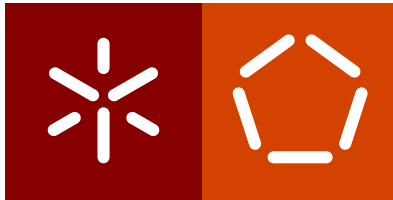


definition



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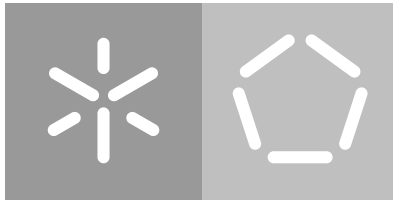
Jaime Santos

Staggered Quantum Walks in Qiskit?? Second Part of Title

First Part of Subtitle

Second part of Subtitle

February 2020



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Staggered Quantum Walks in Qiskit?? **Second Part of Title**

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Second part of Subtitle

Master dissertation
Master Degree in Física da Informação

Dissertation supervised by
Luís Barbosa
Bruno Chagas

February 2020

ACKNOWLEDGEMENTS

Write acknowledgements here

ABSTRACT

Implementation of staggered quantum walks in qiskit.

RESUMO

Pensar no que escrever aqui.

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INTRODUCTION

1.1 BRIEF HISTORY OF QUANTUM COMPUTING

1.1.1 [TEMP ARTIGOS RELEVANTES]

kendon2006 - Introducao historia CQ - Pasta introqw / Coin toffoli1980- Reversible Computing - Pasta intromain

gottesman1998- The Heisenberg Representation of Quantum Computers - Pasta intromain

rebuscado turing1936 - ON COMPUTABLE NUMBERS, WITH AN APPLICATION TO THE ENTSCHEIDUNGSPROBLEM - Pasta intromain

Random walks classicas -

1.2 CLASSICAL AND QUANTUM RANDOM WALKS

From classical random walks to quantum random walks. Balu2017 introdução

1.3 STATE OF THE ART QUANTUM WALKS IMPLEMENTATIONS

Mencionar que o proximo capitulo tem implementacoes de outros algoritmos.

timeline da wikipedia

ler artigos das implementações circuitos locke a e b; douglas wang

1.4 TEXT OVERVIEW AND CONTRIBUTIONS

QUANTUM COMPUTING

qubits
esfera de bloch
rotacoes – implementacoes simples nos pcs da ibm.
grover exemplo. Artigo coles 2018 , livro do nielsen tambem.
isto nao seria state of the art ?
Fazer ao estilo do Nielsen pag. 174, meter exemplos do qiskit

2.0.1 [TEMP ARTIGOS RELEVANTES]

bennet1996- Strengths and Weaknesses of Quantum Computing - Pasta intromain
deutsch1992- Rapid solution of problems by quantum computation - Pasta intromain
gottesman1998- The Heisenberg Representation of Quantum Computers - Pasta intromain
shor1994- Algorithms for quantum computation: discrete logarithms and factoring - Pasta intromain
toffoli1980- REVERSIBLE COMPUTING - Pasta intromain
wootters1982- A single quantum cannot be cloned - Pasta intromain
zalka1999- Grover's quantum searching algorithm is optima - Pasta intromain
aharonov2001.pdf - Modelo computação quântica.

QUANTUM WALKS

Falar dos varios tipos de caminhada quantica sem circuito
talvez simulacoes em python??
ambainis2004 - Pasta introqw/Coin
introducao com random walks classicas
Meter resultados simulacoes de python.

3.1 COINED QUANTUM WALK

3.1.1 *[TEMP Artigos relevantes]*

MAIS MOEDAS. aharonov1993 - Pasta introqw/Coin
aharonov2001 - Pasta introqw/Coin - definicao da QW ;shift operator mod n
ambainis2001 - Pasta introqw/Coin
carteret2005- Implementacao - Pasta introqw/Coin
inui2003 - - Pasta introqw/Coin
kendon2006 - Introducao historia CQ - Pasta introqw/Coin
shenvi2002 - Relacao com grover pg. 10
Resto da pasta.

