Quantum Random Walk: *Mathematica* Syntax and Dirac Notation

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Introduction

Two previous documents showed how to implement the Quantum Random Walk in a "beatiful but slow" way (using Dirac Notation for the Quantum Operators) and an "efficient but specialized" way (using *Mathematica* advanced commands instead of Quantum Operators). In this document a hybrid approach is shown: the Quantum command DefineOperatorOn-Kets is used to create new Quantum Operators that take advantage of the powerful *Mathematica* sintaxis and, once defined, these new Operators can be used inside expresions with kets and bras in Dirac notation.

The quantum random walker (Y. Aharonov, L. Davidovich, and N. Zagury "Quantum random walks" Phys. Rev. A 48, 1687 - 1690 (1993)) is made of a "coin" and a "walker", each one with its own state-space, which will make a composite system with the coin and the walker in entanglement. A unitary operator will be defined to "flip the coin", while another unitary operator will be defined to "move the walker" based on coin's result. The second operator produces entanglement between coin and walker.

Load the Package

First load the Quantum'Notation' package. Write:

Needs["Quantum'Notation'"]

then press at the same time the keys SHET-ENTER to evaluate. Mathematica will load the package:

```
Needs["Quantum`Notation`"]
```

```
Quantum`Notation` Version 2.2.0. (July 2010)

A Mathematica package for Quantum calculations in Dirac bra-ket notation by José Luis Gómez-Muñoz

Execute SetQuantumAliases[] in order to use the keyboard to enter quantum objects in Dirac's notation

SetQuantumAliases[] must be executed again in each new notebook that is created, only one time per notebook.
```

In order to use the keyboard to enter quantum objects write:

SetQuantumAliases[];

then press at the same time the keys shell-enter to evaluate. The semicolon prevents *Mathematica* from printing the help message. Remember that SetQuantumAliases[] must be evaluated again in each new notebook:

SetQuantumAliases[];

Quantum Random Walk using fast Mathematica syntax to define quantum operators

The coin C can have only two states, 0 and 1 (head and tail), while the walker P can be in any (discrete) position from -steps to steps. The coin is inially in state 0 and the walker is initially at the origin 0:

$$| w[0] \rangle = | 0_{\hat{c}} \rangle \otimes | 0_{\hat{p}} \rangle$$

$$| 0_{\hat{c}}, 0_{\hat{p}} \rangle$$

Here we define the "fliping coin" operator, which in this case is a Hadamard operator, but it could be any unitary operator that acts only in the coin C. The coin can have only two states, 0 and 1 (head and tail):

```
DefineOperatorOnKets
  \left\{ \begin{array}{c|c} \mid 0_{\hat{c}} \rangle \Rightarrow \frac{ \left| 0_{\hat{c}} \right\rangle + \left| 1_{\hat{c}} \right\rangle}{\sqrt{2}}, \end{array} \right.
           \left| 1_{\hat{c}} \right\rangle \Rightarrow \frac{\left| 0_{\hat{c}} \right\rangle - \left| 1_{\hat{c}} \right\rangle}{\sqrt{2}} \right\} \right]
```

$$\begin{array}{c} \mid 0_{\hat{c}} \rangle : \rightarrow \frac{\mid 0_{\hat{c}} \rangle + \mid 1_{\hat{c}} \rangle}{\sqrt{2}} \\ \mid 1_{\hat{c}} \rangle : \rightarrow \frac{\mid 0_{\hat{c}} \rangle - \mid 1_{\hat{c}} \rangle}{\sqrt{2}} \end{array}$$

