PHYSICAL REVIEW E **95**, 032141 (2017)

Quantum walks: The first detected passage time problem

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(Received 12 January 2017; published 28 March 2017)

Even after decades of research, the problem of first passage time statistics for quantum dynamics remains a challenging topic of fundamental and practical importance. Using a projective measurement approach, with a sampling time τ, we obtain the statistics of first detection events for quantum dynamics on a lattice, with the detector located at the origin. A quantum renewal equation for a first detection wave function, in terms of which the first detection probability can be calculated, is derived. This formula gives the relation between first detection statistics and the solution of the corresponding Schrödinger equation in the absence of measurement. We illustrate our results with tight-binding quantum walk models. We examine a closed system, i.e., a ring, and reveal the intricate influence of the sampling time τ on the statistics of detection, discussing the quantum Zeno effect, half dark states, revivals, and optimal detection. The initial condition modifies the statistics of a quantum walk on a finite ring in surprising ways. In some cases, the average detection time is independent of the sampling time while in others the average exhibits multiple divergences as the sampling time is modified. For an unbounded one-dimensional quantum walk, the probability of first detection decays like $(\text{time})^{(-3)}$ with superimposed oscillations, with exceptional behavior when the sampling period τ times the tunneling rate γ is a multiple of $\pi/2$. The amplitude of the power-law decay is suppressed as $\tau \to 0$ due to the Zeno effect. Our work, an extended version of our previously published paper, predicts rich physical behaviors compared with classical Brownian motion, for which the first passage probability density decays monotonically like $(\text{time})^{-3/2}$, as elucidated by Schrödinger in 1915.

DOI: 10.1103/PhysRevE.95.032141

I. INTRODUCTION

How long does it take a lion to find its prey, a particle to reach a domain, or an electric signal to cross a certain threshold? These are all examples of the first passage time problem [1–5]. A century ago, Schrödinger showed that a Brownian particle in one dimension, i.e., the continuous limit of the classical random walk, starting at x_0, will eventually reach $x = 0$, with, however, a probability density function (PDF) of the first arrival time that is fat tailed, in such a way that the mean first passage time diverges [6]. Ever since, the classical first passage time problem has been a well studied field of research. More recently, much work has been devoted to the analysis of quantum walks [7–11] (see [12] for a review). These exhibit interference patterns and ballistic scaling and in that sense exhibit behaviors drastically different from the classical random walk. While several variants of quantum walks exist [12], for example discrete time walks, coin tossing walks, and tight-binding models, one line of inquiry addresses a question generally applicable to all these cases, namely, the statistics of first passage or detection times of a quantum particle (to be defined precisely below). Quantum walk search algorithms which are supposed to perform better than classical walk search methods have vitalized this line of research in recent years. A physical example might be the statistics of the time it takes a single electron, ion, or atom to reach a detection device. This question, which at first sight appears well defined and physically meaningful, has nevertheless been the subject of much controversy. The Schrödinger equation and the standard postulates of quantum mechanics [13] do not give a ready-made recipe for calculating these statistics. There are no textbook quantum operators or wave function associated with the first passage time measurements (see [14–16] for related historical accounts). Actually, time is a nonquantum ingredient of quantum mechanics and is treated as an object detached from the probabilistic interpretation inherent to nonclassical reality. From the nondeterministic nature of quantum mechanics, we may expect that the time it takes a single particle to reach a detection point or domain for a given Hamiltonian and initial condition should be random even in the absence of external noise, but how to precisely obtain the distribution of first detection times has remained in our opinion a controversial matter.

The key to the solution is that we must take into consideration the measurement process [17–22]. For example, consider a zebra sitting at the origin waiting for a lion to arrive for the first and, unfortunately for her, the last time. At some rate, the zebra records: did the lion arrive or did it not? The outcome is a string of answers: e.g., no, no, no, ..., and finally yes. If the lion is a quantum particle, then continuous attempts to detect it by the zebra will preserve the zebra's life since the wave function of the lion is collapsed in the vicinity of the zebra; this is the famous quantum Zeno effect [23] (see more details below). On the other hand, if the zebra samples the arrival of the lion at a finite constant rate, its likelihood of death is much higher. In this sense, the measurement of the time of first detection, which implies a set of null measurements for times prior to the final positive recording, is very different than the familiar measurements of canonical variables like position and momentum. There, the system is prepared at time $t = 0$ in some initial state and it evolves free of measurement until time t, at which point an instantaneous recording of some observable is made. Furthermore, we must distinguish between first arrival or first passage problems [15] and first detection at a site. Note that even classically the first detection does not imply that the particle arrived at the site for the first time at the moment of detection if the sampling is not continuous in time. More importantly, arrival times are ill defined in quantum problems [24] because we cannot have a complete record of the trajectory of a quantum particle, whereas the first detection problem under repeated stroboscopic measurements is a well-defined problem, and that is what we treat in this paper.

Here, we investigate the first detection problem of quantum walks following Dhar *et al.* [21,22] who formulated the problem as a tight-binding quantum walk, with projective local measurements every τ units of time (see also [18]). Specifically, we consider a particle on a discrete graph, the quantum evolution determined by the time independent Hamiltonian H. Initially, the particle is localized so that the state function is $|\psi\rangle = |x\rangle$ (some of our general results are not limited to this initial condition, see below). Detection attempts are performed locally at a site we call the origin which is denoted with $|0\rangle$. Measurements at the origin are stroboscopic with the sampling time τ, and as mentioned the measurement stops once the particle is detected after n attempts, so $n\tau$ is the random first detection time. We investigate the statistics of the random observable n. The questions are as follows: Is the particle eventually detected? What is the probability of detection after n attempts? What is the average of number of attempts of detection before a successful measurement? This we investigate both for closed systems and open ones. Below we present a physical derivation of the quantum renewal equation describing the probability amplitude of first detection for the transition $|x\rangle \to |0\rangle$. In classical stochastic theories this corresponds to Schrödinger's renewal equation [6] for the first time a particle starting on x reaches 0 (see details below). We show how the solution of Schrödinger's wave equation free of measurement can be used to predict the quantum statistics of the first detection time. Previously, Grünbaum *et al.* [25] considered the case where the starting point is also the detection site $|x\rangle = |0\rangle$. A topological interpretation of the detection process was provided for that initial condition and among other things they showed that the expected time of first detection is either an integer multiple of τ or infinity. This integer is the winding number of the so called Schur function of the underlying scalar measure; the latter is determined by the initial state and the unitary dynamics. Hence, the expectation of the first detection time is quantized [26]. A vastly different behavior is found when we analyze the transition $|x\rangle \to |0\rangle$ for $x \neq 0$ [18,22]. The average of n is not an integer, nor is detection finally guaranteed. As demonstrated below for a ring geometry, half dark states are observed in some cases while in others the average of n exhibits divergences and nonanalytical behaviors for certain critical sampling times. Finally, we show that critical sampling, including slowing down, is found even for an infinite system. Namely, for the quantum walk on the line, the first detection probability decays like a power law, with additional oscillations, where the amplitude of decay is not a continuous function of the sampling rate. Thus, rich physical behaviors are found for the quantum first detection problem, as compared with the known results of the classical random walker.

