

Counting Statistics of Many-Particle Quantum Walks

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==== [1] Introduction

Ever since the discovery of quantum mechanics people have been puzzled by the counter-intuitive character of the laws of nature. Over time we have learned to accept the more and more effects that unimaginable in a classical world. Recent years research has uncovered many new effects that are strikingly different from their classical counterparts. In this work we will talk about one of the many surprising aspects of quantum world, it is quantum random walk.

To illustrate quantum random walks and give an intuition, we start with an example. We define the model in one dimension, on a line or a circle. Next step, we take the Hilbert space spanned by the positions of the particle. For a circle of size M we have

$$\mathcal{H}_x = \{|x\rangle : x = 0, \dots, M - 1\} \quad (1)$$

The position Hilbert space is extended by a 'coin'-space, which is spanned by two basis states

$$\mathcal{H}_c = \{|\uparrow\rangle, |\downarrow\rangle\} \quad (2)$$

States of the total system are in the space $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_x$. The conditional translation of the system can be described by the following unitary operator

$$S = |\uparrow\rangle\langle\uparrow| \otimes \sum_x |x+1\rangle\langle x| + |\downarrow\rangle\langle\downarrow| \otimes \sum_x |x-1\rangle\langle x| \quad (3)$$

where the index x runs over $0 \leq x \leq M - 1$. S transforms the basis state $|\uparrow\rangle \otimes |x\rangle$ to $|\uparrow\rangle \otimes |x+1\rangle$ and $|\downarrow\rangle \otimes |x\rangle$ to $|\downarrow\rangle \otimes |x-1\rangle$. From now on we will use the standard ordering $\mathcal{H} = \mathcal{H}_x \otimes \mathcal{H}_c$ which is represented by $|x\sigma\rangle$ vectors.

The first step of a random walk is a rotation in the 'coin'-space \mathcal{H}_c . The unitary transformation \mathcal{C} is very arbitrary and therefore a rich family of walks with different behavior can be defined by modifying \mathcal{C} . A frequently used balanced unitary 'coin' is so called Hadamard coin H ,

$$H^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (4)$$

and for M sites it looks like $H^{(M)} = H \otimes H \otimes \dots \otimes H$ ($2M \times 2M$ matrix).

It is easy to see that the Hadamard coin is balanced:

$$H(|0\rangle \otimes |\uparrow\rangle) = \frac{1}{\sqrt{2}} (|0\rangle \otimes (|\uparrow\rangle + |\downarrow\rangle)) \quad (5)$$

$$S \left(\frac{1}{\sqrt{2}} (|0\rangle \otimes (|\uparrow\rangle + |\downarrow\rangle)) \right) = \frac{1}{\sqrt{2}} (|1\rangle \otimes |\uparrow\rangle + |-1\rangle \otimes |\downarrow\rangle) \quad (6)$$

Measuring such coin state in the standard basis gives each of $\{|1\rangle \otimes |\uparrow\rangle, |-1\rangle \otimes |\downarrow\rangle\}$ with probability $\frac{1}{2}$. After this measurement there is no correlation between the positions left. If we continue such a measurement at each iteration we obtain the plain classical random walk on the circle. Its limiting distribution on the line (for a large number of iterations t) approaches a Gaussian distribution with mean zero and variance $\sigma^2 = t$.

In the quantum random walk we will not measure the coin register during intermediate iterations, but keep the quantum correlations between different positions and let them interfere in subsequent steps. This interference will cause a radically different behavior of the quantum walk.

t \ x	-3	-2	-1	0	1	2	3
0				1			
1			1/2		1/2		
2		1/4		1/2		1/4	
3	1/8		3/8		3/8		1/8

(a) The probability of being at position x after t steps of the classical random walk on the line starting at 0.

t \ x	-3	-2	-1	0	1	2	3
0				1			
1			1/2		1/2		
2		1/4		1/2		1/4	
3	1/8		5/8		1/8		1/8

(b) The probability of being at position x after t steps of the quantum random walk on the line with the initial state $|\Phi_{in}\rangle = |\downarrow\rangle \otimes |0\rangle$.