Here we define the "move the walker" operator. Its interpretation is very simple, the walker P moves to the left j-1 if the coin is in state 0, and it moves to the right j+1 if the coin is in state 1:

```
s,
\left\{ \begin{array}{c|c} s, \\ \left| \ 0_{\hat{c}}, \ j_{-\hat{p}} \right\rangle \Rightarrow \ \left| \ 0_{\hat{c}}, \ (j-1)_{\hat{p}} \right\rangle, \\ \left| \ 1_{\hat{c}}, \ j_{-\hat{p}} \right\rangle \Rightarrow \ \left| \ 1_{\hat{c}}, \ (j+1)_{\hat{p}} \right\rangle \\ \end{array} \right\}
```

$$\begin{vmatrix} 0_{\hat{c}}, j_{-\hat{p}} \rangle \leftrightarrow | 0_{\hat{c}}, (j-1)_{\hat{p}} \rangle \\ | 1_{\hat{c}}, j_{-\hat{p}} \rangle \leftrightarrow | 1_{\hat{c}}, (j+1)_{\hat{p}} \rangle \end{vmatrix}$$

This is the evolution of the composite system of coin and walker: flip the coin with the operator h and then move the walker with operator s. This process is repeated "steps" times.

Notice the use of the command Expand at every step. The use of Expand is important when operators created with DefineOperatorOnKets are been used. Expressions can grow very large and calculations become very slow if Expand is Not used, specially with the repeated use of operators that create quantum entanglement. This evaluation does not produce any output, however the evolution of the system is calculted and stored in $|w[0]\rangle$, $|w[1]\rangle$,..., $|w[20]\rangle$

```
steps = 20;
Do[ | \mathbf{w}[\mathbf{k}] \rangle = \text{Expand}[\mathbf{s} \cdot \mathbf{h} \cdot | \mathbf{w}[\mathbf{k} - \mathbf{1}] \rangle],
      \{k, 1, steps, 1\};
```

Each state of the composite system coin-walker is stored. For example this is the state at the second step:

```
| w[2]>
     | 0_{\hat{c}}, (-2)_{\hat{p}} \rangle + \frac{1}{2} | 0_{\hat{c}}, 0_{\hat{p}} \rangle + \frac{1}{2} | 1_{\hat{c}}, 0_{\hat{p}} \rangle - \frac{1}{2} | 1_{\hat{c}}, 2_{\hat{p}} \rangle
```

And this is the state at the fifth step:

```
| w[5]>

\frac{\left|\begin{array}{c} 0_{\hat{c}}, \ (-5)_{\hat{p}} \right\rangle}{4\sqrt{2}} + \frac{\left|\begin{array}{c} 0_{\hat{c}}, \ (-3)_{\hat{p}} \right\rangle}{\sqrt{2}} - \frac{\left|\begin{array}{c} 0_{\hat{c}}, \ 3_{\hat{p}} \right\rangle}{4\sqrt{2}} + \\
\frac{\left|\begin{array}{c} 1_{\hat{c}}, \ (-3)_{\hat{p}} \right\rangle}{4\sqrt{2}} + \frac{\left|\begin{array}{c} 1_{\hat{c}}, \ (-1)_{\hat{p}} \right\rangle}{2\sqrt{2}} - \frac{\left|\begin{array}{c} 1_{\hat{c}}, \ 1_{\hat{p}} \right\rangle}{2\sqrt{2}} + \frac{\left|\begin{array}{c} 1_{\hat{c}}, \ 3_{\hat{p}} \right\rangle}{2\sqrt{2}} + \frac{\left|\begin{array}{c} 1_{\hat{c}}, \ 5_{\hat{p}} \right\rangle}{4\sqrt{2}} \\
\end{array}
```

Here we define the position projector operator pp[j] for each position j of the walker:

```
Do
    With [{j = pos},
     DefineOperatorOnKets
         \left\{ \left( \begin{array}{c} \left| \begin{array}{c} n_{-\hat{e}}, & k_{-\hat{p}} \end{array} \right\rangle /; & k = ! = j \end{array} \right) :> 0, 
          \left| \begin{array}{c} \mathbf{n}_{-\hat{\mathbf{c}}}, \ \mathbf{j}_{\hat{\mathbf{p}}} \right\rangle :> \left| \begin{array}{c} \mathbf{n}_{\hat{\mathbf{c}}}, \ \mathbf{j}_{\hat{\mathbf{p}}} \end{array} \right\rangle
     {pos, -steps, steps}
```

Here we calculate the probabilities for each walker position.

