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Quantum walks on cycles

Małgorzata Bednarska [a], Andrzej Grudka [b], Paweł Kurzyński [b], Tomasz Łuczak [a,*], Antoni Wójcik [b]

[a] *Faculty of Mathematics and Computer Science, Adam Mickiewicz University, Umultowska 87, 61-614 Poznań, Poland*
[b] *Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland*

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Abstract

We consider asymptotic behaviour of a Hadamard walk on a cycle. For the walk which starts with a state in which all the probability is concentrated on one node, we find the explicit formula for the limiting distribution and discuss its asymptotic behaviour when the length of the cycle tends to infinity. We also demonstrate that for a carefully chosen initial state, the limiting distribution of a quantum walk on cycle can lie further away from the uniform distribution than its initial state.

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1. Introduction

Celebrated results of Shor [1] and Grover [2] started a quest for algorithms based on quantum mechanics which can surpass the corresponding classical algorithms. As many classical algorithms employ properties of random walks on graphs, several groups of researchers have begun to study properties of quantum analogues of classical random walks (for a survey see [3]). Two models of quantum random walks have been proposed by Aharonov et al. [4] and Farhi and Gutmann [5]; in this Letter we consider only a discrete quantum walk as defined in [4]. The behavior of quantum random walks has been shown to differ greatly from that of their classical counterparts. Ambainis et al. [6] proved that the spreading time in the quantum walk on line scales linearly with the number of steps, while Aharonov et al. [4] showed that the mixing time for a walk on a cycle grows linearly with the cycle length. Even a more spectacular exponential speed up was discovered by Kempe et al. [7] who studied a quantum random walk on hypercube; this result led to a construction of the first quantum algorithm based on a random walk by Shenvi et al. [8]. The fact that in quantum walks on graphs the probability function spreads out much faster than in the classical case is not the only factor which can be explored in designing new quantum algorithms. In [4] the au-

* Corresponding author.
E-mail address: tomasz@amu.edu.pl (T. Łuczak).

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thors remarked that 'one may try to use quantum walks which converge to limiting distribution which are different than those of the corresponding classical walks'. In this Letter we follow this suggestion and study the limiting distribution of a random walk on a cycle; it turns out that this distribution depends on the length of the cycle in a somewhat surprising way. We also give an example of a quantum walk in which the distance from the initial state to the uniform distribution is larger than the distance between the uniform distribution and the initial state. Finally, we remark that recently Travaglione and Milburn [9] and Dür et al. [10] have proposed a scheme of experiment which realizes a quantum walk on a cycle.

2. Model

We study a quantum random walk on a cycle with d nodes. In the model of such a walk proposed in [4] nodes are represented by vectors $|v\rangle$, $v = 0, 1, \dots, d-1$, which form an orthonormal basis of the Hilbert space H_V. An auxiliary two-dimensional Hilbert space H_A (coin space) is spanned by vectors $|s\rangle$, $s = 0, 1$. The initial state of the walk is a normalized vector

$$|\Psi_0\rangle = \sum_{s,v} \alpha_{sv} |s, v\rangle = \sum_{s,v} \alpha_{sv} |s\rangle |v\rangle \tag{1}$$

from the tensor product $H = H_A \otimes H_V$. In a single step of the walk the state changes according to the equation

$$|\Psi_{n+1}\rangle = U |\Psi_n\rangle, \tag{2}$$

where the operation $U = S(H \otimes I)$ first applies the Hadamard gate operator $H = \sum_{s,s'} (-1)^{ss'} |s\rangle\langle s'|$ to the vector from H_A, and then shifts the state by the operator

$$S = \sum_{s,v} |s\rangle\langle s| \otimes |v + 2s - 1 \ (\mathrm{mod}\, d)\rangle\langle v| \,. \tag{3}$$