3.1.2 *Texto*

In this section, the author will introduce the concept of a *classical random walk*. Consider a one dimensional walker on top of a line, whose decision to go left or right depends on a coin toss. As shown in Portugal (2018), the outcome after many iterations of the coin toss is a binomial distribution centered in the starting position with a standard deviation of \sqrt{t} , where t is the number of time steps. The one dimensional walk can be abstracted to a graph of any dimension, that if allowed to be weighted and directed could also be called a Markov chain, as defined in A.2.

In the quantum case, the walker is a quantum system whose position x on the line is described by a vector $|x\rangle$ in Hilbert Space. The next position of the system is determined by a unitary operator, which can be viewed as a quantum coin. The analogy is, if the coin is tossed and rolls "heads", for example, the system transitions to position $|x + 1\rangle$, otherwise it advances to $|x - 1\rangle$. The Hilbert space of the system is thus $\mathcal{H} = \mathcal{H}_C \otimes \mathcal{H}_P$, where \mathcal{H}_C is the two-dimensional Hilbert space associated with the "coin" and \mathcal{H}_P is the one-dimensional lattice's Hilbert space.

The most commonly used unitary operator is the Hadamard operator, whose actions produce the following states:

$$H |0, x\rangle = \frac{|0, x\rangle + |1, x\rangle}{\sqrt{2}} \quad (1)$$

$$H |1, x\rangle = \frac{|0, x\rangle - |1, x\rangle}{\sqrt{2}} \quad (2)$$

The transition from $|x\rangle$ to either $|x + 1\rangle$ or $|x - 1\rangle$ must be described by a unitary operator, the *shift operator*:

$$S |0, x\rangle = |0, x - 1\rangle \quad (3)$$

$$S |1, x\rangle = |1, x + 1\rangle \quad (4)$$

The entire description of this operator is then:

$$S = |0\rangle \langle 0| \otimes \sum_{x=-\infty}^{x=\infty} |x + 1\rangle \langle x| + |1\rangle \langle 1| \otimes \sum_{x=-\infty}^{x=\infty} |x - 1\rangle \langle x| \quad (5)$$

It then follows that the operator that describes the dynamics of the quantum walk can be given by:

$$U = S(H \otimes I) \quad (6)$$

Consider a quantum system located at $|x = 0\rangle$ with coin state $|0\rangle$, for $t = 0$. It's state will be described by:

$$|\psi(0)\rangle = |0, x = 0\rangle \quad (7)$$

After t steps the walker's state will be given by

$$|\psi(t)\rangle = U^t |\psi(0)\rangle \quad (8)$$

The system's evolution will then be:

$$|\psi(0)\rangle \xrightarrow{U} |\psi(1)\rangle \xrightarrow{U} |\psi(2)\rangle \xrightarrow{U} (\dots) \xrightarrow{U} |\psi(t)\rangle \quad (9)$$

After applying the Hadamard operator followed by the shift operator twice the respective system states are

$$|\psi(1)\rangle = \frac{|0, x = -1\rangle + |1, x = 1\rangle}{\sqrt{2}} \quad (10)$$

$$|\psi(2)\rangle = \frac{|0, x = -2\rangle + |1, x = 0\rangle + |0, x = 0\rangle - |1, x = 2\rangle}{2} \quad (11)$$

If one were to measure the system after each application of U , it would be expected, after the first iteration (10), to see the walker in position $x = 1$ 50% of the time, and at $x = -1$ for the remainder. During the second iteration (11), the walker should be at $x = 2$ or $x = -2$ with 25% chance each. Measure the system t times and the result is a binomial probability distribution. The conclusion is that repetitive measurement of a coined quantum walk system reduces it to the classical case, which means that any desired quantum behaviour is lost.

It is possible, however, to make use of the quantum correlations between different positions to generate constructive or destructive interference, by applying the Hadamard and shift operators successively without intermediary measurements. This course of action results in a probability distribution other than the binomial one, and the standard deviation is not \sqrt{t} .