The spatial quantum first detection problem is a timely subject. Current day experiments on quantum walks can be used to study these problems in the laboratory [27–31]. First passage time statistics in the classical domain are usually recorded based on single particle analysis. Namely, one takes, say, a Brownian particle, releases it from a certain position, and then detects its time of arrival at some other location. This single particle experiment is repeated many times and then a histogram of the first passage time is reported. While in principle one could release simultaneously many particles from the same position, their mutual interaction will influence the statistics of first arrival and similarly statistics of identical particles, either bosons or fermions, alter the many particle statistics compared to the single particle case. Hence, measurement should be made on single particles, or in other words at least classically the first detection time is a property of the single particle path and hence its history. The recent advance of single particle quantum tracking and measurement, for systems where coherence is maintained for relatively long times, is clearly a reason to be optimistic with respect to possible first detection measurements. Such measurements could test our predictions as well as those of a variety of other theoretical approaches [15,24,32–39], some of which are compared with our results towards the end of this paper.

The navigation map of this paper is as follows. We start with the presentation of the quantum walk model and the measurement process in Sec. II. In Sec. III, the first detection wave function formalism is developed. The main tool for actual solution of the problem is based on the generating function formalism given in Sec. IV and in Sec. IV B the quantum renewal equation is discussed. Section V presents the example of first detection on rings, with special emphasis on the peculiar statistics found on a benzene-like ring. In Sec. VI we obtain statistics of first detection times, for a one-dimensional quantum walk on an infinite lattice. We end with further discussion of previous results (Sec. VII) and a summary. A short account of part of our main results was recently published [40].

II. MODEL AND BASIC FORMALISM

We consider a particle whose evolution is described by a time independent Hermitian Hamiltonian H according to the Schrödinger equation $i\hbar|\dot{\psi}\rangle = H|\psi\rangle$. The initial condition is denoted $|\psi(0)\rangle$. For simplicity, we consider a discrete x space. As an example, we shall later consider the tight-binding model

$$H = -\gamma \sum_{x=-\infty}^{\infty} (|x\rangle\langle x+1| + |x+1\rangle\langle x|) \tag{1}$$

on a lattice, although our general results are not limited to a specific Hamiltonian. We denote a subset of lattice points X, and loosely speaking we are interested in the statistics of first passage times from the initial state to any site $x \in X$ in the subset. More generally, X could be any subset of orthogonal states. An example is when X consists of a single lattice point, say $x = 0$, and initially the particle is localized at some other lattice point $|\psi(0)\rangle = |x'\rangle$. We then investigate the distribution of the first detection times. For that we must define the measurement process following [9,17,21].

Measurements on the subset X are made at discrete times $\tau, 2\tau, \ldots, n\tau \ldots$ and hence clearly the first recorded detection time is either $t_f = \tau$ or 2τ, etc. The measurement provides two possible outcomes: either the particle is in $x \in X$ or it is not. Consider the first measurement at time τ. At time $\tau^- = \tau - \epsilon$

with $\epsilon \to 0$ being positive, the wave function is

$$|\psi(\tau^-)\rangle = U(\tau)|\psi(0)\rangle \tag{2}$$

and $U(\tau) = \exp(-iH\tau/\hbar)$ as usual. In what follows, we set $\hbar = 1$. The probability of finding the particle in $x \in X$ is, according to the standard interpretation,

$$P_1 = \sum_{x\in X} |\langle x|\psi(\tau^-)\rangle|^2. \tag{3}$$

If the outcome of the measurement is positive, namely, the particle is found in $x \in X$, the first detection time is $t_f = \tau$. On the other hand, if the particle is not detected, which occurs with probability $1 - P_1$, the evolution of the quantum state will resume. According to collapse theory, following the measurement the particle's wave function in $x \in X$ is zero. Namely, a null measurement alters the wave function in such a way that the probability of detecting the particle in $x \in X$ at time $\tau + \epsilon$ vanishes. 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. Mathematically the measurement is a projection [13], so that at time $\tau^+ = \tau + \epsilon$ we have

$$|\psi(\tau^+)\rangle = N\left(\mathbb{1} - \sum_{x\in X}|x\rangle\langle x|\right)|\psi(\tau^-)\rangle, \tag{4}$$

where $\mathbb{1}$ is the identity operator, and the constant N is determined from the normalization condition. Here, we have used the assumption of a perfect projective measurement that does not alter either the relative phases or magnitudes of the wave function not interacting with the measurement device, i.e., outside the observation domain the wave function is left unchanged beyond a global renormalization. This is the fifth postulate of quantum mechanics [13], though clearly it should be subject to continuing experimental tests. Since just prior to measurement the probability of finding the particle in x not belonging to X is $1 - P_1$, we get

$$\begin{aligned} |\psi(\tau^+)\rangle &= \frac{\mathbb{1} - \sum_{x\in X}|x\rangle\langle x|}{\sqrt{1-P_1}}|\psi(\tau^-)\rangle \\ &= \frac{\mathbb{1} - \sum_{x\in X}|x\rangle\langle x|}{\sqrt{1-P_1}}U(\tau)|\psi(0)\rangle. \end{aligned} \tag{5}$$

In sum, the measurement nullifies the wave functions on $x \in X$ but maintains the relative amplitudes of finding the particles outside the spatial domain of measurement device, modifying only the normalization.

We now proceed in the same way to the second measurement. Between the first and second detection attempts we have $|\psi(2\tau^-)\rangle = U(\tau)|\psi(\tau^+)\rangle$. The probability of finding the particle in $x \in X$ at the second measurement, conditioned on the quantum walker not having been found in the first attempt, is

$$P_2 = \sum_{x\in X} |\underbrace{\langle x|}_{\text{Projection}}\ \underbrace{U(\tau)}_{\text{Evolution}}\ \underbrace{|\psi(\tau^+)\rangle}_{\text{Null } X \text{ state}}|^2. \tag{6}$$

We define the projection operator

$$\hat{D} = \sum_{x\in X}|x\rangle\langle x|, \tag{7}$$

and using Eqs. (5) and (6)

$$P_2 = \frac{\sum_{x\in X}|\langle x|U(\tau)(1-\hat{D})U(\tau)|\psi(0)\rangle|^2}{1-P_1}. \tag{8}$$

This iteration procedure is continued to find the probability of first detection in the nth measurement, conditioned on prior measurements not having detected the particle

$$P_n = \sum_{x\in X}\frac{|\langle x|[U(\tau)(1-\hat{D})]^{n-1}U(\tau)|\psi(0)\rangle|^2}{(1-P_1)\dots(1-P_{n-1})}. \tag{9}$$

