Quantum renewal equation for the first detection time of a quantum walk

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Abstract
We investigate the statistics of the first detected passage time of a quantum walk. The postulates of quantum theory, in particular the collapse of the wave function upon measurement, reveal an intimate connection between the wave function of a process free of measurements, i.e. the solution of the Schrödinger equation, and the statistics of first detection events on a site. For stroboscopic measurements a quantum renewal equation yields basic properties of quantum walks. For example, for a tight binding model on a ring we discover critical sampling times, diverging quantities such as the mean time for first detection, and an optimal detection rate. For a quantum walk on an infinite line the probability of first detection decays like \( t^{-3} \) with a superimposed oscillation, critical behavior for a specific choice of sampling time, and vanishing amplitude when the sampling time approaches zero due to the quantum Zeno effect.

Keywords: first passage time, quantum walk, renewal equation

(Some figures may appear in colour only in the online journal)
0 and returns back after the time interval \( t - t' \). The consequence is a well known renewal formula, the first equation in Redner’s monograph [3], relating occupation probabilities and first passage time statistics.

More recently, quantum walks have attracted much interest both theoretically [6–8] and experimentally [9–11]. These exhibit interference patterns and ballistic scaling and in that sense exhibit behaviors drastically different from the classical random walk. Particularly controversial has been the question of the first passage time for quantum dynamics. As mentioned, the latter is ill-defined, so we consider the first detected passage time to a site (see details below) [12–22]. One motivation for these studies was to characterize running times for quantum search algorithms.

Our main result is the quantum analogue of Schrödinger’s classical renewal equation. With this equation, which deals with amplitudes, rather than probabilities, we calculate some basic properties of quantum walks, for example the first detected passage time statistics on a line. We note that the first passage time in quantum mechanics, and in particular, the quest for the quantum renewal equation has given rise to a number of very different approaches, and so has been the subject of no small controversy.

The quantum walk model under investigation has its origins in the work of Krovi and Brun [14, 15] for a discrete time quantum walk with a measurement at each time-step, while here we use a continuous time process with a stroboscopic projective measurement scheme recently investigated by Dhar et al [21, 22] (see also [16]). This model uses the textbook postulates of quantum measurements, in particular the projective postulate [23], to address the first detection problem of quantum dynamics, the main restriction being that the Hamiltonian is time independent, the latter corresponding to the Markov assumption used by Schrödinger in the classical domain.

**Model and the measurement process.** We consider a single quantum particle on a graph, for example a lattice or a discretized ring, whose state wave function is \( |\psi\rangle \). Under stroboscopic observations at times \( \tau, 2\tau, \cdots \), an observer performs measurements at a spatial position which we may call \( x = 0 \) which is represented as the vector \( |0\rangle \). Such stroboscopic measurements are useful as they capture quantum periodicities as shown below. A measurement provides two possible outcomes: either the particle is detected at \( x = 0 \) or it is not. The experiment provides the string: no, no, no, etc and finally at the \( n \)th attempt a yes so that \( \tau_n \) is the first detected passage time, whose statistics are investigated. For that we must define the measurement process precisely [21, 22].

Just prior to the first measurement the wave function is \( |\psi(\tau^-)\rangle = U(\tau)|\psi(0)\rangle \) and \( U(\tau) = \exp(-iH\tau) \) is the unitary evolution operator, \( H \) the time independent Hamiltonian, \( |\psi(0)\rangle \) is the wave function at the initial time \( t = 0 \) and \( h = 1 \). For example, we will later investigate the tight-binding model

\[
H = -\gamma \sum_{x=-\infty}^{\infty} (|x\rangle\langle x+1| + |x+1\rangle\langle x|).
\]

This describes a quantum particle jumping between nearest neighbours on an infinite one dimensional lattice so \( x \) is an integer and in that sense the model describes a quantum walk [8]. We stress that our main results are not limited to a specific Hamiltonian.

