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# Staggered quantum walk on a line of diamonds

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**Abstract.** The staggered model is a discrete-time quantum walk model, whose evolution operator is obtained from a set of graph tessellations. We use this model to analyze the standard deviation of the probability distribution on a line of diamonds. The results help to understand the dynamics of quantum walks and it can be used as tools for building quantum algorithms.

**Keywords.** Staggered quantum walk, graph tessellation, first and second moments, standard deviation

## 1 Introduction

The staggered quantum walk model [5] was proposed recently and many of its properties have been analyzed, such as searching on two-dimensional lattices [3] and implementation on superconducting quantum circuits [1]. This model is a generalization of the Szegedy model. The staggered quantum walk with Hamiltonians [4] is important because only with the use of Hamiltonians we obtain quantum-walk-based algorithms faster than the classical equivalents.

In this work, we analyze the staggered quantum walk with Hamiltonians on a line of diamonds, which is the graph depicted in Fig. 1. The evolution operator ( $U = e^{i\theta H_1} e^{i\theta H_0}$ ) of the model is obtained from a tessellation cover, which is a set of tessellations that covers the edges of the graph. We analytically calculate the standard deviation of the position of the walker as a function of the number of time steps and we confirmed the result with numerical simulations. The value of  $\theta$  that maximizes the standard deviation is

$$\theta^* = \arctan(3\sqrt{3}), \quad (1)$$

which is different from the optimal value of  $\theta$  for the staggered model on the line, which is  $\theta = \pi/3$  [4]. As far as we know, the results presented in this work are new in the literature.

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## 2 Evolution operator of the staggered model

The line of diamonds is a graph obtained by replacing each vertex of an infinite one-dimensional lattice by a diamond,<sup>4</sup> as depicted in Fig. 1. The labels of the vertices are ordered pairs  $(x, y)$ , where  $x \in \mathbb{Z}$  is the horizontal position and  $y \in \{0, 1\}$  is the vertical position. The Hilbert space  $\mathcal{H}$  associated with this graph is spanned by vectors of the computational basis  $\{|2x, 0\rangle : x \in \mathbb{Z}\} \cup \{|2x + 1, y\rangle : x \in \mathbb{Z}, 0 \leq y \leq 1\}$ .

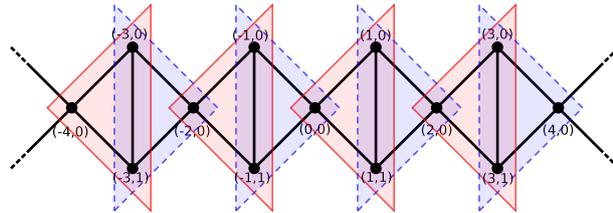


Figure 1: Diamond line with red and blue tessellations.

To obtain the evolution operator of the staggered quantum walk, the first thing we do is a partition of the set of vertices into cliques.<sup>5</sup> We call the partition by tessellation and the elements of the partition by polygons. Fig. 1 shows an example of two tessellations, the red (continuous line) and the blue (dashed line) tessellations. Each polygon consists of the three vertices in the red (blue) triangles, and a tessellation is the set of all red (blue) triangles. An edge  $e$  belongs to a tessellation  $\mathcal{T}$  if the endpoints of  $e$  are in the same polygon of  $\mathcal{T}$  and, in this case, we say that  $\mathcal{T}$  covers  $e$ .

Now we associate each polygon of each tessellation with a unit vector. The most usual association is the uniform superposition. For the red tessellation we have

$$|u_x^0\rangle = \frac{1}{\sqrt{3}} (|2x, 0\rangle + |2x + 1, 0\rangle + |2x + 1, 1\rangle). \quad (2)$$

To make this association, the vectors of the computational basis that represent the vertices of a polygon must have non-zero complex amplitude and all the others vectors must have zero amplitude. The first local operator is

$$H_0 = 2 \sum_{x=-\infty}^{\infty} |u_x^0\rangle\langle u_x^0| - I. \quad (3)$$

Since the red tessellation does not cover all edges of the graph, we need at least a second tessellation, which is associated with a second local operator. Similarly, the unit vector associated with the blue polygons are

$$|u_x^1\rangle = \frac{1}{\sqrt{3}} (|2x, 0\rangle + |2x - 1, 0\rangle + |2x - 1, 1\rangle). \quad (4)$$

<sup>4</sup>A diamond is a complete graph with four vertices minus one edge.

<sup>5</sup>A clique is a subset of the vertex set that induces a complete graph.