In the numerator, the operator $1 - \hat{D}$ appears $n - 1$ times corresponding to the $n - 1$ prior measurements. Similarly, in the denominator we find $n - 1$ probabilities of null measurements $1 - P_j$. Following [21,22] we define the first detection wave function

$$|\theta_n\rangle = U(\tau)[(1-\hat{D})U(\tau)]^{n-1}|\psi(0)\rangle \tag{10}$$

or, equivalently, $|\theta_n\rangle = [U(\tau)(1-\hat{D})]^{n-1}|\theta_1\rangle$ with the initial condition $|\theta_1\rangle = U(\tau)|\psi(0)\rangle$. The bra $|\theta_n\rangle$ is defined only for the moments of detection $n = 1,2,\dots$, unlike $|\psi(t)\rangle$ which is a function of continuous time. With this definition

$$P_n = \frac{\langle\theta_n|\hat{D}|\theta_n\rangle}{\Pi_{j=1}^{n-1}(1-P_i)}. \tag{11}$$

The main focus of this work is on the probability of first detection in the nth measurement, denoted F_n. This is of course not the same as P_n which as mentioned is a conditional probability, namely, the probability of detection on the nth attempt given no previous detection. The conceptual measurement process for the calculation of F_n is as follows. We start with an initial spatial wave function $|\psi(0)\rangle$ and evolve it until time τ when the detection of the particle in $x \in X$ is attempted, and with probability P_1 the first measurement is also the first detection. Hence, to simulate this process on a computer, we toss a coin using a uniform random number generator and, if the particle is detected, the measurement time is τ. If the particle is not detected, we compute P_2. Then, at time 2τ either the particle is detected with probability P_2 or not. Simulating the measurement process we again generate a random variable uniformly distributed in (0,1) and if this variable is smaller then P_2, the first detection time is 2τ. Importantly, the uniform random variables generated in this procedure, corresponding to these first two measurements, are *independent* random variables. Thus, the probability of measuring the particle for the first time after $n = 2$ attempts is $F_2 = (1 - P_1)P_2$.

This process is repeated until a measurement is recorded (see remark below), and that measurement constitutes the random first detection event. In order to gain statistics of the first detection time, we return to the initial step and restart the process with the same initial condition. In this way, repeating this many times, we construct the first detection probability

$$F_n = (1-P_1)(1-P_2)\dots(1-P_{n-1})P_n. \tag{12}$$

Using Eq. (11) we obtain

$$F_n = \langle\theta_n|\hat{D}|\theta_n\rangle. \tag{13}$$

We see that the first detection probability F_n is the expectation value of the projection operator $\hat{D}$ with respect to $|\theta_n\rangle$, which we term the first detection wave function.

Remark. We shall see that not all sequences of measurements, generated on a computer or in the laboratory, yield a detection in the long-time limit. This is not problematic since also classical random walks in say three dimensions are not recurrent and, hence, the total probability of detection is not necessarily unity. In many works one defines the survival probability, i.e., the probability that the particle is not detected in the first n attempts,

$$S_n = 1 - \sum_{n=1}^{n} F_n. \tag{14}$$

The eventual survival probability S_∞ can equal zero or not. If the initial condition and the detection location are identical and $S_\infty = 0$, the quantum walk is called recurrent. We will later investigate whether or not the quantum walk is recurrent, both for the cases of an infinite lattice and a finite ring.

III. FIRST DETECTION AMPLITUDE

In this section, we solve the first detection time problem for quantum dynamics with a single detection site, which we label $x = 0$, so $\hat{D} = |0\rangle\langle 0|$. We define the amplitude of the first detection as

$$\phi_n = \langle 0|\theta_n\rangle \tag{15}$$

so that $F_n = |\phi_n|^2$. Using Eq. (10), $\phi_1 = \langle 0|U(\tau)|\psi(0)\rangle$, $\phi_2 = \langle 0|U(2\tau)|\psi(0)\rangle - \phi_1\langle 0|U(\tau)|0\rangle$, and a short calculation yields

$$\phi_3 = \langle 0|U(3\tau)|\psi(0)\rangle - \phi_1\langle 0|U(2\tau)|0\rangle - \phi_2\langle 0|U(\tau)|0\rangle. \tag{16}$$

In Appendix A, using induction we find our first main equation

$$\phi_n = \langle 0|U(n\tau)|\psi(0)\rangle - \sum_{j=1}^{n-1}\phi_j\langle 0|U[(n-j)\tau]|0\rangle. \tag{17}$$

We call this iteration rule the quantum renewal equation. It yields the amplitude ϕ_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 history of the system. The physical interpretation of Eq. (17) is that the condition of nondetection in previous measurements translates into subtracting wave sources (hence the minus sign) at the detection site $|0\rangle$ following the jth detection attempt. This is due to the nullification of the wave function at the detection site in the jth measurement. The evolution of that wave source from the jth measurement onward is described by the free Hamiltonian, hence, $\langle 0|U[(n-j)\tau]|0\rangle$ which gives the amplitude of return back to the origin in the time interval $(j\tau,n\tau)$.

We now consider the formal solution to the first detection problem for an initial condition on the origin, hence, $|\psi(0)\rangle = |0\rangle$ and as mentioned the origin is also the point at which we perform the detection trials. Clearly, in this case $\phi_1 = \langle 0|U(\tau)|0\rangle$ and since $U(0) = \mathbb{1}$ we get $\phi_1 = 1$ when $\tau \to 0$ which is expected. For $\phi_2 = \langle 0|U^2|0\rangle - \langle 0|U^1|0\rangle^2$ where we use the shorthand notation $U^n \equiv U(n\tau)$. Similarly, $\phi_3 = \langle 0|U^3|0\rangle - 2\langle 0|U^2|0\rangle\langle 0|U^1|0\rangle + \langle 0|U^1|0\rangle^3$. The general solution is obtained by iteration using Eq. (17),

$$\phi_n = \sum_{i=1}^{n}\sum_{\{m_1,\ldots,m_i\}}(-1)^{i+1}\langle 0|U^{m_1}|0\rangle\ldots\langle 0|U^{m_i}|0\rangle. \tag{18}$$

The double sum is over all partitions of n, i.e., all i-tuples of positive integers $\{m_1,\ldots,m_i\}$ satisfying $m_1 + \cdots + m_i = n$. For example, for $n = 5$ we have five partitions corresponding to $i = 1,\ldots,5$, for $i = 1$ the set in the second sum is $\{5\}$, for $i = 2$ we sum over $\{2,3\},\{3,2\},\{1,4\}$, and $\{4,1\}$, for $i = 3$ we use $\{1,1,3\},\{1,3,1\},\{3,1,1\},\{2,2,1\},\{2,1,2\},\{1,2,2\}$, for $i = 4$, $\{1,1,1,2\},\{1,1,2,1\},\{1,2,1,1\},\{2,1,1,1\}$, and for $i = 5$ we have one term $\{1,1,1,1,1\}$. Hence,

$$\begin{aligned}\phi_5 = {} & \langle 0|U^5|0\rangle - 2\langle 0|U^4|0\rangle\langle 0|U^1|0\rangle \\ & + 3\langle 0|U^1|0\rangle^2\langle 0|U^3|0\rangle - 4\langle 0|U^1|0\rangle^3\langle 0|U^2|0\rangle \\ & + 3\langle 0|U^2|0\rangle^2\langle 0|U^1|0\rangle - 2\langle 0|U^3|0\rangle\langle 0|U^2|0\rangle \\ & + \langle 0|U^1|0\rangle^5.\end{aligned} \tag{19}$$

With a symbolic program like *Mathematica* one can obtain similar exact expressions for intermediate values of n. However, to gain some insight, we turn now to the generating function approach [41].