The probability of finding the particle in state \( |0\rangle \), at the first measurement, is \( P_1 = \langle 0|\psi(\tau^-)\rangle^2 \). If the outcome of the first measurement is positive we get \( n = 1 \). On the other hand, if the particle is not detected, with probability \( 1 - P_1 \), Von Neumann’s postulate of collapse states that the null measurement alters the wave function in such a way that the probability of detecting the particle at the detection point \( x = 0 \) at time \( \tau^+ \equiv \tau + 0^+ \) is zero. Afterwards, the evolution of the quantum state will resume until the next measurement time \( 2\tau \) via the transformation
In this sense we are considering projective measurements whose duration is very short, while between the measurements the evolution is according to the Schrödinger equation.

Since the outcome of a null measurement is zero amplitude for finding the particle at \( x = 0 \) at time \( \tau + \) we have

\[
|\psi(\tau^+)\rangle = N(1 - |0\rangle\langle 0|)|\psi(\tau^-)\rangle,
\]

where \( 1 \) is the identity operator, and \( N \) is determined from the normalization condition. Since just prior to the measurement the probability of finding the particle at \( x \neq 0 \) is \( 1 - P_1 \), we get

\[
|\psi(\tau^-)\rangle = \frac{1 - \hat{D}}{\sqrt{1 - P_1}} U(\tau)|\psi(0)\rangle.
\]

Here \( \hat{D} = |0\rangle\langle 0| \) is the measurement’s projection operator. The probability of detecting the particle at the second measurement, conditioned that the quantum walker was not found in the first attempt, is \( P_2 = \langle 0|U(\tau)|\psi(\tau^+)\rangle^2 \). This procedure is continued to find the probability of first detection in the \( n \)th measurement, conditioned that prior measurements did not detect the particle \( [21, 22] \).

\[
P_n = \frac{\langle 0|[U(\tau)(1 - \hat{D})]^{n-1} U(\tau)|\psi(0)\rangle|^2}{(1 - P_1)\ldots(1 - P_{n-1})}.
\]

In the numerator (respectively, the denominator) the operator \( 1 - \hat{D} \) (the probabilities of non-detection \( 1 - P_j \)) is found \( n - 1 \) times corresponding to the \( n - 1 \) prior measurements.

**First detection probability \( F_n \).** The main focus of this work is on the probability of first detection in the \( n \)th attempt, denoted \( F_n \). This detection consists of a set of \( n - 1 \) null measurements, each weighed by the conditional probability \( 1 - P_j \), followed by a positive measurement at attempt \( n \), giving

\[
F_n = (1 - P_1)(1 - P_2)\ldots(1 - P_{n-1})P_n.
\]

Using equation (4), \( F_n = |\phi_n|^2 \) where

\[
\phi_n = \langle 0|U(\tau)(1 - \hat{D})U(\tau)|\psi(0)\rangle
\]

is the first detection amplitude.

**Solution using generating functions.** Equation (6) gives \( \phi_1 = \langle 0|U(\tau)|\psi(0)\rangle \), \( \phi_2 = \langle 0|U(2\tau)|\psi(0)\rangle - \phi_1\langle 0|U(\tau)|0\rangle \) and by induction we find

\[
\phi_n = \langle 0|U(n\tau)|\psi(0)\rangle - \sum_{j=1}^{n-1} \phi_j\langle 0|U[(n-j)\tau]|0\rangle.
\]

This iteration rule yields the amplitude \( \phi_n \) in terms of a propagation free of measurement, i.e. \( \langle 0|U(n\tau)|\psi(0)\rangle \) is the amplitude for being at the origin at time \( n\tau \) in the absence of measurements, from which we subtract \( n - 1 \) terms related to the previous null measurements of the particle. In practice, it is more convenient to work in terms of the generating function [24] also called the \( Z \) transform \( \hat{\phi}(z) = \sum_{n=1}^{\infty} z^n \phi_n \). Multiplying equation (7) by \( z^n \) and summing over \( n \) using the convolution theorem we get

\[
\hat{\phi}(z) = \frac{\langle 0|\hat{U}(z)|\psi(0)\rangle}{1 + \langle 0|\hat{U}(z)|0\rangle}.
\]
where \( \hat{U}(z) \equiv \sum_{n=0}^{\infty} z^n U(n\tau) \). We can now invert the generating function to find the amplitudes \( \phi_n \) and the probabilities \( F_n \), as well as calculate various moments using methods discussed in [24, 25].