The quantum random walk of t steps is defined as the transformation U^t which can be written as

$$U^t = U(t) = UUUU \dots U \quad (7)$$

where U is acting on $\mathcal{H} = \mathcal{H}_x \otimes \mathcal{H}_c$, and is given by

$$U = SH^{(M)} \quad (8)$$

U is represented as a multiplication the following matrices,

$$S = \begin{pmatrix} \ddots & \mathbf{R} & \mathbf{0} & \mathbf{0} \\ \mathbf{R}^\dagger & \mathbf{0} & \mathbf{R} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}^\dagger & \mathbf{0} & \mathbf{R} \\ \mathbf{0} & \mathbf{0} & \mathbf{R}^\dagger & \ddots \end{pmatrix} \quad H^{(M)} = \begin{pmatrix} \ddots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{H} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{H} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \ddots \end{pmatrix} \quad (9)$$

while \mathbf{R} , \mathbf{H} , $\mathbf{0}$ are defined as the following 2×2 matrices

$$\mathbf{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{R}^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (10)$$

To illustrate the difference between the quantum random walk and its classical counterpart let us evolve the walk for some steps starting in the initial state $|\downarrow\rangle \otimes |0\rangle$. The results can be found in Fig(a) and Fig(b) respectively. Below is an example of an algebra used in such calculations.

$$|\downarrow\rangle \otimes |0\rangle \rightarrow U(|\downarrow\rangle \otimes |0\rangle) = \frac{1}{\sqrt{2}} (|\uparrow\rangle \otimes |1\rangle - |\downarrow\rangle \otimes |-1\rangle) \quad (11)$$

This example shows that the probability distribution induced by the quantum walk (fig(b)) differs from the classical one (fig(a)), and that it is asymmetrically distributed on the positions (it is drifting to the left). The drift to the left arises from different treatment of $|\uparrow\rangle$ and $|\downarrow\rangle$ by the Hadamard. Intuitively, this induces more cancellations for paths going right (destructive interference), whereas particles moving to the left interfere constructively. To obtain symmetric distribution of $|\uparrow\rangle$ and $|\downarrow\rangle$ we can use either: define initial state $\frac{1}{\sqrt{2}} (|0\rangle \otimes (|\uparrow\rangle + i|\downarrow\rangle))$ or use a different

balanced 'coin' - $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$.

The classical symmetric random walk on the line after t steps has a variance $\sigma^2 = t$, so the expected distance from the origin is of order $\sigma = \sqrt{t}$. By contrast the quantum random walk has variance that scales with $\sigma^2 \sim t^2$, which implies that the expected distance from the origin is of order $\sigma \sim t$. This result can be understood by thinking of Bloch waves in a periodic lattice, in this case the motion of the waves in a lattice is ballistic, (when a $\sigma \sim t$ the motion is called ballistic).

A simulation that presents both walks can be found here [Quantum Random Walk](#).

Quantum versions of random walks have diverse applications that are motivating experimental implementations, however the main driving behind this interest is the use in quantum algorithms, which have always employed the quantum walks form of a program running on a quantum computer. Moreover, quantum walks used to model transport phenomena in spin chains and bio-molecules broaden their scope beyond algorithms.

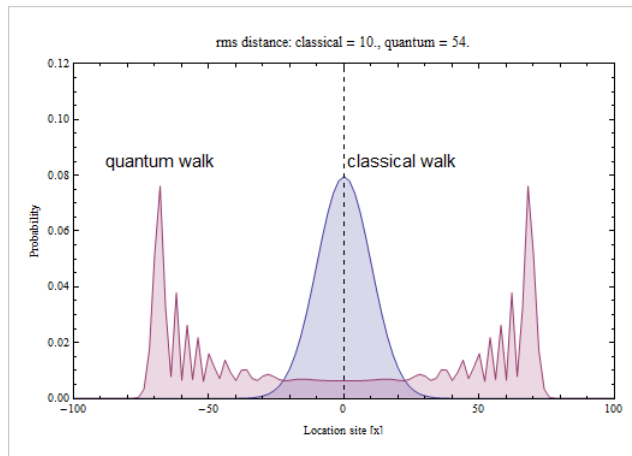


FIG. 1: Quantum random walk vs. classical random walk. The quantum spreading is proportional to t while in classical case it is proportional to \sqrt{t} . Taken from [2].