$$\left\{\left\{-20, \frac{1}{1048576}\right\}, \left\{-19, 0\right\}, \left\{-18, \frac{181}{524288}\right\}, \left\{-17, 0\right\}, \left\{-16, \frac{9257}{524288}\right\}, \left\{-15, 0\right\}, \right\}$$

$$\left\{-14, \frac{95617}{524288}\right\}, \left\{-13, 0\right\}, \left\{-12, \frac{295265}{1048576}\right\}, \left\{-11, 0\right\}, \left\{-10, \frac{965}{32768}\right\}, \left\{-9, 0\right\}, \right\}$$

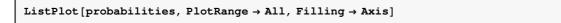
$$\left\{-8, \frac{2501}{32768}\right\}, \left\{-7, 0\right\}, \left\{-6, \frac{2377}{32768}\right\}, \left\{-5, 0\right\}, \left\{-4, \frac{11221}{262144}\right\}, \left\{-3, 0\right\}, \left\{-2, \frac{4165}{131072}\right\}, \right\}$$

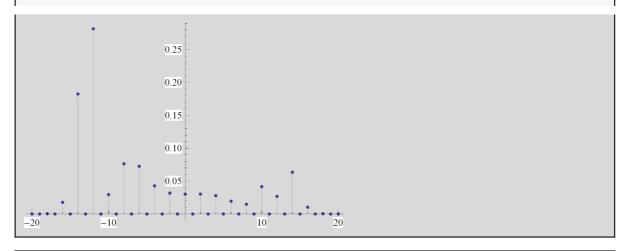
$$\left\{-1, 0\right\}, \left\{0, \frac{3969}{131072}\right\}, \left\{1, 0\right\}, \left\{2, \frac{3969}{131072}\right\}, \left\{3, 0\right\}, \left\{4, \frac{7301}{262144}\right\}, \left\{5, 0\right\}, \left\{6, \frac{637}{32768}\right\}, \right\}$$

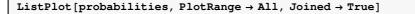
$$\left\{7, 0\right\}, \left\{8, \frac{485}{32768}\right\}, \left\{9, 0\right\}, \left\{10, \frac{1361}{32768}\right\}, \left\{11, 0\right\}, \left\{12, \frac{28097}{1048576}\right\}, \left\{13, 0\right\}, \right\}$$

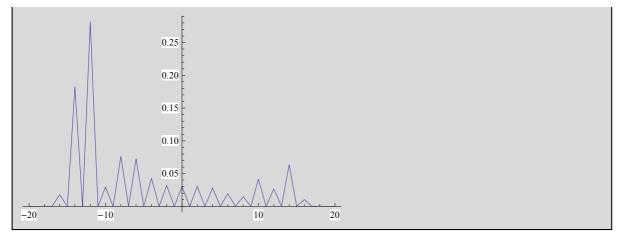
$$\left\{14, \frac{33317}{524288}\right\}, \left\{15, 0\right\}, \left\{16, \frac{5417}{524288}\right\}, \left\{17, 0\right\}, \left\{18, \frac{145}{524288}\right\}, \left\{19, 0\right\}, \left\{20, \frac{1}{1048576}\right\}\right\}$$

Here is a plot of the probabilities for each position of the walker.









Another way to obtain the probabilities is using the Quantum Mathematica command QuantumMeasurement

$qm = \texttt{QuantumMeasurement} \left[~|~ w[\texttt{steps}] \right), ~ \{\hat{p}\}, ~ \texttt{FactorKet} \rightarrow \texttt{False} \right]$