Quantum renewal equation. For a particle free of any measurement, the amplitude of being at the origin at time \( t \) is \( \langle 0 | \psi_f(t) \rangle = e^{iHt}\psi_f(0) \). Here \( \psi_f(t) \) is the solution of the Schrödinger equation \( i\frac{\partial}{\partial t} \psi_f = H\psi_f \), with the same initial conditions as for the first detection problem under investigation \( |\psi_f(0)\rangle = |\psi(0)\rangle \). Let us consider the initial condition where the particle is initially localized at \( x = 0 \) and so \( |\psi(0)\rangle = |0\rangle \). Using \( |0\rangle = 1 \), equation (8) is rewritten

\[
\hat{\phi}(z) = 1 - \frac{1}{\langle 0 | 1 - e^{-iHz} | 0 \rangle}. \quad (9)
\]

We define the measurement-free generating function

\[
\langle 0 | \psi_f(z) \rangle_0 \equiv \sum_{n=0}^{\infty} z^n \langle 0 | \psi_f(n\tau) \rangle,
\]

and clearly \( \langle 0 | \psi_f(z) \rangle_0 = \sum_{n=0}^{\infty} \langle 0 | z^n \exp(-iHn) | 0 \rangle \), the subscript zero denoting the initial condition. Summing the geometric series, we get the appealing result

\[
\hat{\phi}(z) = 1 - \frac{1}{\langle 0 | \psi_f(z) \rangle_0}. \quad (11)
\]

Thus, the generating function of the first detection time amplitude \( \hat{\phi}(z) \) is determined from the \( Z \)-transform of the wave function at the point of detection \( x = 0 \).

Similarly, for an initial condition initially localized at a site \( x \neq 0 \), so that \( |\psi(0)\rangle = |x\rangle \), for detection at site 0 we find that

\[
\hat{\phi}(z) = \frac{\langle 0 | \psi_f(z) \rangle_x}{\langle 0 | \psi_f(z) \rangle_0}, \quad (12)
\]

where \( |\psi_f(z)\rangle_x \) is the \( Z \)-transform of the wave function free of measurements initially localized at site \( x \), \( |\psi_f(z)\rangle_x = \sum_{n=0}^{\infty} z^n |\psi_f(n\tau)\rangle_x \) with \( |\psi_f(n\tau)\rangle_x = \exp(-iHn\tau)|x\rangle \). Equations (11) and (12) are the quantum counterparts of the classical renewal equation (1.2.3) (or equation (I.18)) in [2, 3] respectively. The latter deals with the correspondence between occupation and first passage time probabilities, while we have found the connection between the amplitudes \( \phi_n \) and the wave function \( \psi_f \). In that sense we have reduced the problem of first detection time to the computation of the \( Z \)-transform of the solution of the Schrödinger equation.

Rings. We first consider a tight-binding ring with \( L \) sites, namely the Hamiltonian equation (1) with periodic boundary conditions. The solution of the Schrödinger equation \( |\psi_f\rangle \) is computed with standard methods. To find \( \phi_n \) we use the inverse \( Z \)-transform (see [25] for details). For an \( x = 0 \) initial condition, i.e. \( |\psi(0)\rangle = |0\rangle \), where \( x = 0 \) is also the location of the detector, we find the following three results: (i) The particle is detected with probability 1 and in this sense the quantum walk is recurrent. (ii) Besides isolated sampling times \( \tau \) listed below, the average number of detection attempts is

\[
\langle n \rangle = \begin{cases} 
\frac{L+2}{2} & \text{L is even} \\
\frac{L+1}{2} & \text{L is odd}.
\end{cases} \quad (13)
\]
This result is remarkable since it is independent of the sampling time $\tau$. (iii) Exceptional sam-
ing times $\tau$ are given by the rule

$$\tau \pi = E_n^2,$$

where $n$ is a non-negative integer, and $E = E_i - E_j > 0$ is the energy difference between
pairs of eigenenergies of the underlying Hamiltonian. These exceptional points exhibit non-
analytical behaviors, diverging moments of $n$ and critical slowing down, as we now discuss.