==== [2] Occupation Statistics:

The Classical Problem:

We want to solve the following combinatorial problem. Find the distribution of N identical particles on M sites. In a classical manner we have to count on all the possible arrangements of the system. In the following the arrangement of N particles in the M modes will be denoted by a vector $\mathbf{n}_k = (n_1, n_2, \dots, n_M)$, with n_k the number of orbitals in the “output” mode k , and $\sum_i n_i = N$. For distinguishable, non interacting particles the probability for a certain arrangement \mathbf{n}_k is:

$$P_{cl}(\mathbf{n}_k) = \frac{N!}{M^N} \prod_{i=0}^{M-1} \frac{1}{n_i!} \quad (12)$$

This situation is called classical since there are no interferences between the particles (probabilities are summed instead of amplitudes). Example: (here we take $N = M$) Coincident events $\mathbf{n}_c = (1, 1, \dots, 1)$ are realized with probability $\frac{N!}{N^N}$, and bunching events (all particles are in one specific mode) $\mathbf{n}_b = (0, 0, \dots, N, \dots, 0)$ are realized with probability $\frac{1}{N^N}$. Both events are unlikely for large N .

The Quantum problem:

The analogous problem with identical quantum particles is best formulated in second quantization with the following creation and annihilation rules:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j} ; [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0 \text{ bosons} \quad (13)$$

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{i,j} ; \{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \text{ fermions} \quad (14)$$

Since applications are possible with today’s optical technologies we focus on bosons.

The initial state is defined as

$$|(1, 1, \dots, 1)_x\rangle = \prod_{x=0}^{M-1} \hat{a}_x^\dagger |0\rangle \quad (15)$$

The input creation operators \hat{a}_x^\dagger are mapped to output creation operators \hat{b}_k^\dagger through unitary matrix U , such that

$$\hat{b}_k^\dagger = \sum_{x=0}^{M-1} U_{xk} \hat{a}_x^\dagger \quad (16)$$

Formally, the unbiased Bell multiport beam splitter under consideration corresponds to the unitary operation given by the Fourier matrix, defined for any dimension M by

$$U_{xk} = \frac{e^{\frac{2\pi i}{M} \cdot x \cdot k}}{\sqrt{M}} \quad (17)$$

The possible states with fixed particle number per port after the scattering process read

$$|(n_0, n_1, \dots)_k\rangle = \left(\prod_{k=0}^{M-1} \frac{1}{\sqrt{n_k!}} \left(\hat{b}_k^\dagger \right)^{n_k} \right) |0\rangle \quad (18)$$

In order to describe the event probability of a given arrangement \mathbf{n}_k , we define a vector \mathbf{X} of length N with entries that specify each particle's output port. It is constructed by concatenating n_k times the port number (k), ($\mathbf{X}(\mathbf{n}_k, k)$ maps particle k according to \mathbf{n}_k into output ports).

$$\mathbf{X} = \left(\underbrace{1, 1, \dots, 1}_{n_1}, \underbrace{2, 2, \dots, 2}_{n_2}, \dots, \underbrace{n, n, \dots, n}_{n_n} \right) \quad (19)$$

or in a short way it can be written as $\mathbf{X} = T\mathbf{n}_k$, where T denotes a mapping matrix between two vectors. More comprehensive description of T is that it maps vectors from Fock space to vectors into Hilbert space. One can see that for the vector $\mathbf{n}_k = (3, 2, 3, 0, 2)$ in Fock space, the vector that is accepted in Hilbert space is $\mathbf{X}(\mathbf{n}_k) = (1, 1, 1, 2, 2, 3, 3, 3, 5, 5)$. So we can write the transition probability to a specific output arrangement \mathbf{n}_k as:

$$P_{qm}(\mathbf{n}_k) = |\langle (n_0, n_1, \dots)_k | (1, 1, \dots, 1)_x \rangle|^2 = \prod_{j=0}^{M-1} \frac{1}{\sqrt{n_j!}} \left| \sum_{K \in P_n} \prod_{a=1}^N U_{X_a(\mathbf{n}_k), K(a)} \right|^2 \quad (20)$$

where P_n denotes the set of all permutations of $\{1, \dots, n\}$. $K(a)$ is a permutation function that maps the particles into the orbitals $K(a) = k$. For example: a given permutation K that is defined as:

$$K = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 2 & 1 \end{pmatrix} \quad (21)$$

As an example of use of eq (11): we calculate $P_{qm}(\mathbf{n}_k)$ for different \mathbf{n}_k while the initial state of the system is $|(1, 1)_x\rangle$ and $N = 2$. We calculate explicitly just for a special case, for the output $\mathbf{n}_k = (1, 1) \rightarrow X = (1, 2)$. The algebra shown below can be applied for calculating the other cases, the results are shown in Fig (2).

