Quantum Random Walks with Memory

Michael Mc Gettrick
michael.mcgettrick@nuigalway.ie

The De Brún Centre for Computational Algebra, School of Mathematics, The National University of Ireland, Galway

Winter School on Quantum Information, Maynooth
January 2010

Outline

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

(Classical) Random Walks

A classical random walk can be defined by specifying

1. States: $|n\rangle$ for $n \in \mathbb{Z}$
2. Allowed transitions:

$$|n\rangle \to \begin{cases} |n-1\rangle & \text{a left move} \\ \text{or} & \\ |n+1\rangle & \text{a right move} \end{cases}$$

3. An initial state: $|0\rangle$
4. Rule(s) to carry out the transitions: In our case we toss a (fair) coin , and move left or right with equal probability (0.5).

This defines a 1 dimensional random walk, sometimes known as the "drunk man's walk", which is well understood in mathematics and computer science. Let us denote by $p_c(n, k)$ the probability of finding the particle at position k in an n step walk ($-n \leq k \leq n$). Some of its properties are

1. The probability distribution is Gaussian (plot of $p_c(n,k)$ against k).

2. For an odd (even) number of steps, the particle can only finish at an odd (even) integer position: $p_c(n,k) = 0$ unless $n \mod 2 = k \mod 2$

3. The maximum probability is always at the origin (for an even number of steps in the walk): $p_c(n,0) > p_c(n,k)$ for even n and even $k \neq 0$.

4. For an infinitely long walk, the probability of finding the particle at any fixed point goes to zero: $\lim_{n\to\infty} p_c(n,k) = 0$.

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

Example: A short classical walk

In a 3 step walk, starting at $|0\rangle$, what is the probability of finding the particle at the point $|-1\rangle$?
We denote by $L(R)$ a left (right) step respectively.

- Possible paths that terminate at $|-1\rangle$ are *LLR*, *LRL* and *RLL*, i.e. those paths with precisely 1 right step and 2 left steps. So there are 3 possible paths.
- Total number of possible paths is $2^3 = 8$.

So the probability is $3/8 = 0.375$.

So, how do we calculate the probabilities?

Physicist (Feynman) Path Integral.
Statistician Summation over Outcomes.

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

Let us denote by N_L the number of left steps and N_R the number of right steps. Of course, fixing N_L and N_R fixes k and n, and vice versa: The equations are

$$\begin{aligned} N_R + N_L &= n \\ N_R - N_L &= k \end{aligned}$$

We have an easy closed form solution for the probabilities $p_c(n,k)$: For a fixed N_L and N_R,

$$\frac{n!}{N_L! N_R! 2^n} = \frac{n!}{((n-k)/2)!((n+k)/2)!2^n} = p_c(n,k)$$

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

We can tabulate the probabilities for the first few iterations:

	Number of steps				
position	0	1	2	3	4
4	0	0	0	0	0.0625
3	0	0	0	0.125	0
2	0	0	0.25	0	0.0625
1	0	0.5	0	0.375	0
0	1	0	0.5	0	0.0375
-1	0	0.5	0	0.375	0
-2	0	0	0.25	0	0.0625
-3	0	0	0	0.125	0
-4	0	0	0	0	0.0625

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

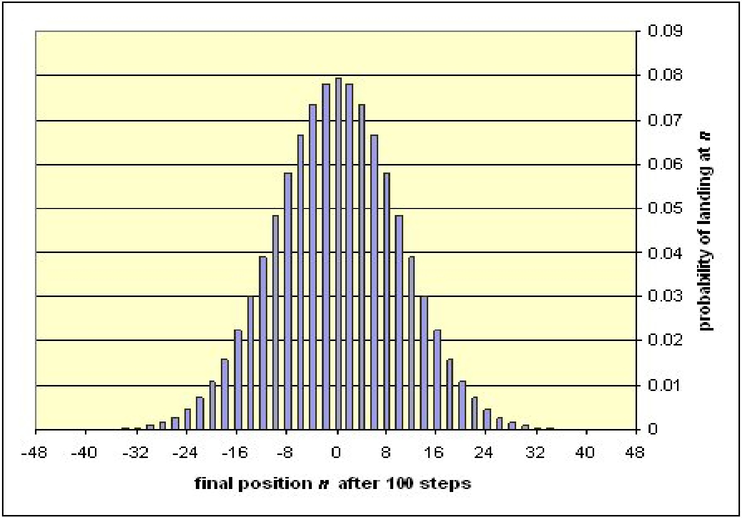


Figure: Probability Distribution after 100 steps

One Dimensional Discrete Quantum Walks (also known as Quantum Markov Chains) take place on the State Space spanned by vectors