For example, for a ring of size $L = 6$, with sites $x = \ldots, 0, 1, 2, 3, \ldots$, equation (13) gives $E_n = n^2$.
The energy levels are $\gamma_+ \pm \gamma_\pm 2$, the former are doubly degenerate. Using equation (11) we
find $E_n$ for the exceptional points given by equation (14) $\gamma \tau = 0, \pi/2, 2\pi/3, \pi \cdots$
which is continued periodically, see figure 1. Physically, the condition equation (14) implies
a partial revival of the wave packet free of measurement, namely two modes of the system
are behaving identically when strobed at period $\tau$. When $\tau = 0$ we get the expected result, the
particle is detected immediately and then $E_n$ diverges, which is also found when $\gamma \tau = 2\pi$, namely
at a full revival period.

Exceptional sampling times manifest themselves in different ways depending on the
observable and the initial condition. For example, consider again the average $\langle n \rangle$ for a ring of
size $L = 6$ but now with the initial condition that the particle is initially localized at the site
$x = 3$ while the detection is at $x = 0$. Equation (12) gives, except for the exceptional $\tau$s,

$$\langle n \rangle = \frac{27 + 23 \cos(\gamma \tau) + 24 \cos(2\gamma \tau) + 9 \cos(3\gamma \tau) - 2 \cos(4\gamma \tau)}{9 \sin^2(\gamma \tau)}.$$

The result, presented in figure 1, shows that $\langle n \rangle$ diverges when $\sin(2\gamma \tau) \rightarrow 0$. When $\tau \rightarrow 0$
the measurements become very frequent and then the probability of measuring the particle
approaches zero and so $\langle n \rangle$ diverges, which is the manifestation of the quantum Zeno
effect [16, 26]. A similar blowup of $\langle n \rangle$ is observed when $\gamma \tau \rightarrow 2\pi$, since the wave packet
fully revives at its initial position $x = 3$ and so the measurements do not detect the particle.
Similarly $\langle n \rangle$ diverges also for $\gamma \tau$ approaching $\pi/2, \pi, 3\pi/2$ due to partial revivals. A far more
subtle effect takes place for the special sampling times $\gamma \tau = 2\pi/3, 4\pi/3$. There $\langle n \rangle$ exhibits a

![Figure 1. The average first successful detection $\langle n \rangle$ versus $\gamma \tau$ for a benzene-like ring
($L = 6$) where the starting point is at $x = 3$ (blue) or $x = 0$ (red) and the detection is
done at $x = 0$. The hollow symbols indicate the jump discontinuities of $\langle n \rangle$ and that it is
single valued. The integer value of $\langle n \rangle$, for the $|0\rangle \rightarrow |0\rangle$ transition, is a general feature
of quantum walks on graphs, related to elegant topological effects [27].](image-url)
discontinuity: on these exceptional points \( n = 43 \) while in their vicinity we find from equation (15) \( \sim n - 2 \). Thus the effects of exceptional points on observables are non-trivial. We have found several other peculiar behaviors for rings [25], but now we turn to the case of an unbounded quantum walk, since the corresponding classical problem is fundamental in stochastic theories, e.g. it gives the random walk exponents through the long tailed first passage PDF [1]. Note that Bach, et al [13] treated the detection problem for a discrete time Hadamard quantum walk, leading to behaviors different from what we find here.

