Excitation transfer by quantum walks on disrupted carbon nanotube structures

Jan Mareš[1]

[1]Department of Physics, Faculty of Nuclear Sciences and Physical Engineering,
Czech Technical University in Prague, Břehová 7, 11000 Prague 1, Czech Republic

Spreading of an excitation governed by laws of quantum physics is of interest in many branches of research. A suitable model for studying transport in microscopic media without specifying any concrete physical system is a quantum walk, where the medium is represented by an abstract undirected graph. The definition of a quantum walk is very versatile and allows for simulation of various scenarios. In this view, quantum walks can serve as a theoretical mediator allowing simulation of one quantum system using some other quantum system.

Since all real systems are subjected to interactions with their environment, it is necessary to deal with the effects of random disturbances of our system resulting in open system dynamics. Quantum walks are also suitable for investigation of transport in disrupted media when we introduce so called dynamical percolation - in every step of the walk some edges of the graph are randomly chosen to be closed (and possibly reopend in future steps). Such system is not only of theoretical interest, but was already realised in a proof-of-principle experiment with a time-multiplexed quantum walk in an optical loop [1].

Instead of investigating rates of spreading on infinite structures, we study long-time limit of transfer from some initial state to a given sink in a finite graph. While for most choices of the quantum walk dynamics the walker will always reach the sink, there are variants with a chance of the walker getting trapped in some part of the graph indefinitely. This can occur in so called lazy quantum walk on a line graph (or a closed ring), where the walker has the possibility of staying in a given vertex during the step instead of moving to either side [2].

We take the investigation to much more complex structures - graphs representing carbon nanotubes. We show, that the effect of trapping is not caused by the presence of the no-movement states but rather by vertices of the degree higher than 2 in the graph. We investigate both the percolated version of the walk and the non-percolated one. The trapping occurs in both variants, but percolation may exclude some of the trapped states from the asymptotics and therefore enhance transfer, as was already reported in [2].

Firstly, we present an analytical approach capable of identifying all the trapped states in the percolated walk and also for the non-percolated walk in all studied cases, allowing us to calculate asymptotic transfer probabilities from one end of the tube to the other. The transfer probability is crucially dependent on the initial state of the walker. Numerical simulations do not allow for exploring sufficient amount of initial states, but our analytical approach allows to identify the states with maximal and minimal transport easily.

In some cases of percolated quantum walks on nanotube structure graphs we observe and interesting phenomenon: the minimal transfer probability increases with the length of the tube (shorter tubes have higher probability to trap the excitation). Again, our insight into the structure of the trapped states allow us to explain this non-intuitive behaviour.

Our second main contribution is a new approach for numerical simulation of percolated quantum walks. For a graph with e undirected edges, there are 2^e possible configurations of the percolated graph with corresponding evolution operators. Direct construction of the evolution super-operator by combining all these operators (sum over all possibilities weighted by their respective probabilities) is impossible for larger graphs. Nevertheless, for a percolated quantum walk we are able to construct the super-operator analytically resulting in an application of a single (non-unitary) operator. This allows us to calculate tens of thousands of steps on graphs like the one in Fig. 1. We can therefore verify our analytical results on asymptotic transport or use the simulation for any further research.

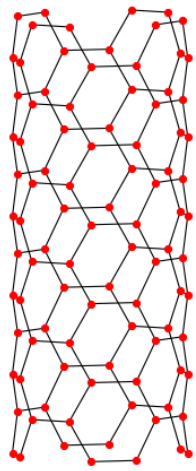

Figure 1: Example nanotube graph with 136 edges (2^{136} possible configurations of the percolated graph).

[1] F. Elster et al. "Quantum walk coherences on a dynamical percolation graph", Scientific Reports. **5**:13495, (2015).

[2] M. Štefaňák et al. "Percolation assisted excitation transport in discrete-time quantum walks", New J. Phys. **18**:023040, (2016).