$$|n, p\rangle \tag{1}$$

where $n \in Z$ (the integers) and $p \in \{0, 1\}$ is a boolean variable. p is often called the 'coin' state or the chirality, with

$0 \equiv$ spin up

$1 \equiv$ spin down

We can view p as the "quantum part" of the walk, while n is the "classical part".

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

One step of the walk is given by the transitions

$$|n,0\rangle \longrightarrow a\,|n-1,0\rangle + b\,|n+1,1\rangle \qquad (2)$$
$$|n,1\rangle \longrightarrow c\,|n-1,0\rangle + d\,|n+1,1\rangle \qquad (3)$$

where

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SU(2), \qquad (4)$$

the group of 2×2 unitary matrices of determinant 1.

Aside

We can view the transitions as consisting of 2 distinct steps, a "coin flip" operation C followed by a shift operation S:

$$C: \quad |n,0\rangle \longrightarrow a\,|n,0\rangle + b\,|n,1\rangle \qquad (5)$$
$$C: \quad |n,1\rangle \longrightarrow c\,|n,0\rangle + d\,|n,1\rangle \qquad (6)$$
$$S: \quad |n,p\rangle \longrightarrow |n \pm 1,p\rangle \qquad (7)$$

These walks have also been well studied: See Kempe (arXiv:quant−ph/0303081) for a thorough review.

The Hadamard Walk

We choose for our coin flip operation the Hadamard matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{8}$$

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

If we start at initial state $|0,0\rangle$, the first few steps of a standard

quantum (Hadamard) random walk would be

$$|0,0\rangle \longrightarrow \frac{1}{\sqrt{2}}(|-1,0\rangle + |1,1\rangle) \longrightarrow \tag{9}$$

$$\frac{1}{2}(|-2,0\rangle + |0,1\rangle + |0,0\rangle - |2,1\rangle) \longrightarrow \tag{10}$$

$$\frac{1}{2\sqrt{2}}(|-3,0\rangle + |-1,1\rangle + |-1,0\rangle - |1,1\rangle + |-1,0\rangle + |1,1\rangle - |1,0\rangle + |3,1\rangle). \tag{11}$$

Thus after the third step of the walk we see
destructive interference (cancellation of 4th. and 6th. terms)
constructive interference (addition of 3rd. and 5th. terms)
which are features that do not exist in the classical case.

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

The calculation of $p_q(n, k)$ proceeds by again looking at all paths that lead to a particular position k, but this time, since we are in the quantum domain:

- We calculate firstly amplitudes $-$ so we have a $1/\sqrt{2}$ factor added at every step, and final probabilities are amplitudes squared (in our examples, with the Hadamard walk there are no imaginary numbers).
- There are also phases that we must take account of in our amplitude calculations.

In particular, note that the phase -1 from the Hadamard matrix arises every time, in a particular path, we follow a right step by another right step.

Brun, Carteret & Ambainis (arXiv:quant−ph/0210161) have calculated explicitly (using combinatorial techniques) the amplitudes:

Amplitude for final state $|k,0\rangle$

$$\frac{1}{\sqrt{2^n}}\sum_{C=1}^{M}(-1)^{N_L-C}\binom{N_L-1}{C-1}\binom{N_R}{C-1}$$

Amplitude for final state $|k,1\rangle$

$$\frac{1}{\sqrt{2^n}}\sum_{C=1}^{M}(-1)^{N_L-C}\binom{N_L-1}{C-1}\binom{N_R}{C}$$

where M has value N_L for $k \geq 0$ and value $N_R + 1$ otherwise.
The analyses of Kempe (and others) show that for the quantum (Hadamard) random walk with initial state $|0,0\rangle$