IV. GENERATING FUNCTION APPROACH

The Z transform, or discrete Laplace transform, of ϕ_n is by definition [41,42]

$$\hat{\phi}(z) = \sum_{n=1}^{\infty} z^n\phi_n. \tag{20}$$

$\hat{\phi}(z)$ is also called the generating function. Multiplying Eq. (17) by z^n and summing over n, we obtain

$$\begin{aligned}\hat{\phi}(z) = {} & \sum_{n=1}^{\infty}\langle 0|z^nU^n|\psi(0)\rangle \\ & - \sum_{n=1}^{\infty}\sum_{j=1}^{n-1}\phi_j z^j\langle 0|z^{n-j}U^{n-j}|0\rangle.\end{aligned} \tag{21}$$

Evaluating the first term on the right hand side we get

$$\hat{U}(z) = \sum_{n=1}^{\infty} z^nU^n = \sum_{n=1}^{\infty}\exp(-iH\tau n)z^n = \frac{ze^{-iH\tau}}{1 - ze^{-iH\tau}}. \tag{22}$$

The second term in Eq. (21) is a convolution term and after rearrangement we find one of our main results [42]

$$\hat{\phi}(z) = \frac{\langle 0|\hat{U}(z)|\psi(0)\rangle}{1 + \langle 0|\hat{U}(z)|0\rangle} \tag{23}$$

or, more explicitly,

$$\hat{\phi}(z) = \frac{\langle 0|\frac{1}{z^{-1}e^{iH\tau}-1}|\psi(0)\rangle}{1 + \langle 0|\frac{1}{z^{-1}e^{iH\tau}-1}|0\rangle}. \tag{24}$$

This equation relates the generating function $\hat{\phi}(z)$ to the Hamiltonian evolution between the initial condition and the detection attempt.

This approach is also valid for other types of measurements, repeatedly performed at times $\tau, 2\tau, \ldots$. For example, the case where we measure a set of points $x \in X$ is given in Eq. (A4) in Appendix A. First detection measurements of general observables are also treated there.

A. Relations between $\hat{\phi}(z)$ and ϕ_n, S_∞, and $\langle n \rangle$

As usual, the amplitudes ϕ_n are given in terms of their Z transforms by the inversion formula

$$\phi_n = \frac{1}{n!}\frac{d^n}{dz^n}\hat{\phi}(z)|_{z=0} \tag{25}$$

or

$$\phi_n = \frac{1}{2\pi i}\oint_C \hat{\phi}(z) z^{-n-1} dz, \tag{26}$$

where C is a counterclockwise path that contains the origin and is entirely within the radius of convergence of $\hat{\phi}(z)$.

The probability of being measured is also related to the generating function $\hat{\phi}(z)$ by

$$\begin{aligned} 1 - S_\infty &= \sum_{n=1}^{\infty} F_n = \sum_{n=1}^{\infty} |\phi_n|^2 \\ &= \frac{1}{2\pi}\int_0^{2\pi} \sum_{k=1}^{\infty} \phi_k e^{i\theta k} \sum_{l=1}^{\infty} \phi_l^* e^{-i\theta l} d\theta \\ &= \frac{1}{2\pi}\int_0^{2\pi} |\hat{\phi}(e^{i\theta})|^2 d\theta. \end{aligned} \tag{27}$$

Similarly,

$$\langle n \rangle = \sum_{n=1}^{\infty} n F_n = \frac{1}{2\pi}\int_0^{2\pi} [\hat{\phi}(e^{i\theta})]^* \left(-i\frac{\partial}{\partial\theta}\right)\hat{\phi}(e^{i\theta}) d\theta. \tag{28}$$

The latter is the average of n only when the particle is detected with probability one, namely, when $S_\infty = 0$. A shorthand notation for Eq. (28) is $\langle n \rangle = \langle \hat{\phi}| - i\partial_\theta |\hat{\phi}\rangle$.

B. Connection between first detection and spatial wave function

In classical random walk theory, the key approach to the first passage time problem is to relate it to occupation probabilities [1]. Let us unravel a similar relation in the quantum domain, connecting between first detection statistics and the corresponding wave packet, namely, the time dependent solution of the Schrödinger equation in the absence of measurement (see also [25] for the $|0\rangle \to |0\rangle$ transition). To that end, we first briefly review the classical random walk.

Consider a classical random walk in discrete time $t = 0, 1, \ldots$, for example, a random walk on a cubic lattice in dimension d with jumps to nearest neighbors. The main assumption is that the random walk is Markovian. Denote $P_{\rm cl}(\mathbf{r}, t)$ as the probability that the walker is at $\mathbf{r}$ at time t when initially the particle is at the origin $\mathbf{r} = 0$ and in the absence of any absorption. Let $F_{\rm cl}(\mathbf{r}, t)$ be the first passage probability: the probability that the random walk visits site $\mathbf{r}$ for the first time at time t with the same initial condition. Following the first equation in the first chapter in [1], $P_{\rm cl}(\mathbf{r}, t)$ and $F_{\rm cl}(\mathbf{r}, t)$ are related by

$$P_{\rm cl}(\mathbf{r}, t) = \delta_{\mathbf{r}0}\delta_{t0} + \sum_{t' \leqslant t} F_{\rm cl}(\mathbf{r}, t') P_{\rm cl}(0, t - t'). \tag{29}$$

This equation [6,43,44], sometimes called the renewal equation, is generally valid for Markov processes in the sense that it is not limited to discrete time and space models; in the continuum one needs only to replace summation with integration and probabilities by probability densities. The idea behind Eq. (29) is that a particle on position $\mathbf{r}$ at time t must have either arrived there previously at time t' *for the first time* and then returned back or it arrived at $\mathbf{r}$ exactly at time t for the first time (the $t' = t$ term) [1,6]. Using the Z transform, the following equations are derived [1]:

$$F_{\rm cl}(\mathbf{r}, z) = \begin{cases} \frac{P_{\rm cl}(\mathbf{r}, z)}{P_{\rm cl}(0, z)}, & \mathbf{r} \neq 0 \\ 1 - \frac{1}{P_{\rm cl}(0, z)}, & \mathbf{r} = 0. \end{cases} \tag{30}$$

From this formula, various basic properties of random walks can be derived. One example is the Pólya theorem which answers the following question: Does a particle eventually return to its origin, i.e., is the random walk recurrent? A second is that in one dimension, for an open system without bias, the famous law $F_{\rm cl}(0, t) \sim t^{-3/2}$ is found for large first passage time t and hence the first passage time has an infinite mean, as mentioned in the Introduction. We will later find the quantum analog to this well known $t^{-3/2}$ behavior.

