LETTER TO THE EDITOR

Pseudo memory effects, majorization and entropy in quantum random walks

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Abstract
A quantum random walk on the integers exhibits pseudo memory effects, in that its probability distribution after N steps is determined by reshuffling the first N distributions that arise in a classical random walk with the same initial distribution. In a classical walk, entropy increase can be regarded as a consequence of the majorization ordering of successive distributions. The Lorenz curves of successive distributions for a symmetric quantum walk reveal no majorization ordering in general. Nevertheless, entropy can increase, and computer experiments show that it does so on average. Varying the stages at which the quantum coin system is traced out leads to new quantum walks, including a symmetric walk for which majorization ordering is valid but the spreading rate exceeds that of the usual symmetric quantum walk.

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During the stochastic evolution of a classical random walk (CRW), correlations are established among the states of its two constituent parts, a *coin* and a *walker*. Because of the widespread use of the CRW in applications involving classical computer simulations [1], recent interest in quantum computation [2] has focussed attention on the notion of a quantum random walk (QRW). The key idea is to replace the classical correlations between coin and walker states in a CRW by the emblematic notion of quantum correlation, i.e. entanglement [2] of the states of suitable quantum analogues of the coin and walker. Of main interest in QRW studies has been the effect of entanglement on various asymptotics, on spreading properties and on hitting and mixing times. From the earliest formulations of QRWs [3, 4], to recent studies on general graphs [5], on the line [6] etc, it has emerged that a number of surprising features distinguish quantum from classical walks, such as their non-Gaussian asymptotics, a quadratic speed up in spreading rate on the line [7], an exponentially faster hitting time in hypercubes [8, 9], and an

exponentially faster penetration time of decision trees [10, 11]. These findings have recently prompted proposals for physical implementation of such processes in experiments, e.g. in ion traps [12], optical lattices [13], or in cavity QED [14]. A review providing a comprehensive introduction and other references has recently appeared [15].

There are two different ways to consider a QRW as a process. In the first, a fixed number N of applications of a unitary quantum evolution to a combined coin–walker system is considered, producing a highly entangled state, and after the last step, the coin degrees of freedom are traced out to determine a reduced density matrix and subsequently $P_Q^{(N)}$, the associated probability distribution (pd) of location probabilities for the walker. In the second, extended interpretation, the QRW is considered as the process that produces *successively* in this way, the pds $P_Q^{(N)}$ for $N = 0, 1, 2, 3, \ldots$. The purpose of the present letter is to indicate some further remarkable properties that differentiate a QRW, interpreted in this extended way, from a CRW.

We construct the QRW on $H = H_c \otimes H_w$, where the coin space is $H_c = l_2(\{0, 1\})$ and the walker space is $H_w = l_2(Z)$, and we consider the unitary evolution operator $V = P_+ U \otimes E_+ + P_- U \otimes E_-$ acting on H. Here U is 2×2 unitary, and acts on H_c along with P_+ and P_-, which are orthogonal projectors onto the coin states $|0\rangle = (1\ 0)^T$ and $|1\rangle = (0\ 1)^T$ respectively. The step operators E_+, E_- act on $|m\rangle \in H_w$ for $m = 0, \pm 1, \pm 2, \ldots$ as $E_\pm |m\rangle = |m \pm 1\rangle$, so that $E_\pm E_\mp = \mathbf{1}$. Together with the *distance operator L* acting as $L|m\rangle = m|m\rangle$, they satisfy the commutation relations $[L, E_\pm] = \pm E_\pm$, $[E_+, E_-] = 0$. With $\rho_c^{(0)} = |\varphi\rangle\langle\varphi|$ chosen as the initial density matrix of the coin and $\rho_w^{(0)} = |0\rangle\langle 0|$ the initial density matrix of the walker, the total initial density matrix $\rho^{(0)}$ is

$$\rho^{(0)} = \rho_c^{(0)} \otimes \rho_w^{(0)} = |\varphi\rangle\langle\varphi| \otimes |0\rangle\langle 0|. \tag{1}$$