The probability distribution on the nodes of the cycle after the first n steps of the walk is given by

$$p_n(v) = \sum_s \bigl|\langle s, v|\Psi_n\rangle\bigr|^2. \tag{4}$$

However, as observed by Aharonov at el. [4], for a fixed v, the probability $p_n(v)$ is 'quasi-periodic' as a function of n and thus, typically, it does not converge to a limit. Thus, instead of $p_n(v)$ the authors of [4] considered

$$\bar{p}_n(v) = \frac{1}{n} \sum_{i=1}^{n} p_n(v), \tag{5}$$

and proved that for any initial state $|\Psi_0\rangle$ and every node $v = 0, 1, \dots, d-1$, the sequence $\bar{p}_n(v)$ converges to the limiting distribution

$$\pi(v) = \sum_{a,a'} \sum_s \Gamma_{aa'} \langle \phi_a|\Psi_0\rangle\langle\Psi_0|\phi_{a'}\rangle \times \langle s, v|\phi_a\rangle\langle\phi_{a'}|s, v\rangle, \tag{6}$$

where $|\phi_a\rangle$ are the eigenvectors of U, and the coefficient $\Gamma_{aa'}$ depends on the eigenvalues corresponding to the eigenvectors $|\phi_a\rangle$ and $|\phi_{a'}\rangle$: if they are the same we take $\Gamma_{aa'} = 1$, otherwise we set $\Gamma_{aa'} = 0$.

In the case of the Hadamard walk on cycle the eigenvalues of U are given by

$$c_{jk} = \frac{1}{\sqrt{2}} \Bigl((-1)^k \sqrt{1 + \cos^2(2\pi j/d)} - i \sin(2\pi j/d)\Bigr), \tag{7}$$

for $j = 0, 1$, and $k = 0, 1, \dots, d-1$, while the corresponding eigenvectors are

$$|\phi_{jk}\rangle = \bigl(a_{jk}|0\rangle + a_{jk} b_{jk}|1\rangle\bigr) \otimes \sum_v \omega_d^{jv} |v\rangle, \tag{8}$$

where $\omega_d = e^{2\pi i/d}$,

$$a_{jk} = 1/\sqrt{d\bigl(1 + |b_{jk}|^2\bigr)}, \tag{9}$$

$$b_{jk} = \omega_d^j \Bigl((-1)^k \sqrt{1 + \cos^2(2\pi j/d)} - \cos(2\pi j/d)\Bigr). \tag{10}$$

Note that $c_{j0} \neq c_{j'1}$ so $\Gamma_{jk,j'k'} = \gamma_{jj'} \delta_{kk'}$, where $\delta_{kk'}$ is the Kronecker delta. Thus, (6) becomes

$$\pi(v) = \sum_{j,j'} \sum_k \gamma_{jj'} \langle \phi_{jk}|\Psi_0\rangle\langle\Psi_0|\phi_{j'k}\rangle A_{jj'k} \omega_d^{v(j-j')}, \tag{11}$$

where $A_{jj'k} = a_{jk} a_{j'k} (1 + b_{jk} b^*_{j'k})$. If d is odd, then all eigenvalues are distinct, $\gamma_{jj'} = \delta_{jj'}$, and $A_{jjk} = 1/d$; consequently,

$$\pi(v) = (1/d) \sum_j \sum_k \bigl|\langle \phi_{jk}|\Psi_0\rangle\bigr|^2 = 1/d.$$

It comes as no surprise, since as was proved by Aharonov et al. [4], the limiting distribution π is always uniform in a non-degenerate case. Thus, we concentrate on a more interesting case of even d. Then, because of the symmetries $c_{d/2-j,k} = c_{j,k}$ and $c_{d/2+j,k} = c^*_{jk} = c_{d-j,k}$, the coefficient $\gamma_{jj'}$ does not vanish when one of the following conditions holds:

(i) $j = j'$;
(ii) $j = 0$, $j' = d/2$;
(iii) $j = t$, $j' = d/2 - t$, for $t = 1, 2, \ldots, t_{\max}$;
(iv) $j = d - t$, $j' = d/2 + t$, for $t = 1, 2, \ldots, t_{\max}$,

where here and below $t_{\max} = \lfloor (d-2)/4 \rfloor$.

3. Result and discussion

We study in detail the limiting distribution π for a quantum walk which starts with a state in which, with probability one, the particle is located at node v_0; more specifically we set

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}\big(|0, v_0\rangle + i|1, v_0\rangle\big). \tag{12}$$

Then $\langle \phi_{jk}|\Psi_0\rangle = g_{jk}\omega_d^{-v_0 j}$, where $g_{jk} = a_{jk}(1 + ib^*_{jk})/\sqrt{2}$, and

$$\pi(v) = \sum_{j,j'}\sum_{k} \gamma_{jj'} f(j, j', k)\omega_d^{(v-v_0)(j-j')}, \tag{13}$$

with $f(j, j', k) = g_{jk} g^*_{j'k} A_{jj'k}$. Since $\gamma_{jj'} = 0$ except for the four cases (i)–(iv) described above, we get

$$\pi(v) = F + (-1)^{\Delta} 2\,\mathrm{Re}(F_0) + (-1)^{\Delta}\,\mathrm{Re}\left(\sum_{i=1}^{t_{\max}} F_t\right), \tag{14}$$

where

$$\Delta = \Delta(v) = \min\big\{|v - v_0|, d - |v - v_0|\big\} \tag{15}$$

denotes the distance between nodes v_0 and v, and

$$F = \sum_{j,k} f(j, j, k),$$
$$F_0 = \sum_{k} f(0, d/2, k),$$
$$F_t = \sum_{k} f(t, d/2 - t, k) + f(d/2 + t, d - t, k). \tag{16}$$

After some elementary but not very exciting calculations (16) reduces to

$$F = \frac{1}{d},$$
$$F_0 = 0,$$
$$F_t = \frac{2}{d^2}\frac{\sin^2(2\pi t/d)}{1 + \cos^2(2\pi t/d)}. \tag{17}$$

We remark that $F_t = 0$ whenever $t_{\max} = 0$, i.e., for $d = 2$ and $d = 4$. Hence, the limiting distribution for even cycles of sizes two and four are uniform, which has also been observed by Travaglione and Milburn [9], who analyzed a quantum walk on cycle of length four step by step. However, for $d \geqslant 6$ we have

$$\pi(v) = \big(1 + \Pi(v)\big)/d, \tag{18}$$

with the 'correction' term $\Pi(v) = (-1)^{\Delta} 4S/d$, where

$$S = \sum_{t=1}^{t_{\max}} \cos(4\pi t\Delta/d)\left(\frac{2}{1 + \cos^2(2\pi t/d)} - 1\right). \tag{19}$$

Setting $z = 3 - 2\sqrt{2} \sim 0.17157\ldots$, one can write (19) as

$$\begin{aligned} S = {} & \left(\frac{8z}{1 - z^2} - 1\right)\sum_{t=1}^{t_{\max}} \cos(4\pi\Delta t/d) \\ & + \frac{8z}{1 - z^2}\sum_{m=1}^{\infty}(-z)^m \sum_{t=1}^{t_{\max}} \cos\big(4\pi(\Delta + m)t/d\big) \\ & + \frac{8z}{1 - z^2}\sum_{m=1}^{\infty}(-z)^m \sum_{t=1}^{t_{\max}} \cos\big(4\pi(\Delta - m)t/d\big), \end{aligned} \tag{20}$$

which, in turn, transforms to

$$\begin{aligned} S = {} & -\frac{d}{4}(\delta_{\Delta,0} + \delta_{\Delta,d/2}) \\ & + (-1)^{\Delta}\frac{d}{4}\frac{8z}{1 - z^2}\frac{z^{-\Delta}(-z)^{d/2} + z^{\Delta}}{1 - (-z)^{d/2}} \\ & + \frac{1 + (-1)^{\Delta}\xi}{2} - \frac{4z}{(1 - z)^2} - \frac{4z(-1)^{\Delta}\xi}{(1 + z)^2}, \end{aligned} \tag{21}$$

where $\xi = (1 + (-1)^{d/2})/2$, i.e., $\xi = 1$ when $d/2$ is

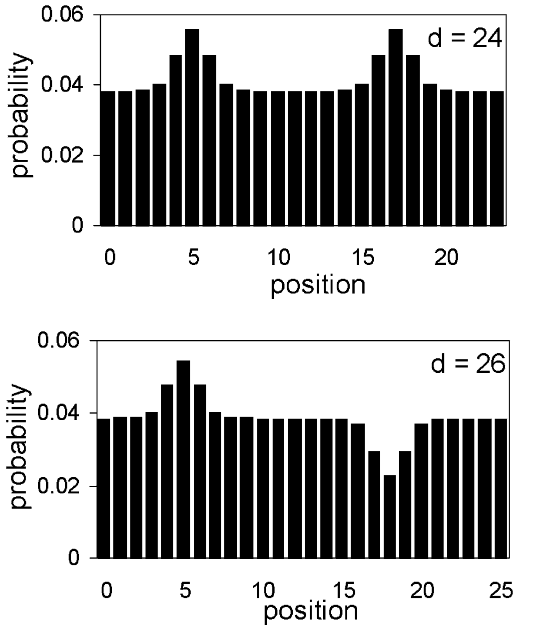

Fig. 1. The limiting distributions for the cases of $d = 24$ and $d = 26$. The walk starts with the state where with probability one a particle is at the node $v_0 = 5$.

even, and $\xi = 0$ if $d/2$ is odd. Thus, we arrive at

$$\begin{aligned}\Pi(v) &= (-1)^{\Delta+1}(\delta_{\Delta,0} + \delta_{\Delta,d/2}) \\ &\quad + \frac{8z}{1-z^2}\,\frac{z^{-\Delta}(-z)^{d/2} + z^{\Delta}}{1-(-z)^{d/2}} \\ &\quad + \frac{4}{d}\left(\frac{\xi + (-1)^{\Delta}}{2} - \frac{4(-1)^{\Delta} z}{(1-z)^2} - \frac{4z\xi}{(1+z)^2}\right).\end{aligned} \tag{22}$$

In Fig. 1 we pictured the resulting limiting distributions for $d = 24$ and $d = 26$. It is easy to see they are almost uniform except for the nodes which lie next to the initially populated node v_0 and the opposite node $\hat{v}_0 = v_0 + d/2 \pmod d$. Indeed, as $d \to \infty$, the last term of (22) vanishes and

$$\bar{\Pi}(v) = \lim_{d\to\infty} \Pi(v) = \eta(\Delta) - (-1)^{\xi}\eta(\Delta'), \tag{23}$$

where

$$\eta(x) = \frac{8z^{1+x}}{1-z^2} - \delta_{x0}, \tag{24}$$

and Δ' is the distance between the nodes v and $\hat{v}_0$. The Eq. (23) shows that the correction term $\bar{\Pi}(v)$ is significant only for v which lie close to either v_0

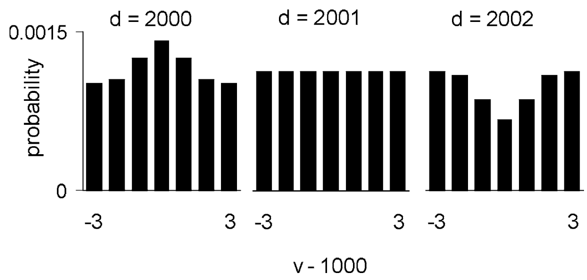

Fig. 2. The limiting distribution for cycles of lengths 2000, 2001 and 2002. In each case the walk starts with a state in which with probability one a particle is at $v_0 = 0$.

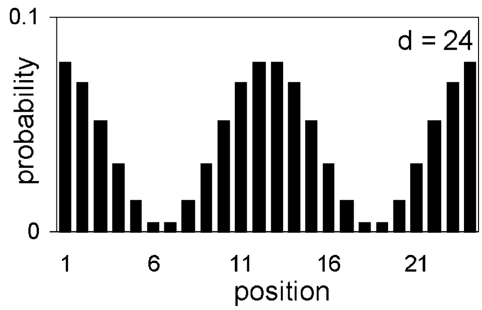

Fig. 3. An example of a non-uniform invariant probability distribution for an initial state of the form $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|\phi_{5,0}\rangle + |\phi_{7,0}\rangle)$.

or $\hat{v}_0$ and decreases exponentially with the distance between v and v_0 and $\hat{v}_0$. Note that the shapes of the cusps near v_0 and $\hat{V}_0$ do not depend very much on d for large d (except of the scaling factor $1/d$). However, if $d/2$ is odd then the limiting distribution $\pi(v)$ has a minimum at $\hat{v}_0$, while if $d/2$ is even the distribution has a peak $\hat{v}_0$, virtually identical with that which appears at v_0 (Figs. 1 and 2, see also [11]). The fact that such a local behaviour of the limiting distribution π depends so strongly on the 'global' properties of space, as the parity of $d/2$, is somewhat surprising. We hope that this and/or analogous phenomena can be used in constructing efficient quantum algorithms.

It is easy to see that despite of narrow cusps near then nodes v_0 and $\hat{v}_0$, the total variation distance d_{TV} between the limiting distribution given by (18) and (22) and the uniform distribution tends to 0 as $d \to \infty$. However, it is not hard as well to construct 'highly non-uniform' distributions which remain invariant during the walk: one can simply take as the initial state a superposition of two degenerated eigenvec-

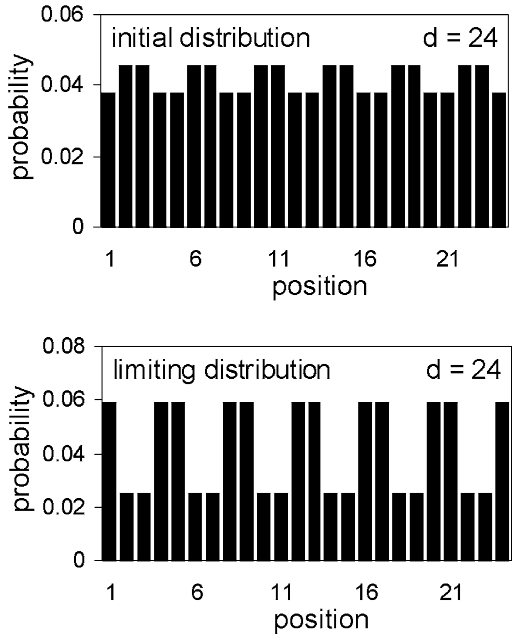

Fig. 4. The initial and limiting distributions for the initial state $|\Psi_0\rangle = \frac{1}{2}(|\phi_{3,0}\rangle + |\phi_{9,0}\rangle - |\phi_{15,0}\rangle - |\phi_{21,0}\rangle)$.

tors (the distribution corresponding to a single eigenvector is always a uniform one). An example of such an invariant nonuniform probability distribution is presented in Fig. 3.

With slightly more work one can construct the initial states which make the differences between the quantum and classical walks on cycles even more distinct. One such example is shown in Fig. 4. Here, the total variation distance from the uniform distribution, defined as

$$\frac{1}{2}\sum_{v=0}^{d-1}\left|p(v) - \frac{1}{d}\right| \qquad (25)$$

is equal 0.046 for the initial state, while for the limiting distribution it grows to 0.204.

4. Conclusion

We study the properties of a Hadamard quantum walk on a cycle with d nodes. In the case of a walk starting from a single node we give an explicit formula for the limiting distribution and show that it is very sensitive to the arithmetic properties d. We hope that this or an analogous mode of behaviour can be used in construction of efficient quantum algorithms.

Furthermore, we present an example of a quantum walk on a cycle, for which the total variation distance between the initial distribution and the uniform distribution is much smaller than the distance between limiting distribution and the uniform one.

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