At first glance, this classical picture might not seem related to ours. However, consider the case where we detect the particle at the origin, so $\hat{D} = |0\rangle\langle 0|$ and initially $|\psi(0)\rangle = |0\rangle$. Then, Eq. (24) reads as

$$\hat{\phi}(z) = \frac{\langle 0|\frac{1}{z^{-1}e^{iH\tau} - 1}|0\rangle}{1 + \langle 0|\frac{1}{z^{-1}e^{iH\tau} - 1}|0\rangle}. \tag{31}$$

We add and subtract one in the numerator and use $\langle 0|0\rangle = 1$ and

$$1 + \frac{1}{z^{-1}e^{iH\tau} - 1} = \frac{1}{1 - ze^{-iH\tau}} \tag{32}$$

to rewrite Eq. (31) as

$$\hat{\phi}(z) = 1 - \frac{1}{\langle 0|\frac{1}{1 - ze^{-iH\tau}}|0\rangle}. \tag{33}$$

Expanding in z we get a geometric series

$$\hat{\phi}(z) = 1 - \frac{1}{\langle 0|\sum_{n=0}^{\infty} z^n \exp(-iH\tau n)|0\rangle}. \tag{34}$$

By definition, the sum $\langle 0|\sum_{n=0}^{\infty} z^n \exp(-iH\tau n)|0\rangle$ is the generating function of the amplitude of being at the origin retrieved from the solution of the Schrödinger equation without detection. Namely, let $|\psi_f(t)\rangle$ be the solution of the Schrödinger equation for the same initial condition $|\psi_f(0)\rangle = |0\rangle$ (the subscript f denotes a wave function free of measurement). The amplitude of being at the origin at time t is $\langle 0|\psi_f(t)\rangle$ and $|\psi_f(t)\rangle = \exp(-iHt)|0\rangle$ as usual. We define the generating function of this amplitude, for the sequence of measurements under consideration,

$$\langle 0|\hat{\psi}_f(z)\rangle_0 \equiv \sum_{n=0}^{\infty} z^n \langle 0|\psi_f(n\tau)\rangle \tag{35}$$

and clearly $\langle 0|\hat{\psi}_f(z)\rangle_0 = \sum_{n=0}^{\infty}\langle 0|z^n \exp(-iH\tau n)|0\rangle$, the subscript zero denotes the initial condition. Hence, we get the appealing result reported already in [25]:

$$\hat{\phi}(z) = 1 - \frac{1}{\langle 0|\hat{\psi}_f(z)\rangle_0}. \tag{36}$$

Thus, the generating function of the first detection time is determined from the Z transform of the spatial wave function at the point of detection $x = 0$. This connection is the quantum analog of the second line in the classical expression (30) since in both cases we start and detect at the origin.

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

$$\hat{\phi}(z) = \frac{\langle 0|\hat{\psi}_f(z)\rangle_x}{\langle 0|\hat{\psi}_f(z)\rangle_0}, \tag{37}$$

where $|\hat{\psi}_f(z)\rangle_x$ is the Z transform of the wave function free of measurements initially localized on site x, $|\hat{\psi}_f(z)\rangle_x = \sum_{n=0}^{\infty} z^n|\psi_f(n\tau)\rangle_x$ with $|\psi_f(n\tau)\rangle_x = \exp(-iHn\tau)|x\rangle$. We see that the ratio of the generating functions of the amplitudes of finding the particle on $|0\rangle$ for initial condition on x and the location of measurement site 0, obtained from the measurement-free evolution, yields the generating function of the measurement process. This is the sought after quantum renewal equation, namely, the amplitude analog of the upper line of the classical Eq. (30).

Remark. In Eq. (35) the lower limit of the sum is $n = 0$, while in Eq. (20) the sum starts at $n = 1$ as noted already [42]. Since $\phi_0 = 0$, one may of course use a summation from 0 also in Eq. (20).

*R*emark. Our formalism is not limited to spatially homogeneous Hamiltonians. Note that in our classical discussion, following the textbook treatment [1] and for the sake of simplicity, we have assumed translation invariant random walks. In nontranslation invariant systems, one should replace $P_{\rm cl}(0,t - t')$ in the left hand side of Eq. (29) with $P_{\rm cl}(\mathbf{r},t - t'|\mathbf{r},0)$. Since the convolution structure of the equation remains, related to the Markovian hypothesis, Eq. (30) can be easily modified to include nonhomogeneous effects.

Remark. Sinkovicz *et al.* [45] found a quantum Kac lemma for recurrence time, thus analogies between quantum and classical walks are not limited to the renewal equation under investigation.

C. Zeno effect

As pointed out in Refs. [20,21], when $\tau \to 0$ we find the Zeno effect [23,46]. Since in that limit $\exp(-iH\tau) = 1$ and $\hat{U}(z) = z/(1 - z)$, using Eq. (23) we get

$$\lim_{\tau\to 0} \hat{\phi}(z) = z\langle 0|\psi(0)\rangle. \tag{38}$$

The amplitude of finding the particle at the origin in the first attempt is given by the initial wave function projected on the origin, i.e., the probability amplitude of finding the particle at the origin at $t = 0$. Hence, the above expression gives an obvious answer for the first measurement; the repeated measurements being very frequent do not allow the wave function to be built up at the origin, and hence $\phi_n = 0$ for all $n > 1$. This means that we may investigate the problem for τ small relative to the time scales of the Hamiltonian, but we cannot take the limit $\tau \to 0$ if we wish to retain information on the measurement process beyond the initial state.

D. Energy representation

Equation (22) for a time-independent Hamiltonian yields

$$\langle E_m|\hat{U}(z)|E_i\rangle = [z^{-1}\exp(iE_m\tau) - 1]^{-1}\delta_{mi} \tag{39}$$

so that the operator $\hat{U}(z)$ is diagonal in the energy representation. Here, $|E_i\rangle$ is a stationary state of the Hamiltonian H, namely, $H|E_i\rangle = E_i|E_i\rangle$. Clearly, it is worthwhile presenting the solution in that basis. Consider the example of the measurement at the spatial origin corresponding to state $|0\rangle$. This state can be expanded in the energy representation $|0\rangle = \sum_k C_k|E_k\rangle$ with $C_k = \langle E_k|0\rangle$. Here as usual $\langle E_m|E_k\rangle = \delta_{mk}$. Similarly, the initial condition is expanded as $|\psi(0)\rangle = \sum_k A_k|E_k\rangle$. The matrix element

$$\langle 0|\hat{U}(z)|\psi(0)\rangle = \sum_k C_k^* A_k[z^{-1}\exp(iE_k\tau) - 1]^{-1} \tag{40}$$

together with

$$\langle 0|\hat{U}(z)|0\rangle = \sum_k |C_k|^2[z^{-1}\exp(iE_k\tau) - 1]^{-1} \tag{41}$$

yields $\hat{\phi}(z)$ using Eq. (23). For the special case where $|\psi(0)\rangle = |0\rangle$, we get $A_k = C_k$ and

$$\hat{\phi}(z) = \frac{\sum_k |C_k|^2[z^{-1}\exp(iE_k\tau) - 1]^{-1}}{1 + \sum_k |C_k|^2[z^{-1}\exp(iE_k\tau) - 1]^{-1}}. \tag{42}$$

Here as usual $\sum_k |C_k|^2 = 1$. It is easy to check that when $\tau \to 0$ we get $F_1 = |\phi_1|^2 = 1$ since a particle starting at the origin is with probability one detected when $\tau \to 0$.

V. RINGS

For our explicit calculations, we will focus on tight-binding models in one dimension [12]. The first model is a quantum walk on a ring of length L:

$$H = -\gamma \sum_{x=0}^{L-1}(|x\rangle\langle x+1| + |x+1\rangle\langle x|). \tag{43}$$

This describes a quantum particle jumping between nearest neighbors on the ring. We use periodic boundary conditions and thus from the site labeled $x = L - 1$ one may jump either to the origin $x = 0$ or to the site labeled $x = L - 2$. In condensed matter physics, the parameter γ is called the hopping rate.

A. Benzene-type ring

As our first example, we consider the tight-binding model on a hexagonal ring illustrated in Fig. 1, namely, a structure similar to the benzene molecule [13,47]. We consider the influence of initial states $|\psi(0)\rangle = |x\rangle$ with $x = 0,1,\ldots,5$ on the statistics of first detection times for detection at site 0 so $\hat{D} = |0\rangle\langle 0|$. According to our theory, to find the generating function we need the energy levels of H and its eigenstates. The six energy levels of the system are $E_k = -2\gamma\cos(\theta_k)$ with $k = 0,\ldots,5$ and the eigenstates are $|E_k\rangle^T =$

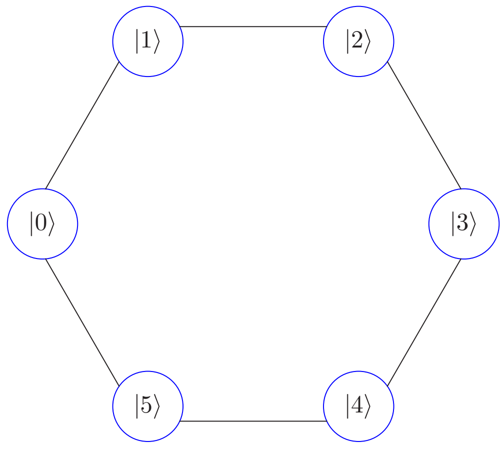

FIG. 1. Schematic model of a benzene ring. In the text, measurement is performed on site 0 and we discuss several initial conditions.

$(1,e^{i\theta_k},e^{2i\theta_k},e^{i3\theta_k},e^{i4\theta_k},e^{i5\theta_k})/\sqrt{6}$ with $\theta_k = 2\pi k/6$ [13] (the superscript T is the transpose). Hence, the coefficients $|C_k|^2 = |\langle E_k|0\rangle|^2 = \frac{1}{6}$, reflecting the symmetry of the problem.

1. Starting at $x = 0$

We use Eq. (42) and find

$$\hat{\phi}(z) = \frac{\frac{1}{6}\sum_{k=0}^{5}\frac{1}{z^{-1}\exp(iE_k\tau)-1}}{1+\frac{1}{6}\sum_{k=0}^{5}\frac{1}{z^{-1}\exp(iE_k\tau)-1}}. \tag{44}$$

The nondegenerate energy levels are -2γ and 2γ while $-\gamma$ and γ are doubly degenerate, hence, for real z

$$\hat{\phi}(z) = \frac{\frac{1}{3}\left\{\mathrm{Re}\left[\frac{1}{z^{-1}e^{2i\gamma\tau}-1}\right]+2\,\mathrm{Re}\left[\frac{1}{z^{-1}e^{i\gamma\tau}-1}\right]\right\}}{1+\frac{1}{3}\left\{\mathrm{Re}\left[\frac{1}{z^{-1}e^{2i\gamma\tau}-1}\right]+2\,\mathrm{Re}\left[\frac{1}{z^{-1}e^{i\gamma\tau}-1}\right]\right\}}. \tag{45}$$

It is interesting to note that the generating function satisfies the identity

$$\hat{\phi}(e^{i\theta})\hat{\phi}(e^{-i\theta}) = 1, \tag{46}$$

an identity we will return to below when discussing $\langle n\rangle$ and S_∞. Inserting Eq. (46) in Eq. (27) and integrating over θ gives $S_\infty = 0$. Thus, the survival probability is zero in the long-time limit. This behavior is classical in the sense that for finite systems a classical random walker is always detected. Note that for a quantum walker this conclusion is not generally valid. If we start at $|1\rangle$ for example and measure at $|0\rangle$, and perform measurements on full revival periods, the particle is never recorded (see further details and other examples below). Hence, for a quantum particle the survival probability S_n does not generally decay to zero as $n \to \infty$, even for finite systems.

For special values of $\gamma\tau$ we get exceptional behaviors. When $\gamma\tau$ is 2π times an integer, we get $\hat{\phi}(z) = z$, namely, the measurement in the first attempt is made with probability 1, so the first detection time is τ, which is expected since the wave function is fully revived at these τ's in its initial state at the origin [12]. If $\gamma\tau = \pi$ we get $\hat{\phi}(z) = z(3z-1)/(3-z)$. Inverting we find $\phi_1 = -\frac{1}{3}$ and $\phi_n = 8/3^n$ for $n \geqslant 2$, thus, the amplitude ϕ_n decays exponentially. It follows that the first detection probabilities are

$$F_n = \begin{cases} \frac{1}{9}, & n = 1 \\ \frac{64}{9^n}, & n \geqslant 2. \end{cases} \tag{47}$$

The average number of detection attempts is $\sum_{n=1}^{\infty} nF_n = 2$. If $\gamma\tau = \pi/2$ we find $\hat{\phi}(z) = -z(1+2z+3z^2)/(3+2z+z^2)$ which has simple poles and, hence,

$$F_n = \begin{cases} \frac{1}{9}, & n = 1 \\ \frac{16}{81}, & n = 2 \\ \frac{24}{3^n}\sin^2[\zeta_1(n-2)-\zeta_2], & n \geqslant 3 \end{cases} \tag{48}$$

where $\zeta_1 = \tan^{-1}(\sqrt{2})$ and $\zeta_2 = \tan^{-1}(\sqrt{2}/5)$. For this case $\langle n\rangle = 3$. Similarly, for $\gamma\tau = 2\pi/3 + 2k\pi$ and $\gamma\tau = 4\pi/3 + 2k\pi$ we get $\langle n\rangle = 2$. The general feature of finite rings is an exponential decay of F_n with a superimposed oscillation determined by the poles of the generating function. However, the sampling times $\gamma\tau = 0,\pi/2,2\pi/3,\pi \ldots$ considered so far exhibit behaviors which are not typical, as we now show.

A surprising behavior is found for the average, with

$$\langle n\rangle = 4 \tag{49}$$

for any sampling rate in the interval $(0,2\pi)$ besides what we call the exceptional sampling times $\gamma\tau = 0,\pi/2,2\pi/3,\pi,\ldots$ where as mentioned $\langle n\rangle = 1,3,2,2,\ldots$, respectively, which is continued periodically (see Fig. 2). This result is derived below. As mentioned in the Introduction, the fact that $\langle n\rangle$ is some integer was already pointed out rather generally by [25] and this is related to topological effects. Except for the exceptional points, the variance of n is

$$\mathrm{Var}(n) = -11 + \frac{27}{4-4\cos\gamma\tau} + \frac{1}{6\cos^2\gamma\tau} + \frac{3}{4+4\cos\gamma\tau} + \frac{3}{(1+2\cos\gamma\tau)^2} \tag{50}$$

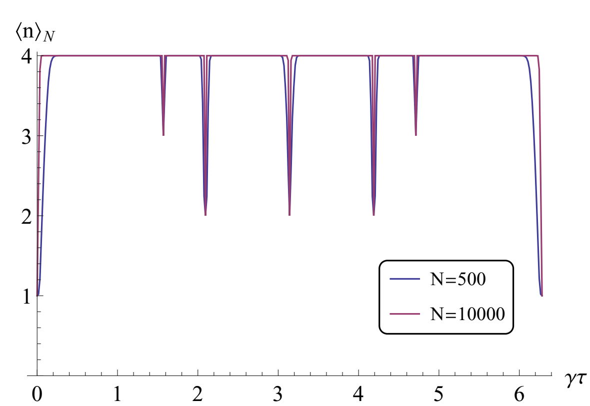

FIG. 2. The average number of detection attempts $\langle n\rangle$ for a quantum walk on a benzene ring, with initial condition $|\psi(0)\rangle = |0\rangle$ and projective measurements on the origin, by Eq. (49), $\langle n\rangle = 4$, except for the cases when $\gamma\tau$ is a multiple of $\pi/2$ or $2\pi/3$. Here, we plot $\langle n\rangle_N = \sum_{n=1}^{N} nF_n$ for $N = 500$ and $10\,000$, the results converging to the analytic result as we increase N further (not shown).

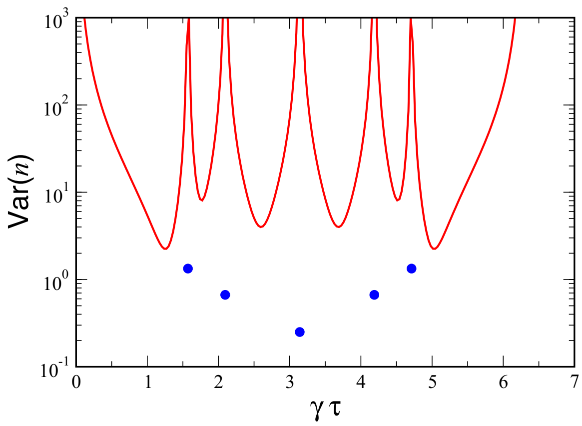

FIG. 3. The variance of n versus $\gamma\tau$ [Eq. (50)] for the $0 \to 0$ first detection problem on the benzene ring. Divergences of the fluctuations are found close to exceptional sampling times, while for these times themselves the fluctuations are finite (blue circles). For $\gamma\tau = 0{,}2\pi$, $\mathrm{Var}(n) = 0$.

so that the first detection time exhibits large fluctuations near these points. Thus, for the 0 to 0 transition it is only the average $\langle n\rangle$ that is nearly always not sensitive to the sampling rate, not the full distribution of first detection times. In Fig. 3, we plot the variance of n versus the sampling time $\gamma\tau$ including also the exceptional points. As mentioned a measurement of $\langle n\rangle$ gives 4 for nearly all values of $\gamma\tau$; the discontinuities for special sampling times are point discontinuities and hence exceptional sampling times seem difficult to detect in measurements of the mean. In contrast, the blowup of the fluctuations in the vicinity of the critical sampling times, presented in Fig. 3, seems to provide a more realistic way to detect critical sampling times in the laboratory.

There are numerous methods to find $\langle n\rangle = \sum_{n=1}^{\infty} nF_n$. For the exceptional points we used the exact solution for F_n (as mentioned). For other sampling times we use two approaches: the first using *Mathematica* and is based on a Taylor expansion of $\hat{\phi}(z)$ and the second is an analytic calculation. The former approach is very general in the sense that it can be used in principle for general initial conditions and other problems beyond the benzene ring.

Specifically, we calculate F_n exactly using the expansion of $\hat{\phi}(z)$ with symbolic programming on *Mathematica*. This is performed up to some large N. We then calculate $\langle n\rangle_N = \sum_{n=1}^{N} nF_n$. Clearly, $\langle n\rangle > \langle n\rangle_N$, and increasing N we see convergence towards $\langle n\rangle = 4$ except for the mentioned exceptional points. An example is shown in Fig. 2 for the cases $N = 500$ and 10 000.

Even better is to write $\hat{\phi}(z) = z^4 H(1/z)/H(z)$, which is the extension to general z of the identity (46) that we used to show $S_\infty = 0$. To find $\langle n\rangle$ we use Eq. (44) to find

$$\begin{aligned} H(z) = {} & [2\cos(\gamma\tau) + \cos(2\gamma\tau)]z^3 \\ & - [3 + 6\cos(\gamma\tau)\cos(2\gamma\tau)]z^2 \\ & + [4\cos(\gamma\tau) + 5\cos(2\gamma\tau)]z - 3, \end{aligned} \tag{51}$$

and with Eq. (28)

$$\begin{aligned} \langle n\rangle &= \frac{1}{2\pi i}\int_0^{2\pi} \frac{e^{-4i\theta}H(e^{i\theta})}{H(e^{-i\theta})}\frac{\partial}{\partial\theta}\left[\frac{e^{4i\theta}H(e^{-i\theta})}{H(e^{i\theta})}\right]d\theta \\ &= 4 - \frac{1}{i\pi}\int_0^{2\pi}\frac{\partial}{\partial\theta}\ln H(e^{i\theta})d\theta. \end{aligned} \tag{52}$$

Rewriting $H(z) = a(z - z_1)(z - z_2)(z - z_3)$ we can proceed to show that

$$\langle n\rangle = 4 - \frac{1}{i\pi}\sum_{j=1}^{3}\int_0^{2\pi}\frac{\partial}{\partial\theta}\ln(e^{i\theta} - z_j)d\theta = 4 - 2\alpha - \beta, \tag{53}$$

where α (or β) is the number of zeros of $H(z)$ for z within (or on) the unit circle, respectively. As explained in Appendix B, $\alpha = 0$ for otherwise we would find $F_n > 1$. For the exceptional values of $\gamma\tau$ we find $\beta > 0$, as follows:

$$\beta = \begin{cases} 1, & \gamma\tau = \frac{1}{2}\pi + \pi k \\ 2, & \gamma\tau = \frac{2}{3}\pi + 2\pi k, \pi + 2\pi k, \frac{4}{3}\pi + 2\pi k \\ 3, & \gamma\tau = 2\pi k \\ 0, & \text{otherwise.} \end{cases} \tag{54}$$

This agrees with the values of $\langle n\rangle$ we have found at the exceptional points. This exercise shows that mathematically, at least for this example, the exceptional points are those specific values of τ where some of the zeros of the polynomial $H(z)$ are found to lie on the unit circle in the complex plane. We will soon find a by far more physical and explicit formula for these points Eq. (58) below.