The second local operator is

$$H_1 = 2 \sum_{x=-\infty}^{\infty} |u_x^1\rangle\langle u_x^1| - I. \tag{5}$$

Since the red and blue tessellations cover all edges of the graph, we define the evolution operator by

$$U = e^{i\theta H_1} e^{i\theta H_0}, \tag{6}$$

where  $\theta$  is an angle. The state of the quantum walk at time  $t \in \mathbb{Z}^+$  is

$$|\psi(t)\rangle = U^t |\psi(0)\rangle, \tag{7}$$

where  $|\psi(0)\rangle$  is the initial state, and the probability of finding the walker on vertex  $(x, y)$  after  $t$  time steps is  $p_{x,y}(t) = |\langle x, y | \psi(t) \rangle|^2$ . When we fix  $t$ ,  $p_{x,y}(t)$  is a probability distribution.

### 3 Standard deviation

The standard deviation of the position of the walker using the probability distribution  $p_{x,y}(t)$  describes how far we can find the walker with respect to its initial position, which is given by  $(x, y) = (0, 0)$ . We want to determine the value of  $\theta$  that yields the largest standard deviation.

Let us define the staggered Fourier basis as

$$|\psi_k^0\rangle = \sum_{x=-\infty}^{\infty} e^{-ik(2x)} |2x, 0\rangle, \tag{8}$$

$$|\psi_k^1\rangle = \frac{1}{\sqrt{2}} \sum_{x=-\infty}^{\infty} e^{-ik(2x+1)} (|2x+1, 0\rangle + |2x+1, 1\rangle), \tag{9}$$

$$|\psi_k^2\rangle = \frac{1}{\sqrt{2}} \sum_{x=-\infty}^{\infty} e^{-ik(2x+1)} (|2x+1, 0\rangle - |2x+1, 1\rangle), \tag{10}$$

where  $k \in (-\pi, \pi)$ . For a fixed  $k$ , the set of vectors  $\{|\psi_k^0\rangle, |\psi_k^1\rangle, |\psi_k^2\rangle\}$  spans a hyperplane  $\Omega_k$  that is invariant under the action of  $H_0$  and  $H_1$ .

Consider an operator from  $\mathcal{H}$  to  $\Omega_k$ , which maps  $|\psi_k^p\rangle$  to the 3-dimensional vector  $|p\rangle$ . We define  $H_i^k$  as  $H_i$  restricted to  $\Omega_k$  for  $i \in \{0, 1\}$  and consequently we obtain (see details in [7])

$$H_i |\psi_k^p\rangle = \sum_{p'=0}^2 \langle p' | H_i^k | p \rangle |\psi_k^{p'}\rangle. \tag{11}$$

Define  $U_k = e^{i\theta H_1^k} e^{i\theta H_0^k}$ . Since  $H_0^k$  and  $H_1^k$  are involutory matrices, it follows that  $e^{i\theta H_{0,1}^k} = \cos \theta I + i \sin \theta H_{0,1}^k$ . We also have that

$$U |\psi_k^p\rangle = \sum_{p'=0}^2 \langle p' | U_k | p \rangle |\psi_k^{p'}\rangle. \tag{12}$$

Let  $\lambda_k^p$  be the eigenvalues of  $U_k$  and  $|w_k^p\rangle$  be the corresponding eigenvectors. The eigenvalues of  $U$  are  $\lambda_k^p$  and the corresponding eigenvectors are

$$|v_k^p\rangle = \sum_{p'=0}^2 \langle p'|w_k^p\rangle |\psi_k^{p'}\rangle. \tag{13}$$

By right-multiplying (12) by  $\langle \psi_k^p|$ , summing on  $p$ , integrating on  $k$ , and using the completeness relation, we obtain [7]

$$U^t = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{p=0}^2 \sum_{p'=0}^2 \langle p'|U_k^t|p\rangle |\psi_k^{p'}\rangle \langle \psi_k^p|. \tag{14}$$

### 3.1 Moments of the probability distribution

To calculate the  $n$ -th moment [6], we utilize the characteristic function  $\langle e^{ik_0\hat{D}} \rangle_t = \langle \psi(t)|e^{ik_0\hat{D}}|\psi(t)\rangle$ , where  $\hat{D}$  is the linear operator  $\hat{D}|x, y\rangle = x|x, y\rangle$ , that is, the action of  $\hat{D}$  on a vector of the computational basis returns the distance to the origin. Using Eqs. (7) and (14), we obtain

$$\langle e^{ik_0\hat{D}} \rangle_t = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{p,p'} \langle p|(U_k^t)^\dagger U_{k^*}^t|p'\rangle \langle \psi(0)|\psi_k^p\rangle \langle \psi_{k^*}^{p'}|\psi(0)\rangle, \tag{15}$$

where  $k^* = k + k_0$ . Using that  $|\psi(0)\rangle = |0, 0\rangle$ , we obtain  $\langle \psi(0)|\psi_k^p\rangle = \delta_{p0}$ . Eq. (15) becomes

$$\langle e^{ik_0\hat{D}} \rangle_t = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \langle 0|(U_k^t)^\dagger U_{k^*}^t|0\rangle. \tag{16}$$