In order to study this distribution, a simulation of the coined quantum walk was coded in *Python*, [PRESENTE ONDE?]. Using the Hadamard coin and the aforementioned initial condition, the resulting probability distribution is:

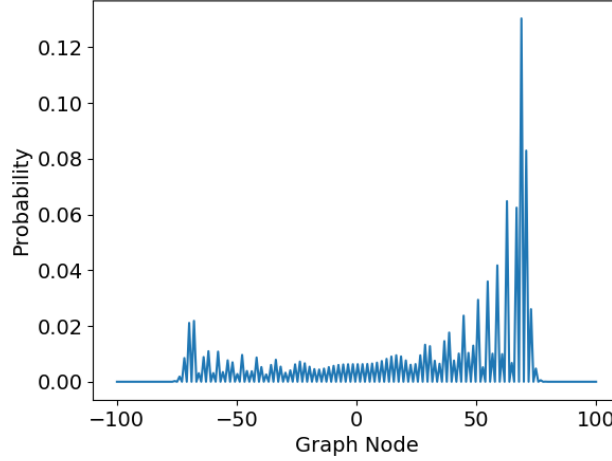


Figure 1: Probability distribution for the coined quantum walk on a line, after 100 steps, with initial condition $|\psi(0)\rangle = |0, x = 0\rangle$ and the Hadamard coin.

Analyzing the plot, it is noticeable that the distribution is asymmetric, the probability amplitude of finding the walker at the right-hand side is much larger than at the left, with a peak around $x = \frac{100}{\sqrt{2}}$ [COMO POSSO PROVAR ISTO? Confirmar atraves de graficos]. Regardless of number of steps, this peak is always present (albeit in varying positions), which is to say that the walker can always be found moving in a uniform fashion away from the origin, implying that the quantum walk has *ballistic* behaviour.

Another interesting case study is to find if this behaviour is preserved for a symmetric distribution around the origin. For this purpose, one must first understand where the asymmetry comes from. The Hadamard operator induces a sign flip [in OU on ?] state $|1\rangle$, hence more terms are cancelled when the coin state is $|1\rangle$ [FAZER DEMONSTRAÇÃO?]. Since $|0\rangle$ was defined to induce movement to the right, the result is as shown in 1. It then follows that the initial condition

$$|\psi(0)\rangle = -|1, x = 0\rangle \quad (12)$$

Will return a mirror image of 1:

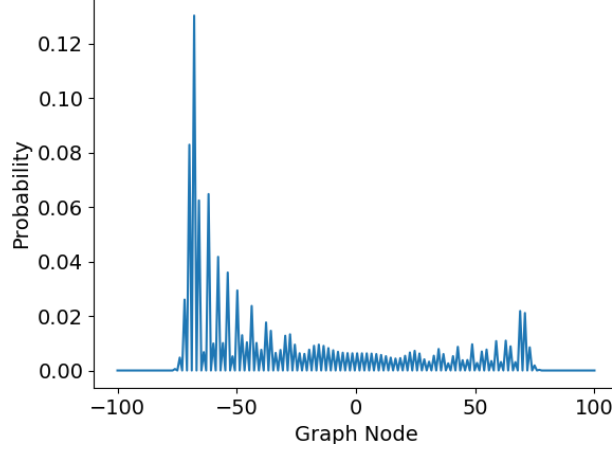


Figure 2: Probability distribution for the coined quantum walk on a line, after 100 steps, with initial condition $|\psi(0)\rangle = -|1, x=0\rangle$ and the Hadamard coin.