1. The probability distribution $p_q(n,k)$ is not gaussian – it oscillates with many peaks.
2. It is not even symmetric.

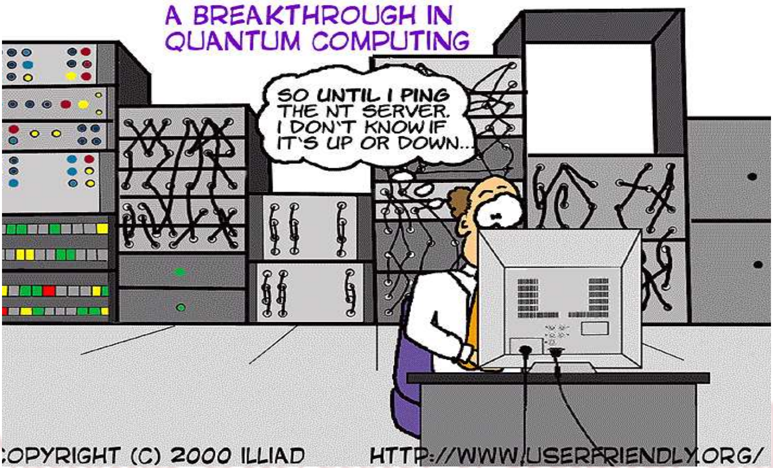
National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

3. For large n, the place at which the particle is most likely to be found is not at the origin: rather it is most likely to be at distance $n/\sqrt{2}$ from the origin.

4. In some general sense, the particle "travels further": The probability distribution is spread fairly evenly between $-n/\sqrt{2}$ and $n/\sqrt{2}$, and only decreases rapidly outside these limits.

5. The asymmetric nature of $p_q(n, k)$ is a figment of the initial state chosen: We can choose a more symmetric initial state to give a symmetric probability distribution.

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh



Ollscoil na hÉireann, Gaillimh

The state space is spanned by vectors of the form

$$|n_r, n_{r-1}, \ldots, n_2, n_1, p\rangle \tag{12}$$

where $n_j = n_{j-1} \pm 1$, since the walk only takes one step right or left at each time interval. n_j is the position of the walk at time $t - j + 1$ (so n_1 is the current position).

The transitions are of the form

$$\begin{aligned} |n_r, n_{r-1}, \ldots, n_2, n_1, 0\rangle \longrightarrow a\,&|n_{r-1}, \ldots, n_2, n_1, n_1 \pm 1, 0\rangle \\ &+ b\,|n_{r-1}, \ldots, n_2, n_1, n_1 \pm 1, 1\rangle \end{aligned} \tag{13}$$

$$\begin{aligned} |n_r, n_{r-1}, \ldots, n_2, n_1, 1\rangle \longrightarrow c\,&|n_{r-1}, \ldots, n_2, n_1, n_1 \pm 1, 0\rangle \\ &+ d\,|n_{r-1}, \ldots, n_2, n_1, n_1 \pm 1, 1\rangle \end{aligned} \tag{14}$$

Order 2

The state space is composed of the families of vectors

$$|n-1,n,0\rangle\,,\qquad |n-1,n,1\rangle\,,\qquad |n+1,n,0\rangle\,,\qquad |n+1,n,1\rangle \tag{15}$$

for $n \in Z$. For obvious reasons, we call

$|n-1,n,p\rangle$ a right mover

$|n+1,n,p\rangle$ a left mover

As before, we can split the transitions into two steps, a "coin flip" operator C and a "shift" operator S:

$$C: \qquad |n_2,n_1,0\rangle \longrightarrow a\,|n_2,n_1,0\rangle + b\,|n_2,n_1,1\rangle \tag{16}$$

$$C: \qquad |n_2,n_1,1\rangle \longrightarrow c\,|n_2,n_1,0\rangle + d\,|n_2,n_1,1\rangle \tag{17}$$