After N successive applications of the unitary evolution defined by V, the coin degrees of freedom are traced out, so that $\rho_w^{(0)}$ evolves to $\rho_w^{(N)}$, given by the action of a trace preserving completely positive (CP) map ε_{V^N} [16]

$$\rho_w^{(N)} = \varepsilon_{V^N}\left(\rho_w^{(0)}\right) \equiv \mathrm{Tr}_c\left[V^N\left(\rho_c^{(0)} \otimes \rho_w^{(0)}\right)(V^\dagger)^N\right]$$
$$= \sum_{k=0,1} A_k^{(N)} \rho_w^{(0)} A_k^{(N)\dagger}. \tag{2}$$

Here the Kraus operators are given for $k = 0, 1$ by $A_k^{(N)} = \langle k|V^N|\varphi\rangle$, and satisfy

$$\sum_{k=0,1} A_k^{(N)\dagger} A_k^{(N)} = \mathbf{1}. \tag{3}$$

The diagonal element $\langle k|\rho_w^{(N)}|k\rangle$ of the walker density matrix, for $k \in \{-N, -N+2, \ldots, N\}$, is the probability $P_Q^{(N)}(k)$ of occupation of the site k by the walker after the Nth step. It follows from (1) that $P_Q^{(0)}(k) = \delta_{k0}$.

With V defined as above we have $V^N = \begin{pmatrix} \alpha^{(N)} & \beta^{(N)} \\ \gamma^{(N)} & \delta^{(N)} \end{pmatrix}$, for suitable operators $\alpha^{(N)}$, etc acting on H_w. For the general choice $|\varphi\rangle = c|0\rangle + d|1\rangle$, with c, d complex, we have that $A_0^{(N)} = c\alpha^{(N)} + d\beta^{(N)}$, $A_1^{(N)} = c\gamma^{(N)} + d\delta^{(N)}$. We choose $U = U(p) = \begin{pmatrix} \sqrt{p} & \sqrt{1-p} \\ \sqrt{1-p} & -\sqrt{p} \end{pmatrix}$, with $0 \leqslant p \leqslant 1$, without any significant loss of generality [5]. The choice $c = 1/\sqrt{2}$, $d = \mathrm{i}/\sqrt{2}$ and $p = 1/2$ is known [5, 12] to result in $P_Q^{(N)}(-k) = P_Q^{(N)}(k)$ for all k, but a QRW is not symmetric in general. In what follows, we utilize the elementwise or Hadamard product $\Delta = A \circ B$, defined between matrices A, B of the same size by $(A \circ B)_{ij} = A_{ij} B_{ij}$, and we call *doubly stochastic* [17] a square matrix Δ (of finite size, or with columns and rows of finite support, as is the case here), with nonnegative elements, which has unit column and row sums.

Our first result is summarized as:

Proposition 1. *There exists a doubly stochastic matrix $\Delta_Q^{(N)} = A_0^{(N)} \circ \bar{A}_0^{(N)} + A_1^{(N)} \circ \bar{A}_1^{(N)}$, that connects the initial pd $P_Q^{(0)}$ with the pd $P_Q^{(N)}$ of the Nth step. These matrices satisfy the inhomogeneous recurrence relation*

$$\Delta_Q^{(N+1)} = A_0^{(N+1)} \circ \bar{A}_0^{(N+1)} + A_1^{(N+1)} \circ \bar{A}_1^{(N+1)}$$
$$= ((1-p)E_+ + pE_-))\Delta_q^{(N)} + (E_+ - E_-)$$
$$\times \left[\sqrt{p(1-p)}\left(A_0^{(N)} \circ \bar{A}_1^{(N)} + A_1^{(N)} \circ \bar{A}_0^{(N)}\right) + (2p-1)A_0^{(N)} \circ \bar{A}_0^{(N)} \right]. \tag{4}$$

By means of this relation, $P_Q^{(N)}$ is related to the classical pds $\{ P_C^{(N)}, P_C^{(N-1)}, \ldots, P_C^{(1)}, P_C^{(0)} = P_Q^{(0)} \}$, arising from the first N steps of a CRW, via the map $\delta^{(N)}$ given by

$$P_Q^{(N)} = \delta^{(N)}\left(P_C^{(N)}, \ldots, P_C^{(0)}\right)$$
$$= P_C^{(N)} + \omega^{(1)}P_C^{(N-1)} + \omega^{(2)}P_C^{(N-2)} + \cdots + \omega^{(N-1)}P_C^{(1)} + \omega^{(N)}P_C^{(0)} \tag{5}$$

where we have introduced the reshuffling matrices $\omega^{(i+1)} = (E_+ - E_-)M^{(i)}$, $i > 0$ with $M^{(i)} = \sqrt{p(1-p)}\left(A_0^{(i)} \circ \bar{A}_1^{(i)} + A_1^{(i)} \circ \bar{A}_0^{(i)}\right) + (2p-1)A_0^{(i)} \circ \bar{A}_0^{(i)}$ and with $M^{(0)} = 0$, $\omega^{(1)} = 0$.