In order to obtain a symmetrical distribution, one must superpose 7 and 31 carefully, as to not cancel terms before the calculation of the probability distribution, by multiplying 31 by the imaginary unit. This works because the entries of the Hadamard operator are real numbers; terms with the imaginary unit will not cancel out with terms without it[FAZER DEMONSTRAÇÃO?], thus the walk can proceed to both left and right. The initial condition is then:

$$|\psi(0)\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}} |x=0\rangle \quad (13)$$

With a corresponding plot:

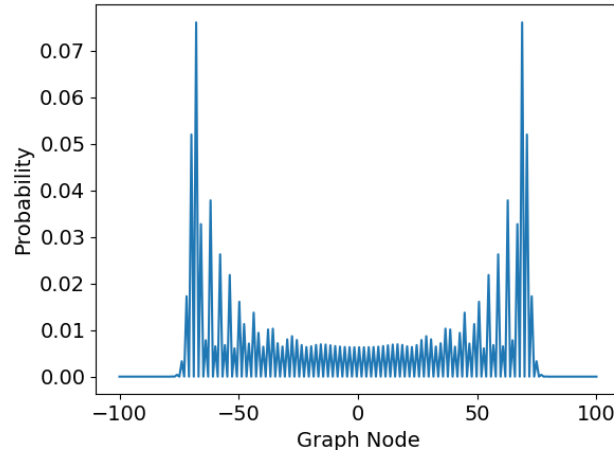


Figure 3: Probability distribution for the coined quantum walk on a line, after 100 steps, with initial condition $|\psi(0)\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}} |x=0\rangle$ and the Hadamard coin.

3.2 CONTINUOUS-TIME QUANTUM WALK

3.2.1 [TEMP Artigos relevantes]

Loke2016b- Pasta introqw childs2001 childs2004 dam2002 pg 204 nielsen fazer mais conds
iniciais

3.2.2 [Text]

The transition from the classical random walk model (A.2) to the coined quantum model was done by replacing the probability vector by a state vector of probability amplitudes and the transition matrix by a unitary matrix. The position Hilbert space was also extended with the coin Hilbert space, through the tensor product. The same will be done for A.3 resulting in the *continuous-time Quantum Walk*.

In this case, the nodes can be viewed as quantum states that form the basis for the Hilbert space, and the first step is to create an Hamiltonian with non-zero matrix elements only between states that are adjacent (connected) in the graph. Matrix \hat{H} is Hermitan and matrix M is not necessarily unitary, which can be fixed by replacing the generating matrix \hat{H} by $i\hat{H}$.

The quantum system is then started in the state corresponding to the topmost node and has a time evolution determined by \hat{H} so that the unitary time evolution operator is

$$U(t) = e^{-iHt} \quad (14)$$

The quantum state at time t , for the corresponding state $|\psi(0)\rangle$, will be

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle \quad (15)$$

With a probability distribution

$$p_k = |\langle k|\psi(t)\rangle|^2 \quad (16)$$

where k is a vertex and $|k\rangle$ is the state of the computational basis relative to k .

Considering the line example, matrix H will reduce to

$$H_{ij} = \begin{cases} 2\gamma, & \text{if } i = j; \\ -\gamma, & \text{if } i \neq j \text{ and adjacent;} \\ 0, & \text{if } i \neq j \text{ and not adjacent.} \end{cases} \quad (17)$$

And, when applied to a position:

$$H|x\rangle = -\gamma|x-1\rangle + 2\gamma|x\rangle - \gamma|x+1\rangle \quad (18)$$

Coding this into Python [METER AQUI A REFERENCIA], the following plot was obtained setting the transition rate to $\gamma = \frac{1}{2\sqrt{2}}$ the initial condition to $|\psi(0)\rangle = |0\rangle$:

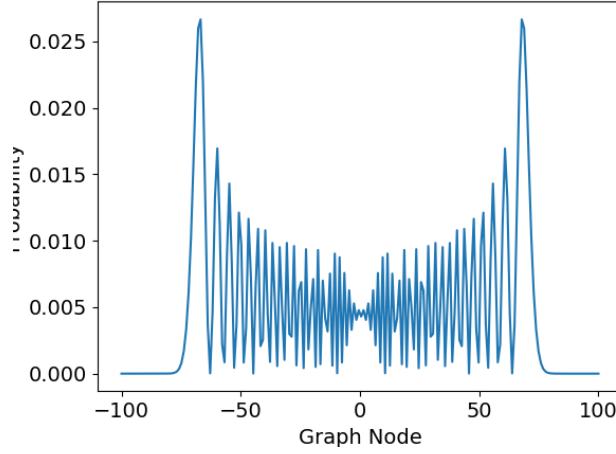


Figure 4: Probability distribution for the continuous-time quantum walk on a line, after 100 steps, with initial condition $|\psi(0)\rangle = |0\rangle$ and the Hadamard coin.