$$S: \qquad |n_2,n_1,p\rangle \longrightarrow |n_1,n_1\pm 1,p\rangle \tag{18}$$

To construct a unitary transition on the states, our possibilities are

Initial State	Final State			
	Case a	Case b	Case c	Case d
$\|n-1,n,0\rangle$	$\|n,n+1,0\rangle$	$\|n,n+1,0\rangle$	$\|n,n-1,0\rangle$	$\|n,n-1,0\rangle$
$\|n-1,n,1\rangle$	$\|n,n+1,1\rangle$	$\|n,n-1,1\rangle$	$\|n,n+1,1\rangle$	$\|n,n-1,1\rangle$
$\|n+1,n,0\rangle$	$\|n,n-1,0\rangle$	$\|n,n-1,0\rangle$	$\|n,n+1,0\rangle$	$\|n,n+1,0\rangle$
$\|n+1,n,1\rangle$	$\|n,n-1,1\rangle$	$\|n,n+1,1\rangle$	$\|n,n-1,1\rangle$	$\|n,n+1,1\rangle$

Table: Action of Shift Operator S

A simpler way to view these cases follows. Depending on the value of the coin state p, one either transmits or reflects the walk:

Transmission corresponds to $|n-1,n,p\rangle \longrightarrow |n,n+1,p\rangle$ and $|n+1,n,p\rangle \longrightarrow |n,n-1,p\rangle$ (i.e. the particle keeps walking in the same direction it was going in)

Reflection corresponds to $|n-1,n,p\rangle \longrightarrow |n,n-1,p\rangle$ and $|n+1,n,p\rangle \longrightarrow |n,n+1,p\rangle$ (i.e. the particle changes direction)

so we can re draw the table as

Value of p	Action of S			
	Case a	Case b	Case c	Case d
0	Transmit	Transmit	Reflect	Reflect
1	Transmit	Reflect	Transmit	Reflect

Table: Action of Shift Operator S

Case a 0 and 1 both give rise to transmission This does not give an interesting walk: particle moves uniformly in one direction. For an initial state which is a superposition of left and right movers, the walk progresses simultaneously right **and** left.

Case d 0 and 1 both give rise to reflection The walk "stays put", oscillating forever between 0 and -1 (for initial state $|-1, 0, p\rangle$)

In both these cases in fact, the coin flip operator C plays no role (since the action of S is independent of p), so there is nothing quantum about these walks.

We analyse in detail Case (c), where 0 corresponds to reflection and 1 to transmission. For the Hadamard case, the coin flip operator C behaves as

$$C: \qquad |n_2, n_1, 0\rangle \longrightarrow \frac{1}{\sqrt{2}}(|n_2, n_1, 0\rangle + |n_2, n_1, 1\rangle) \tag{19}$$

$$C: \qquad |n_2, n_1, 1\rangle \longrightarrow \frac{1}{\sqrt{2}}(|n_2, n_1, 0\rangle - |n_2, n_1, 1\rangle) \tag{20}$$

Aside: Classical Order 2 Random Walk

It should be clear that the classical order 2 random walk corresponding to our quantum order 2 Hadamard walk behaves exactly like a standard (order 1) classical walk.

Classical Order 1 0 always means move left (e.g.) and 1 always means move right.

Classical Order 2 0 means reflect and 1 means transmit: So e.g. 0 will sometimes mean "move left" and sometimes "move right", but always 1 will mean to move in the opposite direction to 0.

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

The first few steps of the Order 2 Hadamard walk for case (c)

are

$$|-1,0,0\rangle \longrightarrow \frac{1}{\sqrt{2}}(|0,-1,0\rangle + |0,1,1\rangle) \longrightarrow \tag{21}$$

$$\frac{1}{2}(|-1,0,0\rangle + |-1,-2,1\rangle + |1,0,0\rangle - |1,2,1\rangle) \longrightarrow \tag{22}$$

$$\begin{aligned}\frac{1}{2\sqrt{2}}(&|0,-1,0\rangle + |0,1,1\rangle + |-2,-1,0\rangle - |-2,-3,1\rangle \\ &+ |0,1,0\rangle + |0,-1,1\rangle - |2,1,0\rangle + |2,3,1\rangle) \longrightarrow\end{aligned} \tag{23}$$

$$\begin{aligned}\frac{1}{4}(&|-1,0,0\rangle + {\color{red}|-1,-2,1\rangle} + {\color{blue}|1,0,0\rangle} - |1,2,1\rangle \\ &+ |-1,-2,0\rangle + |-1,0,1\rangle - |-3,-2,0\rangle + |-3,-4,1\rangle \\ &+ {\color{blue}|1,0,0\rangle} + |1,2,1\rangle + |-1,0,0\rangle - {\color{red}|-1,-2,1\rangle} \\ &- |1,2,0\rangle - |1,0,1\rangle + |3,2,0\rangle - |3,4,1\rangle).\end{aligned} \tag{24}$$