The proof is straightforward.

Comments.

(1) Since the $A_{0,1}^{(N)}$ are polynomials of degree N in the commuting step operators $E_\pm$, they are normal operators, i.e. $A_k^{(N)}A_k^{(N)\dagger} = A_k^{(N)\dagger}A_k^{(N)}$ for $k = 0, 1$. This means that in addition to (3), there is a similar relation with $A_k^{(N)}$, $A_k^{(N)\dagger}$ interchanged. Together, these two relations lead to the double stochasticity of $\Delta_Q^{(N)}$ [18]. This simple method of constructing doubly stochastic matrices by convex sums of Hadamard products of Kraus generators of CP maps, being normal operators, together with the question of the ensuing entropy increase, to be discussed shortly, is a nontrivial extension of Uhlmann's theory which addresses those questions for unitary CP maps only (cf [19] and references therein).

(2) The general form of (4) is $\Delta_Q^{(N+1)} = \Delta_C \Delta_Q^{(N)} + (E_+ - E_-)M^{(N)}$, and we see that the final N-dependent inhomogeneous term, which must have zero column and row sums, distinguishes a QRW from a CRW and moreover carries the burden of possible breaking of the majorization ordering, as will be seen shortly.

(3) Proposition 1 shows that the effect of tracing out the coin system after N applications of V to $\rho^{(0)}$, results in a kind of pseudo memory effect (or pseudo non-Markovian effect), in that determination of the quantum occupation probabilities at step N involves the occupation probabilities of an N-step CRW, reshuffled from step to step as in (5). This suggests a modified QRW where the coin system is traced out after every m steps, for some fixed m, rather than after 1 or 2 or ... N steps as in the QRW as considered to date. The case $m = 1$ defines a scheme that *promptly traces* the coin system after each V action. With $U(p)$ as above and $\rho^{(0)}$ as in (1), this yields the occupation probabilities of a $(p, 1-p)$ biased CRW. Indeed if $\rho_w^{(N+1)} = (\varepsilon_V)^{N+1}(\rho_w^{(0)}) = \varepsilon_V(\rho_w^{(N)}) \equiv \text{Tr}_c[V(\rho_c^{(0)} \otimes \rho_w^{(N)})V^\dagger]$, then we have at each step, along the diagonal of the reduced density matrix, the probabilities of the corresponding row of the classical Pascal triangle i.e. $\langle k|\rho_w^{(N)}|k\rangle = (P_Q^{(N)})(k) = (P_C^{(N)})(k)$. In this case no memory effects are present and $P_Q^{(N+1)} = \Delta_C P_Q^{(N)}$, where $\Delta_C = (1-p)E_+ + pE_-$ is a doubly stochastic matrix that repeatedly mixes the evolving probability distribution and extends its support by one unit to the left and right at each time step of the walk.

(4) Proposition 2 is devoted to the case $m = 2$, where a pseudo memory effect is also exhibited, since here also the determination of the quantum pd at step N involves classical occupation probabilities from the first N steps. However now the reshuffling matrix Φ is fixed (as in (6)).

Proposition 2. *There exists a doubly stochastic matrix* $\Delta_Q = B_0 \circ \bar{B}_0 + B_1 \circ \bar{B}_1$ *that connects the Nth step pd* $P_Q^{(N)}$ *identified with the diagonal elements of* $\rho_w^{(N)}$, *with* $P_Q^{(N+1)}$ *at the* $(N+1)th$ *step, identified with the diagonal elements of* $\rho_w^{(N+1)} = \varepsilon_{V^2}(\rho_w^{(N)})$. *Here the Kraus generators are*

$$B_0 = (pc + \sqrt{p(1-p)}d)E_+^2 + ((1-p)c - \sqrt{p(1-p)}d)\mathbf{1}$$
$$B_1 = (pd - \sqrt{p(1-p)}c)E_-^2 + ((1-p)d + \sqrt{p(1-p)}c)\mathbf{1}.$$