Deckaritie	M	05-55-
Probability	Measurement	State
1 0 4 8 5 7 6	$\left\{\left\{\left(-20\right)_{\hat{p}}\right\}\right\}$	0 _ĉ , (-20) _ĝ
181 524 288	{{(-18) _{p̂} }}	$\frac{19 \left 0_{\hat{c}}, (-18)_{\hat{p}} \right\rangle + \left 1_{\hat{c}}, (-18)_{\hat{p}} \right\rangle}{\sqrt{-18}}$
9257		$ \sqrt{362} $ 135 $ 0_{\hat{c}}, (-16)_{\hat{p}}\rangle + 17 1_{\hat{c}}, (-16)_{\hat{p}}\rangle$
524 288	$\left\{\left\{\left(-16\right)_{\hat{p}}\right\}\right\}$	$\frac{\sqrt{18514}}{\sqrt{18514}}$
95 617	{{(-14) _p }}	$\frac{425 \left 0_{\hat{c}}, (-14)_{\hat{p}} \right\rangle + 103 \left 1_{\hat{c}}, (-14)_{\hat{p}} \right\rangle}{}$
524 288	((, ,b))	√191 234
295 265 1 048 576	$\left\{\left\{\left(-12\right)_{\hat{p}}\right\}\right\}$	$\frac{484 \left 0_{\hat{c}}, (-12)_{\hat{p}} \right\rangle + 247 \left 1_{\hat{c}}, (-12)_{\hat{p}} \right\rangle}{\sqrt{295265}}$
965	{{(-10) _{p̂} }}	$-33 \mid 0_{\hat{c}}, (-10)_{\hat{p}} \rangle + 29 \mid 1_{\hat{c}}, (-10)_{\hat{p}} \rangle$
32 768	[[(±o/p]]	√1930
2501 32 768	$\{\{(-8)_{\hat{p}}\}\}$	$-\frac{49 \left 0_{\hat{c}}, (-8)_{\hat{p}}\right> + 51 \left 1_{\hat{c}}, (-8)_{\hat{p}}\right>}{\sqrt{5002}}$
2377	[[(<)]]	$65 \mid 0_{\hat{c}}, (-6)_{\hat{p}} \rangle + 23 \mid 1_{\hat{c}}, (-6)_{\hat{p}} \rangle$
32 768	$\left\{\left\{\left.\left(-6\right)_{\hat{p}}\right\}\right\}\right.$	
11 221 262 144	$\left\{\left\{\left(-4\right)_{\hat{p}}\right\}\right\}$	$\frac{-15 \left 0_{\hat{c}}, (-4)_{\hat{p}} \right\rangle + 2 \left 1_{\hat{c}}, (-4)_{\hat{p}} \right\rangle}{\sqrt{229}}$
4165	(((0)))	11 $ 0_{\hat{c}}, (-2)_{\hat{p}}\rangle - 7 1_{\hat{c}}, (-2)_{\hat{p}}\rangle$
131 072	$\left\{\left\{\left(-2\right)_{\hat{p}}\right\}\right\}$	√170
3969 131 072	$\{\{0_{\hat{p}}\}\}$	$\frac{-\left 0_{\hat{c}},0_{\hat{p}}\right\rangle+\left 1_{\hat{c}},0_{\hat{p}}\right\rangle}{\sqrt{2}}$
3969	((0))	$ 0_{\hat{c}},2_{\hat{p}}\rangle - 1_{\hat{c}},2_{\hat{p}}\rangle$
131 072	$\left\{\left\{2_{\hat{p}}\right\}\right\}$	$\sqrt{2}$
7301 262 144	$\left\{\left\{4_{\hat{p}}\right\}\right\}$	$\frac{-10 \mid 0_{\hat{c}}, 4_{\hat{p}} \rangle + 7 \mid 1_{\hat{c}}, 4_{\hat{p}} \rangle}{\sqrt{149}}$
637	((c))	$5 \left 0_{\hat{c}}, 6_{\hat{p}} \right\rangle - \left 1_{\hat{c}}, 6_{\hat{p}} \right\rangle$
32 768	$\{\{6_{\hat{p}}\}\}$	$\sqrt{26}$
485 32 768	{{8 _ĝ }}	$-\frac{21 \left 0_{\hat{c}}, 8_{\hat{p}} \right\rangle + 23 \left 1_{\hat{c}}, 8_{\hat{p}} \right\rangle}{\phantom{aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa$
		$\sqrt{970}$ -11 $ 0_{\hat{c}}, 10_{\hat{p}}\rangle + 51 1_{\hat{c}}, 10_{\hat{p}}\rangle$
1361 32 768	$\left\{ \left\{ 10_{\hat{p}}\right\} \right\}$	$\frac{\frac{11 \left \sigma_{c} / 10_{p} / 101 \right \left \Gamma_{c} / 10_{p} / 101 \right }{\sqrt{2722}}$
28 097	$\{\{12_{\hat{p}}\}\}$	$\frac{121 \left 0_{\hat{c}}, 12_{\hat{p}} \right\rangle - 116 \left 1_{\hat{c}}, 12_{\hat{p}} \right\rangle}{}$
1 0 4 8 5 7 6	[[±²p]]	√28097
33 317 524 288	$\left\{ \left\{ 14_{\hat{p}}\right\} \right\}$	$\frac{75 \left 0_{\hat{c}}, 14_{\hat{p}} \right\rangle - 247 \left 1_{\hat{c}}, 14_{\hat{p}} \right\rangle}{\sqrt{66634}}$
5417	$\{\{16_{\hat{p}}\}\}$	$15 \mid 0_{\hat{c}}, 16_{\hat{p}} \rangle - 103 \mid 1_{\hat{c}}, 16_{\hat{p}} \rangle$
524 288		√10834
145 524 288	$\{\{18_{\hat{p}}\}\}$	$\frac{\left 0_{\hat{c}},18_{\hat{p}}\right\rangle-17\left 1_{\hat{c}},18_{\hat{p}}\right\rangle}{\sqrt{290}}$
1 1 0 4 8 5 7 6	{{20 _{p̂} }}	$- \left 1_{\hat{c}}, 20_{\hat{p}} \right\rangle$
Probability	Measurement	State
	1	