After three steps, there is no interference (constructive or destructive), but the interference appears after step four (e.g.,

in expression 24, we can cancel the 2nd. and 12th. terms, and we can add term 3 and term 9, etc.). We use combinatorial techniques to find all paths leading to a final position k; for each path we determine the amplitude contribution and phase (± 1). There are 4 possible "final states" leading to the particle being found at position$k$:

$|k-1, k, 0\rangle$ (Denote the amplitude by a_{kLR})

$|k-1, k, 1\rangle$ (Denote the amplitude by a_{kRR})

$|k+1, k, 0\rangle$ (Denote the amplitude by a_{kRL})

$|k+1, k, 1\rangle$ (Denote the amplitude by a_{kLL})

Written as a sequence of left/right moves, these correspond to the sequence of Ls and Rs ending in

$\ldots LR \ |k-1, k, 0\rangle$

$\ldots RR \ |k-1, k, 1\rangle$

$\ldots RL \ |k+1, k, 0\rangle$

$\dots LL \ |k+1, k, 1\rangle$

Lemma

We refer to an 'isolated' L (respectively R) as one which is not bordered on either side by another L (respectively R). Let N_L^1 (respectively N_R^1) be the number of isolated Ls (respectively isolated Rs) in the sequence of steps of the walk. Then, the quantum phase associated with this sequence is

$$(-1)^{N_L+N_R+N_L^1+N_R^1} \tag{25}$$

Proof.

- We analyze firstly the contribution of clusters of Ls.
- Clusters of various size contribute as follows:

Cluster	L	LL	LLL	$LLLL$	$LLLLL$	$LLLLLL$
Phase Contribution	+	+	-	+	-	+

- The -1 phase comes from a *transmission* followed by another *transmission*. So the cluster of 3 Ls is the first to contribute.
- For $j > 2$ a cluster of j Ls gives a contribution of $(-1)^j$.
- For clusters of size at least 3:
  - Moving an L from one cluster to another does not change overall phase contribution.

□

Proof.

- So, do this repeatedly until we have only one cluster of size at least 3:

$$\ldots RLR \ldots RLLR \ldots RLR \ldots RLLR \ldots R \quad \underbrace{LLLLL \ldots L}_{\text{One large cluster of } Ls} \quad R \ldots$$

- In this (rearranged) path, the total number of L clusters of size 2 is $C_L - N_L^1 - 1$ (where C_L is the total number of clusters).
- Therefore, the size of the one "large" cluster is

$$N_L - N_L^1 - 2(C_L - N_L^1 - 1) = N_L + N_L^1 - 2C_L + 2$$

□

Proof.

- Since this is the only cluster to contribute, the contribution is

$$(-1)^{N_L+N_L^1}$$

- Analogous arguments apply for right moves $-$ so the overall phase is

$$(-1)^{N_L+N_L^1+N_R+N_R^1}$$

$\square$

We need to know how many paths have particular values of N_L^1 (and N_R^1). Straight forward combinatorics gives

$$\text{Number of compositions of } N_L \text{ into } C_L \text{ parts with exactly } N_L^1 \text{ ones} = \begin{pmatrix} C_L \\ N_L^1 \end{pmatrix} \begin{pmatrix} N_L - C_L - 1 \\ C_L - N_L^1 - 1 \end{pmatrix} = \begin{pmatrix} C_L \\ N_L^1 \\ N_L \end{pmatrix}.$$

Example: Compositions with restrictions

Number of compositions of 5 into 3 parts with 1 one The formula gives

$$\binom{3}{1}\binom{1}{1} = 3$$

which are the compositions $\{122, 212, 221\}$

Number of compositions of 8 into 4 parts with 2 ones The formula gives

$$\binom{4}{2}\binom{3}{1} = 18$$

which are the compositions $\{1142, 1124, 1133\}$ and rearrangements of the 2 ones therein.