The recurrence relation satisfied by $P_Q^{(N)}$, *and its solution, are given by*

$$P_Q^{(N)} = \Delta_Q P_Q^{(N-1)} = (\Delta_C + \Phi)P_Q^{(N-1)}$$

and

$$P_Q^{(N)} = \Delta_Q^N P_Q^{(0)} = (\Delta_C + \Phi)^N P_Q^{(0)}$$

$$= \sum_{k=0}^{N} \binom{N}{k} \Phi^{N-k} \Delta_C^k P_Q^{(0)} = \sum_{k=0}^{N} \binom{N}{k} \Phi^{N-k} P_C^{(k)}$$

where $\Delta_Q = \Delta_C + \Phi$, *and where the matrix* Φ *with null column and row sums is given explicitly by*

$$\Phi = B_0 \circ \bar{B}_0 + B_1 \circ \bar{B}_1 - \Delta_c$$
$$= |pc + \sqrt{p(1-p)}d|^2 E_+^2 + |\sqrt{p(1-p)}c - pd|^2 E_-^2 + (|(1-p)c - \sqrt{p(1-p)}d|^2$$
$$+ |(1-p)d + \sqrt{p(1-p)}c|^2)\mathbf{1} - (1-p)E_+ - pE_-. \tag{6}$$

Once it is seen that in this case the analogue of (2) reads $\rho_w^{(N+1)} = \varepsilon_{V^2}(\rho_w^{(N)}) \equiv \mathrm{Tr}_c[V^{2N}(\rho_c^{(0)} \otimes \rho_w^{(0)})(V^{2\dagger})^N] = \sum_{k=0,1} B_k \rho_w^{(0)} B_k^\dagger$, the rest of the proof is similar to that for proposition 1. Generalization to the case $m > 2$ is straightforward.