You can extract the list of probabilities using standard Mathematica notation. Remember that the measurement results were stored in the variable qm:

```
qm[[1, All, 1]]
```

```
\left\{\frac{1}{1\,048\,576}, \frac{181}{524\,288}, \frac{9257}{524\,288}, \frac{95\,617}{524\,288}, \frac{295\,265}{1\,048\,576}, \frac{965}{32\,768}, \frac{2501}{32\,768}, \frac{2377}{32\,768}, \frac{11\,221}{32\,768}, \frac{4165}{131\,072}, \frac{3969}{131\,072}, \frac{3969}{131\,072}, \frac{7301}{262\,144}, \frac{637}{32\,768}, \frac{485}{32\,768}, \frac{1361}{32\,768}, \frac{28\,097}{1\,048\,576}, \frac{33\,317}{524\,288}, \frac{5417}{524\,288}, \frac{145}{524\,288}, \frac{1}{1\,048\,576}\right\}
```

The standard *Mathematica* command N[] gives the numerical values of the probabilities:

N[qm]

Probability	Measurement	State
9.53674×10 ⁻⁷	{{(-20) _{p̂} }}	$\left 0_{\hat{c}}, (-20)_{\hat{p}} \right\rangle$
0.00034523	{{(-18) _{p̂} }}	$0.0525588 \left(19. \mid 0_{\hat{c}}, (-18)_{\hat{p}}\right) + \mid 1_{\hat{c}}, (-18)_{\hat{p}}\right)\right)$
0.0176563	{{(-16) _{p̂} }}	0.00734937 (135. $ 0_{\hat{c}}, (-16)_{\hat{p}}\rangle + 17. 1_{\hat{c}}, (-16)_{\hat{p}}\rangle)$
0.182375	{{(-14) _{p̂} }}	$0.00228674 \left(425. \mid 0_{\hat{c}}, (-14)_{\hat{p}}\right) + 103. \mid 1_{\hat{c}}, (-14)_{\hat{p}}\right)$
0.281587	{{(-12) _{p̂} }}	$0.00184032 \left(484. \mid 0_{\hat{c}}, (-12)_{\hat{p}}\right) + 247. \mid 1_{\hat{c}}, (-12)_{\hat{p}}\right)\right)$
0.0294495	$\left\{\left\{\left.\left(-10\right)_{\hat{p}}\right\}\right\}\right.$	$0.0227626 \left(-33. \mid 0_{\hat{c}}, (-10)_{\hat{p}}\right) + 29. \mid 1_{\hat{c}}, (-10)_{\hat{p}}\right)$
0.0763245	{{(-8) _{p̂} }}	$-0.0141393 \left(49. \mid 0_{\hat{c}}, (-8)_{\hat{p}}\right) + 51. \mid 1_{\hat{c}}, (-8)_{\hat{p}}\right)\right)$
0.0725403	{{(-6) _{p̂} }}	0.0145034 (65. $ 0_{\hat{c}}, (-6)_{\hat{p}}\rangle + 23. 1_{\hat{c}}, (-6)_{\hat{p}}\rangle)$