The  $n$ -th moment at time  $t$  can be obtained from the  $n$ -th derivative of  $\langle e^{ik_0\hat{D}} \rangle_t$  with respect to  $k$  evaluated at  $k_0 = 0$ . In fact,

$$\langle \hat{D}^n \rangle_t = \left(-i \frac{\delta}{\delta k_0}\right)^n \langle e^{ik_0\hat{D}} \rangle_t \Big|_{k_0=0} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \langle 0|(U_k^t)^\dagger \left(-i \frac{\delta}{\delta k}\right)^n U_k^t|0\rangle. \tag{17}$$

Define  $\Lambda_k = [|w_k^0\rangle, |w_k^1\rangle, |w_k^2\rangle]$  as the  $3 \times 3$  matrix whose columns are the eigenvectors of  $U_k$ . Let  $D[a_j]$  be the diagonal matrix with entries  $a_1, \dots, a_n$ . Then,  $U_k = \Lambda_k D[\lambda_k^p] \Lambda_k^\dagger$ . Using that  $\Lambda_k \Lambda_k^\dagger = I$ , we obtain

$$U_k^t = \Lambda_k D[(\lambda_k^p)^t] \Lambda_k^\dagger. \tag{18}$$

Then, we have  $\left(-i \frac{\delta}{\delta k}\right)^n U_k^t = \left(-i \frac{\delta}{\delta k}\right)^n \left(\Lambda_k D[(\lambda_k^p)^t] \Lambda_k^\dagger\right)$  and after using the product rule, we obtain for large  $t$

$$\left(-i \frac{\delta}{\delta k}\right)^n U_k^t = \Lambda_k D\left[t^n (\lambda_k^p)^t \left(\frac{\delta \ln(\lambda_k^p)}{i \delta k}\right)^n\right] \Lambda_k^\dagger + O(t^{n-1}). \tag{19}$$

Using Eqs. (17)-(19),  $\Lambda_k \Lambda_k^\dagger = I$ , and  $D[a_j]D[b_j] = D[a_j b_j]$ , we obtain

$$\langle \hat{D}^n \rangle_t = t^n \int_{-\pi}^{\pi} \frac{dk}{2\pi} \langle 0 | \Lambda_k D \left[ \left( \frac{\delta \ln(\lambda_k^p)}{i \delta k} \right)^n \right] \Lambda_k^\dagger | 0 \rangle + O(t^{n-1}). \tag{20}$$

Next step is the calculation of the eigenvectors and eigenvalues of  $U_k$ .

### 3.2 The eigenvectors and eigenvalues of $U_k$

In the next calculations we use wxMaxima<sup>6</sup> and Maple.  $U_k$  is given by

$$\begin{bmatrix} a_k & b_k & 0 \\ b_k & \bar{a}_k & 0 \\ 0 & 0 & e^{-2i\theta} \end{bmatrix}, \tag{21}$$

where

$$a_k = \frac{1}{9} (4 + 5 \cos(2\theta) - 3i \sin(2\theta) - 8e^{2ik} \sin^2 \theta), \tag{22}$$

$$b_k = -\frac{4\sqrt{2}i \sin \theta}{9} (\sin k \sin \theta - 6 \cos k \cos \theta). \tag{23}$$

The eigenvalues are  $\lambda_k^0 = e^{i\phi_k}$ ,  $\lambda_k^1 = e^{-i\phi_k}$ , and  $\lambda_k^2 = -e^{-2i\theta}$ , where

$$\cos(\phi_k) = 1 - \frac{2(8 \cos^2 k + 1) \sin^2 \theta}{9}. \tag{24}$$

The nontrivial eigenvectors of  $U_k$  are

$$|w_0\rangle = \frac{1}{\sqrt{c_k^+}} \begin{bmatrix} b_k \\ e^{i\phi_k} - a_k \\ 0 \end{bmatrix} \text{ and } |w_1\rangle = \frac{1}{\sqrt{c_k^-}} \begin{bmatrix} b_k \\ e^{-i\phi_k} - a_k \\ 0 \end{bmatrix}, \tag{25}$$

where

$$c_k^\pm = 2(1 - \Re(a_k) \cos(\phi_k) \mp \Im(a_k) \sin(\phi_k)),$$

and  $\Re(a_k)$  and  $\Im(a_k)$  are the real and imaginary parts of  $a_k$ , respectively.