3.3 STAGGERED QUANTUM WALK

Similarly to the continuous-time quantum walk, the staggered case aims to spread a transition probability to neighboring vertices. The notion of adjacency now comes from cliques¹, and the initial stage of this walk consists in partitioning the graph in several different cliques. This is called a tessellation, and it is defined as the division of the set of vertices into disjoint cliques. An element of tessellation \mathcal{T} is called a polygon, and it's only valid if all of its vertices belong to the clique in \mathcal{T} . The set of polygons of each tessellation must cover all vertices of the graph, and the set of tessellations $(\mathcal{T}_1, \mathcal{T}_2, \dots, \mathcal{T}_k)$ must cover all edges.

These definitions allow the construction of operators H_1, H_2, \dots, H_k that will be used to propagate the probability amplitude locally, in each polygon. The state associated to each polygon is

$$|u_j^k\rangle = \frac{1}{\sqrt{|\alpha_j^k|}} \sum_{l \in \alpha_j^k} |l\rangle \quad (19)$$

where α_j^k is the j -th polygon in the k -th tessellation.

The unitary and Hermitian operator H_k , associated to each tessellation is defined in [Portugal et al. \(2017\)](#) as:

$$H_k = 2 \sum_{j=1}^p |u_j^k\rangle \langle u_j^k| - I \quad (20)$$

¹ A clique is defined as the subset of vertices of an undirected graph such that every two distinct vertices in each clique are adjacent.

The authors also show that the evolution operator can be generalized with Hamiltonians

$$U = e^{i\theta_k H_k} \dots e^{i\theta_2 H_2} e^{i\theta_1 H_1} \quad (21)$$

where

$$e^{i\theta_k H_k} = \cos(\theta_k)I + i \sin(\theta_k)H_k \quad (22)$$

and $H_k^2 = I$.

The simplest use case of this quantum walk model is the one-dimensional lattice, where the minimum tessalations are:

$$\mathcal{T}_\alpha = \{\{2x, 2x+1\} : x \in \mathbb{Z}\} \quad (23)$$

$$\mathcal{T}_\beta = \{\{2x+1, 2x+2\} : x \in \mathbb{Z}\} \quad (24)$$

Each element of the tessellation has a corresponding state, and the uniform superposition of these states is:

$$|\alpha_x\rangle = \frac{|2x\rangle + |2x+1\rangle}{\sqrt{2}} \quad (25)$$

$$|\beta_x\rangle = \frac{|2x+1\rangle + |2x+2\rangle}{\sqrt{2}} \quad (26)$$

One can now define operators H_α and H_β as:

$$H_\alpha = 2 \sum_{x=-\infty}^{+\infty} |\alpha_x\rangle \langle \alpha_x| - I \quad (27)$$

$$H_\beta = 2 \sum_{x=-\infty}^{+\infty} |\beta_x\rangle \langle \beta_x| - I \quad (28)$$

The next step is to define the Hamiltonian evolution operator as

$$U = e^{i\theta H_\beta} e^{i\theta H_\alpha} \quad (29)$$

and apply it to an initial condition $|\psi(0)\rangle$, resulting in the time evolution operator

$$U |\psi(t)\rangle = U^t |\psi(0)\rangle \quad (30)$$

Coding and plotting this algorithm in Python, the following graphs will help analysing the behaviour of the staggered quantum walk.

3.4 DESVIO PADRAO

-grafico com a media dependendo da cond inicial - grafico do quadrado da media

IMPLEMENTATIONS AND APPLICATIONS

meter aqui os circuitos.

Pagerank? paparo2012 tem coisas

Simulações em python?

mencionar PC IBMQ

DISCUSSIONS AND CONCLUSION

discutir os resultados encontrados, o future work, o que falta fazer etc.