$$P_{qm}(1, 1) = |\langle (1, 1)_k | (1, 1)_x \rangle|^2 = \prod_{j=0}^{M-1} \frac{1}{\sqrt{n_j!}} \left| \sum_{K \in P_n} \prod_{a=1}^N U_{X_a(1,1), K(a)} \right|^2 \quad (22)$$

$$= \frac{1}{1!1!} |U_{X_1(1,1), K_1(1)} U_{X_2(1,1), K_1(2)} + U_{X_1(1,1), K_2(1)} U_{X_2(1,1), K_2(2)}|^2 \quad (23)$$

$$= \frac{1}{1!1!} |U_{1,0} U_{2,1} + U_{1,1} U_{2,0}|^2 \quad (24)$$

$$= \left| \frac{e^{\frac{2\pi i}{2} \cdot 0} e^{\frac{2\pi i}{2} \cdot 1}}{\sqrt{2}} + \frac{e^{\frac{2\pi i}{2} \cdot 0} e^{\frac{2\pi i}{2} \cdot 0}}{\sqrt{2}} \right|^2 = \left| \frac{1}{\sqrt{2}} \frac{-1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \right|^2 = 0 \quad (25)$$

It is possible to recover a general bosonic behavior by grouping many final arrangements in larger classes which are characterized by the number of occupied ports k or by the number of particles in one port m . The event probability for such a class is given by the sum of the probabilities of the single events that pertain to the class. Very generally,

$ \Phi_k\rangle$	$ \mathbf{n}_k\rangle$	P_{cl}	P_{qm}
$k=1$ ——— $k=0$ ●●●	$(2,0)_k$	1/4	1/2
$k=1$ ●—— $k=0$ ●——	$(1,1)_k$	1/2	0
$k=1$ ●●—— $k=0$ ———	$(0,2)_k$	1/4	1/2

FIG. 2: The probability to find two bosons in s state $|\Phi_k\rangle$ while beginning at the state $|(1,1)_x\rangle$. The probabilities of quantum and classical cases are shown.

for bosons, quantum states with large occupation numbers are favored. This behavior is reflected by the formalism. According to eq(20), the probabilities $P_{qm}(\mathbf{n}_k)$ are given in terms of sum over permutations of scattering amplitudes (over complex numbers of equal modulus - products of matrix elements of $U_{x,k}$). Since these numbers typically have different phases, they tend to add up destructively. However, all $n_j!$ permutations K that interchange the n_j particles that exit in port j leave the scattering amplitude invariant, so that $n_j!$ terms in the sum have equal phases and add up constructively. This motivates the following approximation for the translation probability:

$$P_{approx}(\mathbf{n}_k) = \frac{\left(\prod_j n_j!\right) P_{cl}(\mathbf{n}_k)}{\sum_{\mathbf{r}} \left(\prod_j r_j!\right) P_{cl}(\mathbf{r})} \quad (26)$$

We present probability distribution for the number of occupied ports, for the classical calculation eq(12), for the bosonic quantum case eq(20) and for the approximation eq(26), for $k=14$ in Fig(3).

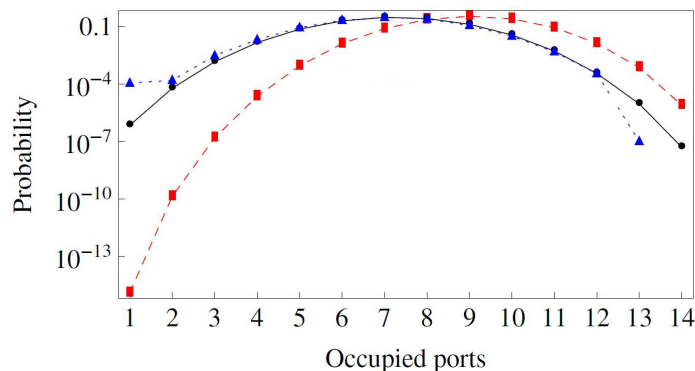


FIG. 3: Events probability for a given number of occupied ports, for $k=14$. (red) Rectangles indicate classical combinations, (blue) triangles the quantum mechanical probability distribution, and (black) circles (bosonic) approximation for the quantum result. [5]

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