The standard deviation over the number of steps is

$$\frac{\sigma(t)}{t} = \sqrt{\frac{\langle \hat{D}^2 \rangle}{t^2} - \left( \frac{\langle \hat{D} \rangle}{t} \right)^2}, \tag{26}$$

where  $\langle \hat{D} \rangle$  and  $\langle \hat{D}^2 \rangle$  are the first and second moments, which can be calculated explicitly using the expressions of the eigenvalues and Eqs. (20) and (25), resulting in

$$\frac{\langle \hat{D} \rangle}{t} = \frac{4}{3} + \frac{2}{3} \cos^2 \theta - \frac{2}{3} |\cos \theta| \sqrt{\cos^2 \theta + 8}, \tag{27}$$

$$\frac{\langle \hat{D}^2 \rangle}{t^2} = \frac{8}{3} + \frac{4}{3} \cos^2 \theta - \frac{4}{3} |\cos \theta| \sqrt{\cos^2 \theta + 8}. \tag{28}$$

<sup>6</sup>wxMaxima is a document based interface for the computer algebra system Maxima.

Then,

$$\frac{\sigma(t)}{t} = \frac{2}{3} \sqrt{2 - 9 \cos^2 \theta - 2 \cos^4 \theta + |\cos \theta| \sqrt{\cos^2 \theta + 8} (2 \cos^2 \theta + 1)}. \quad (29)$$

The value  $\theta^*$  that maximizes  $\sigma(t)$  is

$$\tan \theta^* = 3\sqrt{3}. \quad (30)$$

## 4 Numerical simulations

In this section, we analyze the standard deviation via numerical simulations. The numerical calculations were performed using the program Hiperwalk [2].<sup>7</sup> The input to Hiperwalk is matrices  $e^{i\theta H_0}$  and  $e^{i\theta H_1}$ . Since  $|\psi(t)\rangle$  has a finite number of nonzero amplitudes in the computational basis, we use a sufficiently large number of vertices (in a finite graph) so that the walker does not reach the border. In the simulations, we take 60,000 vertices (20,000 diamonds) and 10,000 time steps. The input is two  $60000 \times 60000$  complex matrices, which are sparse.

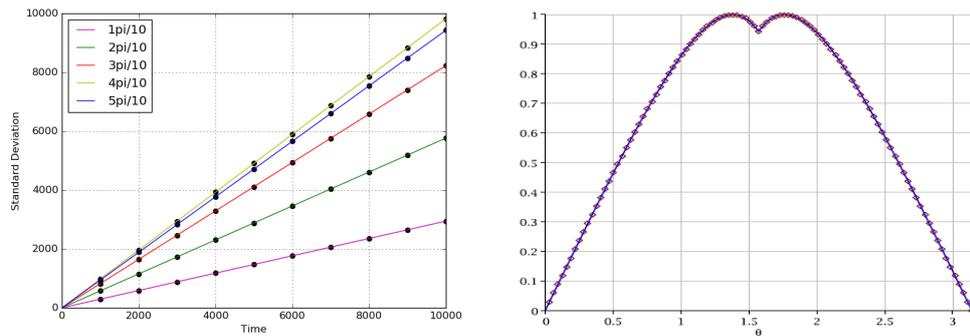


Figure 2: Left-hand panel: standard deviation as a function of  $t$  for  $\theta = \pi/10, \pi/5, 3\pi/10, 2\pi/5$ , and  $\pi/2$ . Right-hand panel: red diamonds are the numerical results for  $\sigma(t)/t$  and the blue curve is the analytical result.

The left-hand panel of Fig. 2 depicts the standard deviation  $\sigma(t)$  as a function of  $t$  for some values of  $\theta$ . These results show that  $\sigma(t)$  is a linear function of  $t$ , whose slope depends on  $\theta$ . The value of  $\theta$  that maximizes  $\sigma(t)/t$  can be obtained from the right-hand panel, which depicts  $\sigma(t)/t$  as a function of  $\theta$ . The blue curve is the analytical result and the red diamonds are obtained via numerical simulations.

## 5 Conclusion

We analyzed the staggered quantum walk with Hamiltonians on a line of diamonds and we calculated the standard deviation of the walker's position as a function of the

<sup>7</sup>Hiperwalk is a freeware open-source program that allows the user to perform simulations of quantum walks on graphs using HPC.

number of steps. We also determined the optimal value of  $\theta$  that maximizes the standard deviation, which is  $\theta^* = \arctan(3\sqrt{3})$ . The numerical simulations confirmed our analytical results. For future works, we can obtain the expression of the standard deviation of more general graphs. We can also obtain the expression of the hitting time.

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