0.0428047	$\left\{ \left\{ \left. \left(-4\right) _{\hat{p}}\right\} \right\} \right.$	0.0660819 $\left(-15. \mid 0_{\hat{c}}, (-4)_{\hat{p}}\right) + 2. \mid 1_{\hat{c}}, (-4)_{\hat{p}}\right)$
0.0317764	$\left\{\left\{\left(-2\right)_{\hat{p}}\right\}\right\}$	$0.0766965 \left(11. \mid 0_{\hat{c}}, (-2)_{\hat{p}} \right) - 7. \mid 1_{\hat{c}}, (-2)_{\hat{p}} \right)$
0.0302811	$\left\{ \left\{ 0_{\hat{\mathbf{p}}}\right\} \right\}$	0.707107 $\left(-1. \mid 0_{\hat{c}}, 0_{\hat{p}}\right) + \mid 1_{\hat{c}}, 0_{\hat{p}}\right)\right)$
0.0302811	$\left\{ \left\{ 2_{\hat{p}}\right\} \right\}$	0.707107 ($ 0_{\hat{c}}, 2_{\hat{p}} \rangle - 1. 1_{\hat{c}}, 2_{\hat{p}} \rangle$)
0.0278511	$\left\{ \left\{ 4_{\hat{p}}\right\} \right\}$	0.0819232 (-10. $ 0_{\hat{c}}, 4_{\hat{p}} \rangle + 7. 1_{\hat{c}}, 4_{\hat{p}} \rangle$)
0.0194397	$\{\{6_{\hat{p}}\}\}$	0.196116 (5. $ 0_{\hat{c}}, 6_{\hat{p}} \rangle - 1. 1_{\hat{c}}, 6_{\hat{p}} \rangle)$
0.014801	$\{\{8_{\hat{p}}\}\}$	$-0.0321081 \left(21. \mid 0_{\hat{c}}, 8_{\hat{p}}\right) + 23. \mid 1_{\hat{c}}, 8_{\hat{p}}\right)\right)$
0.0415344	$\left\{ \left\{ 10_{\hat{p}}\right\} \right\}$	0.0191671 $\left(-11. \mid 0_{\hat{c}}, 10_{\hat{p}}\right) + 51. \mid 1_{\hat{c}}, 10_{\hat{p}}\right)\right)$
0.0267954	$\left\{\left\{12_{\hat{p}}\right\}\right\}$	0.00596582 (121. \mid 0 _ĉ , 12 _{\hat{p}}) - 116. \mid 1 _{\hat{c}} , 12 _{\hat{p}}))
0.0635471	$\left\{ \left\{ 14_{\hat{p}}\right\} \right\}$	0.00387393 (75. $\left 0_{\hat{c}}, 14_{\hat{p}} \right\rangle - 247. \left 1_{\hat{c}}, 14_{\hat{p}} \right\rangle \right)$
0.0103321	$\left\{\left\{16_{\hat{p}}\right\}\right\}$	0.00960739 (15. $\left 0_{\hat{c}}, 16_{\hat{p}} \right\rangle - 103. \left 1_{\hat{c}}, 16_{\hat{p}} \right\rangle \right)$
0.000276566	$\left\{\left\{18_{\hat{p}}\right\}\right\}$	0.058722 (\mid 0 _ĉ , 18 _{\hat{p}} \rangle -17. \mid 1 _{\hat{c}} , 18 _{\hat{p}} \rangle)
9.53674×10^{-7}	$\left\{ \left\{ 20_{\hat{p}}\right\} \right\}$	-1. 1 _ĉ , 20 _ĝ)
Probability	Measurement	State