Now, knowing the number of paths, and their phase and amplitude contributions, we can do the summations (**....gory details skipped!**). The 4 cases are treated separately. As an

example, the finaly amplitude a_{kLL} is

$$2^{\frac{n}{2}} a_{kLL} = \sum_{C=2}^{N_L-1} \sum_{\substack{N_L^1 = \max(1, \\ 2C - N_L)}}^{C-1} \sum_{\substack{N_R^1 = \max(0, \\ 2C - N_R - 2)}}^{C-2} (-1)^{n+N_L^1+N_R^1} \frac{N_L^1(C-N_L^1)}{C(C-1)} \begin{pmatrix} C \\ N_L^1 \\ N_L \end{pmatrix} \begin{pmatrix} C-1 \\ N_R^1 \\ N_R \end{pmatrix} + \sum_{\substack{N_L^1 = \max(1, \\ 2N_R - N_L + 2)}}^{N_R} (-1)^{N_L+N_L^1} \frac{N_L^1(N_R - N_L^1 + 1)}{N_R(N_R+1)} \begin{pmatrix} N_R+1 \\ N_L^1 \\ N_L \end{pmatrix} \tag{26}$$

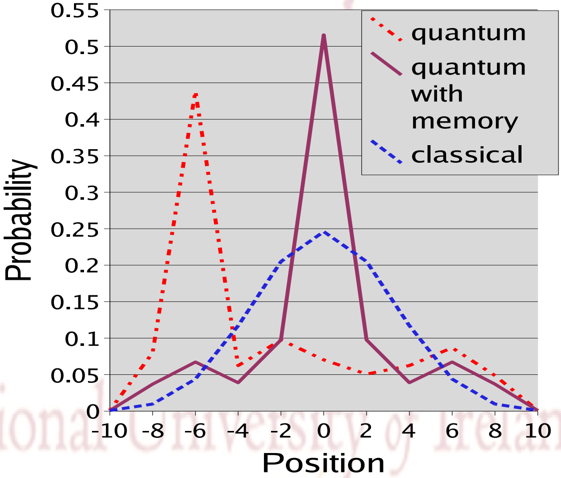


Figure: Probability Distribution after 10 steps

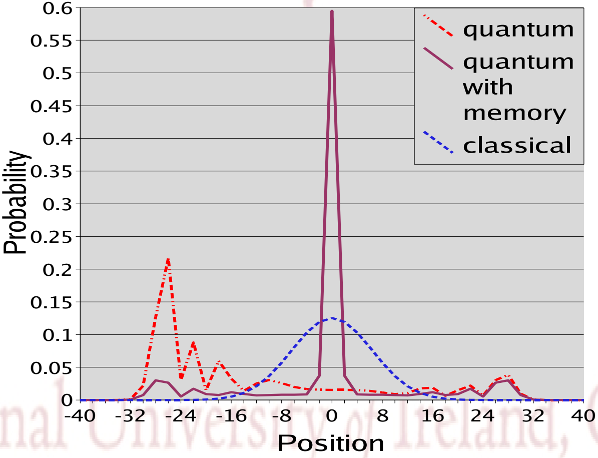


Figure: Probability Distribution after 40 steps

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

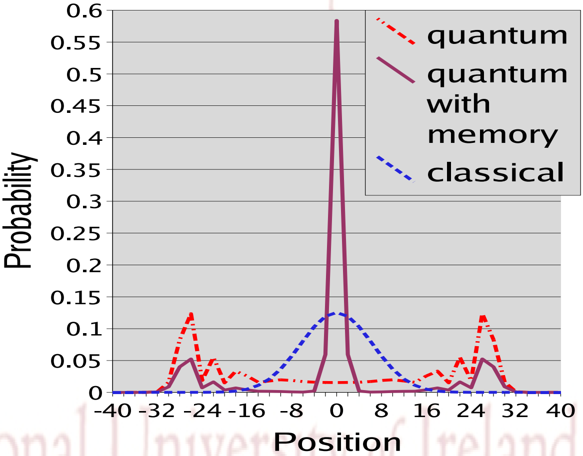


Figure: Probability Distribution after 40 steps for symmetric initial state

We say a particle is **localized** if $\lim_{k\to\infty} p(n,k) \neq 0$. The spike

at the origin leads us to suspect localization for the 2nd. order Hadamard walk.