5.1 CONCLUSIONS

5.2 PROSPECT FOR FUTURE WORK

BIBLIOGRAPHY

Renato Portugal. *Quantum Walks and Search Algorithms*. Springer, 2018.

Renato Portugal, M. C. de Oliveira, and J. K. Moqadam. Staggered quantum walks with hamiltonians. *Physical Review A*, 95(1):012328, 2017.

SUPPORT MATERIAL

A.1 GRAPHS

A.2 CLASSICAL DISCRETE-TIME MARKOV CHAINS

A *classical Markov Chain* is a stochastic process that assumes discrete values and whose next state depends only on the current state, which is ruled by a deterministic or random rule based only on the current state. This can be viewed as a directed graph where the states are represented by *nodes* and the transitions between states by *edges*. In the case of the classical discrete-time Markov chain, each transition has an associated probability distribution and, after choosing an order for the states, this distribution is described by a vector:

$$\vec{p}(t) = \begin{bmatrix} p_1(t) \\ p_2(t) \\ \vdots \\ p_n(t) \end{bmatrix}$$

where $p_i(t)$ is the probability of the walker being on vertex x_i at time t . Due to the probabilistic nature of the transitions, one cannot tell the exact node the walker will be at a future time. One can instead determine the probability distribution, which will require the *transition matrix* M . **[POR ACABAR]**

A.3 CLASSICAL CONTINUOUS-TIME MARKOV CHAINS

Previously in [A.2](#), the *classical discrete-times Markov chains* were defined in order to make the transition from the *classical random walk* to the *coined quantum walk* ([3.1](#)). This appendix comes as an additional tool to better understand [3.2](#).

Continuous time can be considered a stochastic process where time can be any non-negative real number, and the walker can now transition from vertex x_i to x_j at any time.

Eventually, the probability of the walker being found in adjacent vertices will increase and the probability of staying on x_i decrease. This is called the *transition rate*, γ , and it is homogeneous and uniform¹. The probability of this transition is γ over time.

In order to deal with continuous variables, one must consider an *infinitesimal* time interval, τ , and solve the problem's differential equation. The probability of a transition during this time interval is thus $\gamma\tau$. The degree of vertex x_j is defined as d_j , will also be a component of the probability since it relates to how many other vertices it is connected to. After τ time, it is expected to see a transition with probability $d_j\gamma\tau$ and a standstill with $1 - d_j\gamma\tau$ probability. It is now possible to define a transition matrix as

$$M_{ij} = \begin{cases} 1 - d_j\gamma\tau + O(\tau^2), & \text{if } i = j; \\ \gamma\tau + O(\tau^2), & \text{if } i \neq j; \end{cases} \quad (31)$$

[Perceber o O] And an auxiliary generating matrix as

$$H_{ij} = \begin{cases} d_j\gamma, & \text{if } i = j; \\ -\gamma, & \text{if } i \neq j \text{ and adjacent}; \\ 0, & \text{if } i \neq j \text{ and not adjacent.} \end{cases} \quad (32)$$

Since the next state of a Markov state only depends on the current state, the probability of two independent events is given by their multiplication. The transition matrix at different times will then be

$$M_{ij}(t + \tau) = \sum_k M_{ik}(t)M_{kj}(\tau) \quad (33)$$

By noticing that one needs only to calculate the transitions for vertices adjacent to x_j and after some manipulation of 34, as was done in Portugal (2018), one arrives at the following differential equation

$$\frac{dM_{ij}(t)}{dt} = - \sum_k H_{kj}M_{ik}(t) \quad (34)$$

Setting the initial condition $M_{ij}(0) = \delta_{ij}$ [Perceber a cond inicial - e simplesmente a identidade], the solution for the differential equation is

$$M(t) = e^{-Ht} \quad (35)$$

With the transition matrix defined, the corresponding probability distribution will be

$$\vec{p}(t) = M(t)\vec{p}(0) \quad (36)$$

[Tentar completar mais isto e alterar um bocado o texto.]

¹ It is the same for all vertices and times, respectively.