It is known that CRW pds become more entropic as N increases. This can be attributed to the fact that they are ordered by majorization [20]. Thus, for two consecutive classical pds $P_C^{(N)}$ and $P_C^{(N+1)}$, each with elements arranged in nondecreasing order, it is true that $P_C^{(N)} \succ P_C^{(N+1)}$, and *therefore* that $S(P_c^{(N)}) \leqslant S(P_c^{(N+1)})$, for the respective Shannon entropies, defined as $S(P) = -\sum_k P(k) \log P(k)$. To facilitate a comparison with the corresponding behaviour in the symmetric QRW of proposition 1, we set the classical pd $P_C^{(N)}$ in the upper horizontal line in figure 1, and the quantum pd $P_Q^{(N)}$ in the lower horizontal line. We find the remarkable result that in certain cases, though QRW pds are becoming more entropic in the course of time, namely $S(P_Q^{(N)}) \leqslant S(P_Q^{(N+1)})$, majorization breaks down, i.e. $P_Q^{(N)} \not\succ P_Q^{(N+1)}$, even in the early stages. This is illustrated in figure 2, which refers to steps $N = 6, 7, 8$ and 9 of the symmetric QRW. Here the entropy is increasing, with $S^Q(6) \approx 1.6551$, $S^Q(7) \approx 1.8138$, $S^Q(8) \approx 1.8909$, $S^Q(9) \approx 1.9295$, but majorization ordering is violated, as can be seen at once from the corresponding Lorenz curves. The Lorenz curve of a pd P whose elements $P(k)$ have been arranged in nonincreasing order is the plot of the points $(n/N, \gamma_n(P))$ for $n = 0, 1, \ldots N$, where $\gamma_n(P) = \sum_{k=1}^{n} P(k)$, and $\gamma_0(P) = 0$, $\gamma_N(P) = 1$. If $P \prec P'$ then the Lorenz curve of P' always lies below that of P and never crosses it. Thus *crossing of Lorenz curves implies majorization breakdown*
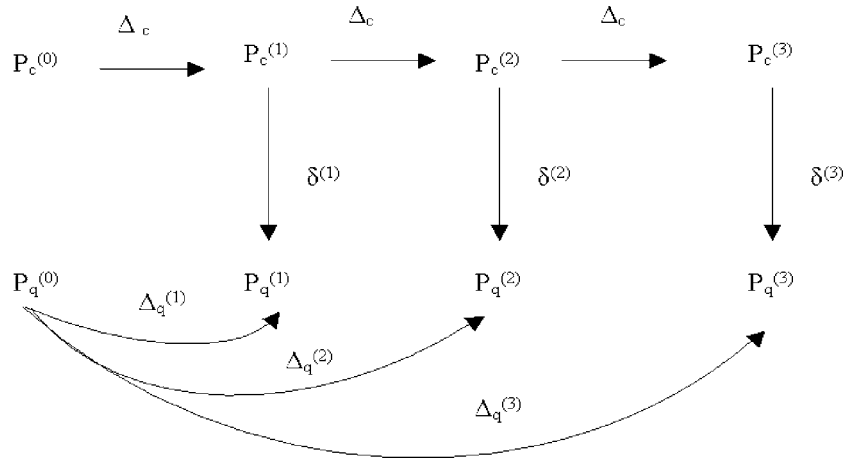
Figure 1. Successive distributions of a CRW (upper horizontal line) obtained by action of Δ_c, and of a QRW as in proposition 1 (lower horizontal line), obtained by the action of $\Delta_q^{(N)}$. The pseudo memory effect is shown by the vertical arrows $\delta^{(N)}$.
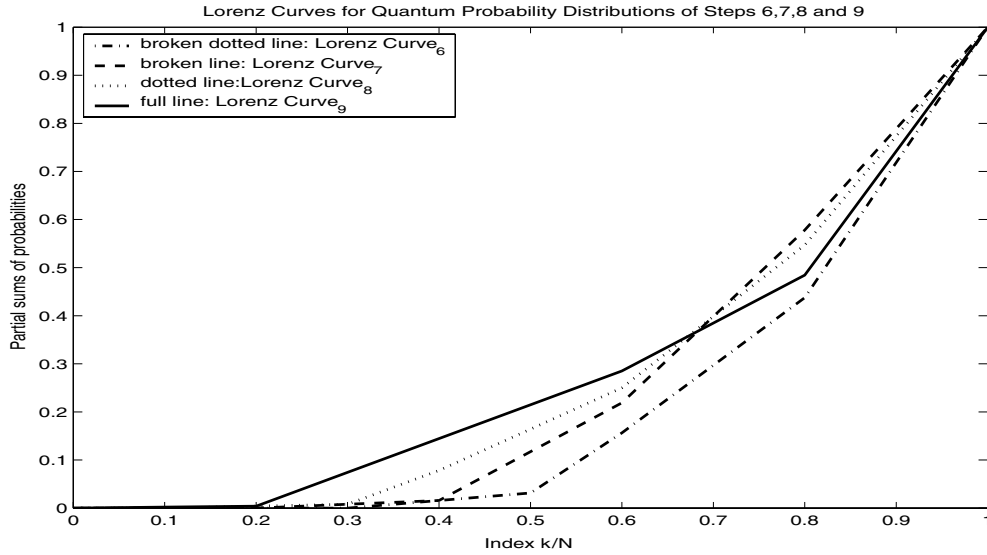
Figure 2. Lorenz curves for the distributions of steps 6–9 of the symmetric QRW of proposition 1.

and vice versa. Such a breakdown of majorization takes place in the symmetric QRW as is seen in figure 2, while entropy increases as seen in figure 3. Remarkably, this is not the case for the QRW of proposition 2, since in this case the mixing matrix from step to step remains N-independent, fixed and doubly stochastic, guaranteeing majorization ordering [20, 21].