Lemma

$$\lim_{k\to\infty} p_m(n,k) > 0.5$$

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

Proof.

We proceed by induction. Consider the set

$$S = \{a_{0LR}(n), a_{0RL}(n)\}$$

We analyze how these amplitudes depend on the corresponding amplitudes 2 steps earlier

$$S^{\dagger} = \{a_{0LR}(n-2), a_{0RL}(n-2)\}$$

Base Case For $n = 2$, $a_{0LR}(2) = a_{0RL}(2) = 1/2$ are the only terms contributing to the probability at the origin.

Inductive Step We assume the amplitudes $a_{0LR}(n-2)$ and $a_{0RL}(n-2)$ are both positive and sum to 1 (as in the base case).

$\square$

Proof.

Amplitude of $|-1,0,0\rangle$ This corresponds to $a_{0LR}(n)$. There are 2 contributions from $a_{0**}(n-2)$:

Contribution from $a_{0LR}(n-2)$ The particle moves left and then right. The phase contribution stays positive. The amplitude factor is $(1/\sqrt{2})^2 = 0.5$.

Contribution from $a_{0RL}(n-2)$ The particle moves left and then right. The phase contribution stays positive. The amplitude factor is $(1/\sqrt{2})^2 = 0.5$.

The total amplitude contribution is
$0.5a_{0LR}(n-2) + 0.5a_{0RL}(n-2) =$
$0.5a_{0LR}(n-2) + 0.5(1 - a_{0LR}(n-2)) = 0.5$ $\square$

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

Proof.

Amplitude of $|1,0,0\rangle$ This corresponds to $a_{0RL}(n)$. There are 2 contributions from $a_{0**}(n-2)$:

Contribution from $a_{0LR}(n-2)$ The particle moves right and then left. The phase contribution stays positive. The amplitude factor is $(1/\sqrt{2})^2 = 0.5$.

Contribution from $a_{0RL}(n-2)$ The particle moves right and then left. The phase contribution stays positive. The amplitude factor is $(1/\sqrt{2})^2 = 0.5$.

Thus the total amplitude contribution is
$0.5a_{0LR}(n-2) + 0.5a_{0RL}(n-2) =$
$0.5a_{0LR}(n-2) + 0.5(1 - a_{0LR}(n-2)) = 0.5$ $\square$

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

Proof.

We need to prove also that contributions from $a_{0LL}(n-2)$ and $a_{0RR}(n-2)$ will not break the inductive step. Consider $a_{0LL}(n-2)$. The two contributions arise from moving either *RL* or *LR*.

The amplitude factor, as before, is 0.5. But the phase factor contributions are opposite: For *RL* it is positive, while for *LR* it is negative. This adds $0.5a_{0LL}(n-2)$ to the amplitude $a_{0RL}(n)$ and subtracts $0.5a_{0LL}(n-2)$ from the amplitude $a_{0LR}(n)$. Letting $\epsilon = 0.5a_{0LL}(n-2)$, since $a_{0LR}(n-2)$ and $a_{0RL}(n-2)$ are two positive numbers summing to 1, so are $a_{0LR}(n-2) - \epsilon$ and $a_{0RL}(n-2) + \epsilon$. □

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

Conclusions

- Quantum random walks with memory exhibit new features not found elsewhere.
- Localization occurs in the order 2 case.
- We have exact analytic expressions for the probability distributions (...but the formulae are awful!)

Future Work

- What about higher orders?
- Alternative approach $-$ transform to Fourier domain, analytics are harder but asymptotics are easier (current work).
- What about non$-$Hadamard transitions?
- Is localization unique to the order 2 case?

National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh