical physics and computational sciences, quantum walks found their applications in quantum physics and quantum information theory. For example, they are suitable models for describing quantum transport, scattering and topological effects in solid state materials. In quantum information theory, quantum walks are widely used to construct quantum algorithms, in particular, search on unstructured databases. Quantum walks are also universal primitives of quantum computation: On a quantum computer, the computational process is described by unitary (reversible) transitions between elements of the state space. One can consider these elements as vertices of a graph, and the unitary computation process as a quantum walk on this very graph.

The universality and other promising aspects of quantum walks have caught the attention of experimentalists: Quantum walks have been successfully demonstrated in optical lattices using single neutral atoms and trapped ions. These experiments all have a similar approach: the internal state of the atom is rotated by an electromagnetic field, then the atom is coherently displaced in the lattice corresponding to its internal state. The repetition of this process realizes a discrete time quantum walk. A nuclear-magnetic-resonance-based experiment (realizing a quantum information processor consisting of three qubits) was also reported. Another promising way to realize quantum walks is the photonic approach: These experiments are quite diverse considering the media where the photons propagate. In integrated waveguide arrays photons scatter between parallel waveguides of close proximity; their final position density is determined by a continuous time quantum walk. These arrangements are very well suited to study multi-photon (i.e. multi-particle) walks and decoherence, as well. Experiments are also performed with linear optics mimicking the so-called optical Galton board, and by the time bin encoding of the position of the walker. This latter approach is also suitable for studying higher dimensional walks, multi-particle walks with interaction, and decoherence.

Scientific background

Quantum walks obey unitary evolution by design — they correspond to a deterministic, closed-system dynamics. A unitary and homogeneous quantum walk on a lattice usually exhibits ballistic spreading, which is quadratically faster in contrast with its classical diffusively spreading counterpart. However, in nature physical processes are subject to noise, which might disturb the unitary evolution of closed quantum systems, essentially leading to an open-system dynamics. Under such noisy condisitons quantum walks exhibit a rich variety of behaviors, for example fractional scaling in their spreading, or Anderson-localization. On the other hand, in some cases noise can enhance the spreading.

Errors in the underlying graph or lattice are special sources of noise in walks. For example, hot water (liquid) passing through ground coffee (porous or granular material) or the robustness of computer networks under attacks or power outage can be modeled with graphs, where connections are broken with some probability. This concept is called *percolation.* Percolation is extensively studied in relation to classical walks, leading to interesting phenomena, in particular, phase transitions in higher dimensional lattices. On the other hand, the question of the effect of percolation on quantum walk models is rather new and there exists only a few studies in this topic. Most of the known results are either numerical or phenomenological, due to the “size" of the problem: A quantum walk spread on a bigger graph means a bigger territory for percolation, and the number of actual percolation graphs (configurations) grows exponentially with the size of the graph. Thus, even purely numerical results are hard to obtain due to the required computational power.

In physics, entropy is the most well-known measure of information content. However, the definition of entropy is very special, since it is the average asymptotic information content *per sample* for an independent and identically distributed sequence of random variables, thus, for a stochastic process. Even for simple stochastic processes, e.g. Markov chains, which, in fact, can be interpreted as classical walks on weighted, directed graphs, entropy is not a suitable measure for the asymptotic per sample information content. In information theory, however, there exists a generalization, which is a suitable measure for general stochastic processes: the *entropy rate*. It is a rather interesting (and open) question whether for a quantum mechanical system the (classical) concept of entropy rate is applicable.

Motivations and goals

In our research we focused on the *discrete time quantum walk*, which is a non-trivial extension of the classical random walk. Here, the non-triviality is given by the introduction of the so-called *coin space*, an internal Hilbert space, by which the scalarity of classical random walks is lost. This particular model is a universal quantum computational primitive, and is also the most well-known definition of quantum walks. The time evolution of such walks effectively mimics classical discrete time walks, i.e. is given by the repeated application of a coin toss and a step operation. Albeit being very simple, this model is frequently used in theoretical physics to study transport, topological phases, multiparticle systems, and quantum algorithms. Early experiments were mostly directed to study the basic properties of discrete time quantum walks, whereas state-of-the-art experiments are aimed to explore and exploit quantum walks in a more general setting. In summary, the simple but universal definition of the model and the increasing number of experimental realizations motivated us to study this system.

The question considering the behavior of quantum walks on percolation graphs is rather new and still open. As the computational cost of the problem is exponential with respect to the size of the underlying graph, any brute force numerical simulations are doomed to fail. Analytical results on this topic were mostly phenomenological so far. We first aimed to perform efficient numerical simulations to aid the analytical studies. Our next goal was to develop analytical methods which allow for solving the general problem. Our final goal was to deploy the developed methods in order to learn about the physics of some particularly interesting quantum walks on percolation graphs.

Entropy rate is an interesting concept generalizing entropy for stochastic processes. As classical walks are the textbook examples of Markov chains, on which entropy rate is a meaningful definition, it is a rather interesting question whether the concept of entropy rate is applicable in the case of quantum walks (which are quantum Markov chains). A further interesting fact is that unitary quantum processes can be disturbed by measurements. It is known that frequent measurements on a quantum system can result in interesting phenomena, e.g. the quantum Zeno effect. We aimed at answering the following questions: What happens with a periodically measured quantum walk? If one has access to the measurement data only, is it possible to say something regarding the quantumness of the system? Does the classical concept of entropy rate reflect the non-classicality of a frequently measured quantum system?

Applied methods

In the first model we studied, the transport process (step) of the walk was disturbed by some noise corresponding to classical randomness. We described this noise as a change in the connectivity of the underlying graph given by dynamical percolation. To study this problem, we employed the asymptotic theory of random unitary operations. As a by-product we proposed an ansatz based on pure eigenstates, in order to get a better physical insight. To check our analytical results, we have also performed numerical studies. As the computational cost of the problem is exponential with respect to the size of the underlying lattice, we took advantage of the nearest neighbour interactions of the model to develop a more efficient algorithm, which ultimately resulted in a polynomial scaling.

For our studies considering the entropy rate of quantum walks, we employed the tools of classical information theory. To give a reference we determined the entropy rate of some periodically measured classical walks. Then, we numerically checked whether the concept of entropy rate is applicable for quantum systems as well. These checks were performed using two different approaches: First, by calculating the "partial entropy rate" up to a finite number of steps and by predicting its convergence. Next, we employed Monte Carlo simulations to predict the convergence. As entropy rate is an asymptotic quantity, we needed to perform an elaborate analysis in order to solve the problem formally. For this analysis we used the homogeneity of the system. We also employed the hidden Markov model to give an upper bound approximation for the entropy rate. We used the so-called *weak limit* (i.e. an asymptotic rescaled position distribution) of the model to determine the scaling of the entropy rate in the rare measurement limit. To compare different possible approaches known form the literature, we calculated the entropy rate considering other definitions and measurement processes.

New scientific results

1. I have developed a general method for solving the asymptotics of discrete time quantum walks on percolation graphs. This general method is based on the attractor-space formalism of the asymptotic method of random unitary operations, which I separated into two parts by making a difference between the coin toss and position step. I have shown that the separation process allows for solving the problem for whole families of graphs and coins. I have also shown that the superoperator describing the dynamics of the percolation quantum walk can be constructed polynomially on regular graphs with respect to the number of sites [I].
2. I presented a method for determining the asymptotic attractors of random unitary operations. The core of this method is to find the common eigenstates of the dynamics, which can be used to form attractors with a direct physical meaning. I have shown that these common eigenstates span a decoherence-free subspace. I have also shown that in some cases the complete attractor space can be determined via common eigenstates and the trivial attractor (corresponding to the completely mixed state). I determined the formula of the asymptotic time evolution in this case, which is given as an incoherent mixture of the unitary dynamics on the decoherence-free subspace spanned by common eigenstates and the completely mixed state on its orthogonal complement. I have also illustrated the method on discrete time quantum walks on dynamical percolation graphs and pointed out the important differences with respect to the general method [II].