Figure 3 illustrates three notable features of entropy dynamics common to three symmetric QRWs as in proposition 1, with $U(p)$ having $p = 1/3 = \cos^2(\pi/6)$, $p = 1/2 = \cos^2(\pi/4)$ and $p = 3/4 = \cos^2(\pi/3)$, respectively: firstly, *an increase of entropy on average*, e.g. in the case $p = 1/4$, the sequence of steps $45, 51, 57, 63, \ldots$ has monotonically increasing entropy values; secondly, clusters of steps with *decreasing entropy*, e.g. $S\left(P_Q^{(49)}\right) \approx$
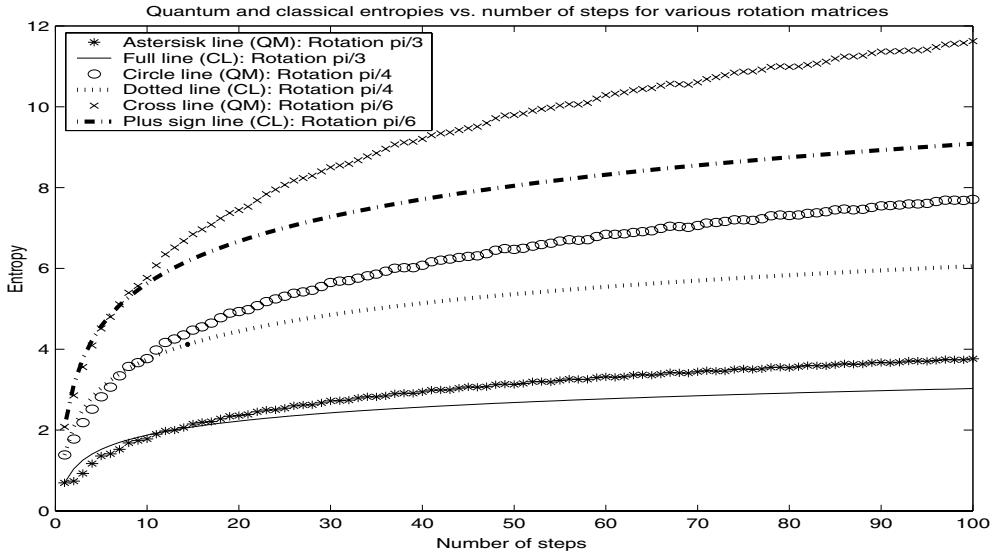
Figure 3. Quantum and classical entropies versus number of steps. The symmetric QRW is as in proposition 1 in each case.

3.3498, $S(P_Q^{(50)}) \approx 3.3467$, $S(P_Q^{(51)}) \approx 3.3408$; and thirdly, *a larger rate of increase* of quantum entropy cf classical entropy on average.

Finally, we indicate that a symmetric QRW with a constantly delayed tracing scheme, as in proposition 2, shows an even greater rate of spreading than the usual symmetric QRW, which in turn is known to spread quadratically faster than a CRW [5, 7].

Define the mth order statistical moment of the distance operator L at step N by $\langle L^m \rangle_N \equiv \mathrm{Tr}(\rho_w^{(N)} L^m)$, where for the 'classical' case corresponding to the 'promptly traced' QRW, $\rho_w^{(N)} = (\varepsilon_V)^N(\rho_w^{(0)})$, and for the cases of quantum walks described in propositions 1 and 2, $\rho_w^{(N)} = \varepsilon_{V^N}(\rho_w^{(0)})$ and $\rho_w^{(N)} = (\varepsilon_{V^2})^N(\rho_w^{(0)})$, respectively. Consider symmetric walks in each case, with $p = 1/2$. All first moments are zero in each case, i.e. $\langle L \rangle_N = 0$, for all N, so that the standard deviation at step N is given by $\sigma_N = \sqrt{\langle L^2 \rangle_N}$. For the CRW we have $\sigma_N^C = \sqrt{N}$ as is well known [1]. Our methods allow us to calculate σ_N easily for QRWs, for a given N. For the first five steps of the QRW of proposition 1 we get $\sigma_1^{Q1} = \sigma_1^C, \sigma_2^{Q1} = \sigma_2^C, \sigma_3^{Q1} = \sigma_3^C, \sigma_4^{Q1} = (\sqrt{5}/2)\sigma_4^C, \sigma_5^{Q1} = \sqrt{8/5}\sigma_5^C$. The enhanced rate of growth in the quantum case, which is known [5, 7] to be given as $N \to \infty$ by $\sigma_N^{(Q1)} \sim \sqrt{N(2-\sqrt{2})/2}\sigma_N^C$, is soon clear.

For the first five steps of the QRW of proposition 2 we have $\sigma_1^{Q2} = \sigma_1^C, \sigma_2^{Q2} = \sqrt{5/2}\sigma_2^C, \sigma_3^{Q2} = \sqrt{3}\sigma_3^C, \sigma_4^{Q2} = \sqrt{7/2}\sigma_4^C, \sigma_5^{Q2} = 2\sigma_5^C$.

We see that the standard deviations for this 'delayed tracing' QRW grow even faster than those of the first type of QRW. Since this second type of walk has constant Kraus generators, it may well be more easily implemented experimentally than the first type [12–14].

Acknowledgments

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