First detection time for an unbounded quantum walk described by the tight binding Hamiltonian equation (1) is now investigated. For a particle starting at the origin, we use \( \psi(z) = \sum_{n=0}^{\infty} a_n J_n(2\sqrt{r}n) \), equation (11)

\[
\phi(z) = 1 - \frac{1}{\langle 0|\psi(z)\rangle_0} = 1 - \frac{1}{\sum_{n=0}^{\infty} a_n J_n(2\sqrt{r}n)}.
\]

where \( J_n(x) \) is the Bessel function of the first kind. Employing \( J_n(2\sqrt{r}n) \sim \cos(2\sqrt{r}n - \pi/4) / \sqrt{\pi\sqrt{r}n} \) we obtain the large \( n \) limit of \( \phi_n \). From this asymptotic property of the Bessel function it becomes clear that the generating function \( \langle 0|\psi(z)\rangle_0 \) does not converge when \( z = r \exp(i\theta) \) with \( \theta = \pm 2\gamma\tau \) and \( r \gg 1 \). Thus, as shown in [25], when we invert \( \phi(z) \) to find \( \phi_n \), we find two branch cuts in the complex \( (r, \theta) \) plane. These branch cuts merge when \( \gamma\tau \) is an integer multiple of \( \pi \), a mathematical observation which is behind the critical behavior we find below.

Our renewal equation leads to another central result [25], the probability of measuring the unbounded quantum walker returning to its origin for the first time after \( n \) attempts,

\[
F_n \sim \frac{4\gamma\tau}{\pi n^3} \cos^2 \left(2\gamma\tau n + \frac{\pi}{4}\right).
\]

This formula, which is valid for large \( n \), is the quantum version of the first passage time problem of a classical one dimensional non-biased walker which exhibits the well known power law and monotonic tail \( F_{\text{classical}} \propto n^{-3/2} \) [1, 3]. The role of sampling time in the quantum problem is crucial. When \( \tau \to 0 \) the prefactor of the \( n^{-3} \) power law in equation (17) vanishes, a manifestation of the quantum Zeno effect (a similar effect is found for all initial conditions). Furthermore, the formula predicts that when \( \gamma\tau/\pi \) is rational the probability \( F_n \) multiplied
by $n^3$ is periodic. In contrast if $\gamma \pi / n$ is not rational the asymptotic behavior appears irregular (see figure 2). In the limit $2\gamma \pi \to \pi$ equation (17) gives $F_n \sim n^3$ which is a pure power law. However the sampling time $2\gamma \pi = \pi$ is exceptional and for this case a detailed calculation [25] reveals $F_n \sim n^{-3}/4$ so a factor of 4 mismatch is found. In this sense exceptional points are found also for an infinite system. This in turn implies a critical slowing down when $2\gamma \pi \approx \pi$, a behavior that cannot be anticipated without a detailed calculation. Physically, the energy band width of a ring of size $L \to \infty$ is $\Delta E = 4\gamma$ and inserting that in equation (14) with $n = 1$ we get the exceptional sampling time of the infinite system.

1. Summary and discussion

Previously Krovi and Brun found a general trace formula for the average hitting time of a discrete time quantum walk [14] (see also [16]). That method is based on a density matrix approach, while our solution shows how the measurement-free wave function yields the full statistics of the quantum first detection problem, and not just the average.

We have derived the quantum renewal equation, obtaining the first detection probability of an unbounded quantum walk in one dimension, and finding unusual non-analytical behavior even for a small benzene-like ring with $L = 6$ sites. Our results are thus the quantum version of Schrödinger’s pioneering work on the classical first passage time problem from a century ago [1]. The applications of our main formulas are vast, since they are not limited to a specific Hamiltonian. We believe that the powerful quantum renewal approach considered here will be as valuable a tool as its classical counterpart [3]. Indeed we already see unexpected novel behaviors such as critical sampling. We note that stroboscopic sampling is very useful in quantum systems, since this reveals revivals, critical points, and periodicities, though in principle the method used in this work could be extended to other measurement protocols, e.g. sampling at a Poissonian rate [16].

After completion of the manuscript, it was brought to our attention that some of our results, in particular the $0 \to 0$ renewal equation, have been obtained previously by Grünbaum, et al [27]. We thank Dr J Asboth for alerting us to this work.

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