3. I have explicitly solved the asymptotic dynamics of one-dimensional percolation quantum walks by employing the methods I developed. I have given the attractor space in a closed form for the percolation cycle and linear graph for the complete $SU(2)$ problem. I have shown that there are non-trivial asymptotics: stationary states with quantum coherences and limit cycles can appear. I have analyzed the physical form of the solutions and discovered that on the linear graph the solutions are edge states for most of the coin operators [III].

4. I have explicitly solved the asymptotic dynamics of the two-dimensional Hadamard and Grover walks on the percolation torus and carpet. I have shown that in contrast to its one-dimensional counterpart, the Hadamard walk exhibits asymptotic position inhomogeneity. I have also discovered that the percolation model in certain cases is sensitive to rotation, in contrast with the corresponding undisturbed (unitary) quantum walk. I have found that the common eigenstates of the Grover walk have finite support, thus the walk keeps its trapping property in the percolation case [II].

5. I have defined a stochastic process based on the periodically measured quantum and classical walks. I have given a general method for calculating the classical entropy rate of these stochastic processes. I have shown that the frequently measured quantum walk behaves as a classical Markov chain in the position-coin state basis, and the entropy rate of this Markov chain is equal to the entropy rate of the previously defined

stochastic process. I have also given a method for calculating the lower and upper bounds of this entropy rate. I have found that in the regime of frequent measurements, the entropy rate of the quantum-walk-based model is usually lower, due to the memory effect of the coin state of the particle [IV].

6. I have developed an approximation protocol to give an upper bound to the exact entropy rate of the periodically measured quantum walks. I have estimated the scaling of the entropy rate of the one-dimensional Hadamard walk with respect to the time (number of discrete steps) between measurements using the so-called weak limit theorem. I have found that for rare measurements the entropy rate is dominated by the ballistic spreading of the quantum walk, thus the entropy rate is higher than in the classical case. I have also studied finite systems and discovered that collapses and revivals can occur in the quantum walk based system. I have also calculated the "most quantum case" and the quantum entropy rate of the model to give a comparison. I found that both of these models are inconclusive for periodically measured walks. On the other hand, the classical-entropy-rate approach I proposed is a suitable tool to capture some of the quantum features of the system [IV].

List of publications

Related publications

[I] B. Kollár, T. Kiss, J. Novotný, I. Jex, *Asymptotic Dynamics of Coined Quantum Walks on Percolation Graphs*, Phys. Rev. Lett. **108**, 230505 (2012)

[II] B. Kollár, J. Novotný, T. Kiss, I. Jex, *Percolation induced effects in two-dimensional coined quantum walks: analytic asymptotic solutions*, New J. Phys. **16**, 023002 (2014)

[III] B. Kollár, J. Novotný, T. Kiss, I. Jex, *Discrete time quantum walks on percolation graphs*, Eur. Phys. J. Plus **129**, 103 (2014)

[IV] B. Kollár, M. Koniorczyk, *Entropy rate of message sources driven by quantum walks*, Phys. Rev. A **89**, 022338 (2014)

Other publications

[V] B. Kollár, M. Štefaňák, T. Kiss, I. Jex, *Recurrences in three-state quantum walks on a plane*, Phys. Rev. A **82**, 012303 (2010)

[VI] M. Štefaňák, B. Kollár, T. Kiss, I. Jex, *Full revivals in 2D quantum walks*, Phys. Scr. **T140**, 014035 (2010)

[VII] M. Štefaňák, S. M. Barnett, B. Kollár, T. Kiss, I. Jex, *Directional correlations in quantum walks with two particles*, New J. Phys. **13**, 033029 (2011)