2. *Half dark states*

Another peculiar behavior is found if the detection is at the origin $\hat{D} = |0\rangle\langle 0|$ and the starting point is $|i\rangle$ with $i = 1,2,4,5$. The total probability of detection is found to be, by the method explained in Appendix B,

$$1 - S_\infty = 1/2 \tag{55}$$

for all values of $0 < \gamma\tau < 2\pi$ aside from exceptional points which are listed in Table I. The exceptions include the case when τ is the full revival time, for which case the probability of being detected is of course 0. The behavior (55) was observed in [21,22] for even larger systems. It is remarkable that for

TABLE I. Total detection probability $1 - S_\infty$ for a quantum walker on a benzene ring, for different localized starting points $|\psi(0)\rangle = |x\rangle$. Measurements are performed at $x = 0$, hence, initial conditions on sites 1 and 2 are equivalent to initial conditions on 5 and 4, respectively. Values of the parameter $\gamma\tau$ are listed in the first row, and $0 < \gamma\tau < 2\pi^*$ implies all values of $\gamma\tau$ in the interval, aside from the listed special cases, e.g., $\gamma\tau = \pi$.

x	$0 < \gamma\tau < 2\pi^*$	$\gamma\tau = 0$	$\frac{1}{2}\pi$	$\frac{2}{3}\pi$	π	$\frac{4}{3}\pi$	$\frac{3}{2}\pi$	2π
0	1	1	1	1	1	1	1	1
1	1/2	0	1/6	0	0	0	1/6	0
2	1/2	0	1/2	0	1/2	0	1/2	0
3	1	0	2/3	1	0	1	2/3	0

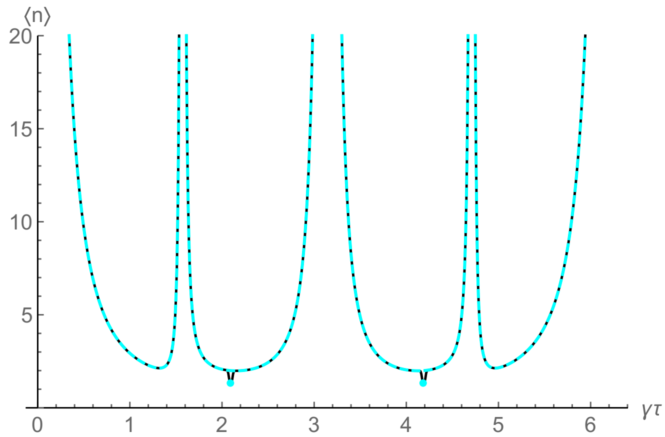

FIG. 4. The average $\langle n\rangle$ versus $\gamma\tau$ [Eq. (56)]. When $\tau\to 0$ we find $\langle n\rangle\to\infty$ due to the Zeno effect, another expected divergence of $\langle n\rangle$ is found when the sampling time is the full revival time $\gamma\tau=2\pi$. In addition to these two points, we find singularities also for $\pi/2,\pi,3\pi/2$. Notice the discontinuities of $\langle n\rangle$ for the exceptional sampling times $\gamma\tau=2\pi/3$ and $\gamma\tau=4\pi/3$ which are discussed in the text. Here, $|\psi(0)\rangle=|3\rangle$ and the detection is on the origin. The plot of $\langle n\rangle$ for this choice of initial condition is vastly different from that presented in Fig. 2. The blue line is the analytic result (56). The blue circles represent the values at the exceptional sampling times. The black dashed line is the result of a numerical evaluation of $\sum_n nF_n$ up to a large finite N.

certain initial conditions, the detection of the particle is not guaranteed, and only in half of the measurement processes we detect the particle, hence, we call these initial conditions half dark states.

3. Starting on site 3 measuring on 0

In contrast, if the starting state is $|3\rangle$ the total probability of detection is found to be 1, if the measurement time τ is not the full revival time $\gamma\tau=2\pi$, or one of the exceptional sampling times listed in Table I. In Appendix B, we find

$$\langle n\rangle=\frac{4}{9}+\frac{9}{8-8\cos\gamma\tau}+\frac{1}{36\cos^2\gamma\tau}-\frac{1}{9\cos\gamma\tau}+\frac{17}{72(1+\cos\gamma\tau)},\tag{56}$$

an equation valid for all $\gamma\tau$ aside from the exceptional points. The general behavior of $\langle n\rangle$ is obviously quite different from the case when the initial location is 0 (compare Figs. 2 and 4 indicating that the initial condition plays a crucial rule). As shown in Fig. 4, the average $\langle n\rangle$ exhibits nontrivial behavior as it diverges as it approaches some of the exceptional points. These singularities are found near those exceptional sampling times where the total probability of measurement is not one. Interestingly, the values of $\langle n\rangle$, conditioned on return, are finite at the exceptional points themselves.

An analytical calculation for the exceptional sampling times $\gamma\tau=2\pi/3$ or $4\pi/3$ finds $\langle n\rangle=\frac{4}{3}$. This sampling time is unique since the average $\langle n\rangle$ exhibits a discontinuity: for $\gamma\tau$ in the vicinity of $2\pi/3$ and $4\pi/3$ we find using Eq. (56) $\langle n\rangle=2$ (so at these points the equation is not valid). Similar to any discontinuity at a point, the discontinuity of $\langle n\rangle$ at $\gamma\tau=2\pi/3,4\pi/3$ might not be detectable in experiment. However, one finds critical slowing down, namely, the convergence of $\langle n\rangle$ for any point in the vicinity of these exceptional points is very slow, as demonstrated in Fig. 4.

B. Rings of size *L*

While the benzene ring is instructive, one must wonder how general are the main results. In Appendix B, we derive the following four results:

(i) For a ring of size L and for a particle initially on site $x=0$ where the measurements are performed, the particle is detected with probability unity, and in this sense the motion is recurrent. We emphasize that this result is a property of the specified initial condition.

(ii) For these same initial conditions, aside from those isolated exceptional sampling times τ listed below, the average number of detection events is

$$\langle n\rangle=\begin{cases}\frac{L+2}{2}, & L \text{ is even}\\ \frac{L+1}{2}, & L \text{ is odd.}\end{cases}\tag{57}$$

This result is remarkable since the average is independent of the sampling time τ. Here, we see that $\langle n\rangle$ is the number of distinct energy levels of the system. In the language of [25] it is the winding number of the Schur function, or the effective dimension of the Hilbert space. For large systems, $\langle n\rangle$ grows linearly with the size of the system L. This is the same as a classical random walk on a ring where for the case of starting and detecting at the same point, one finds from Kac's return theorem $\langle n\rangle^{\text{cl}}=L$ [see Eq. (1) in [5]]. The quantum search for large systems seems slightly faster since $\langle n\rangle^{Qu}=\langle n\rangle^{cl}/2$, however, in the presence of the slightest disorder, which still removes the degeneracy of the energy levels, we will get $\langle n\rangle^{\text{Qu}}=\langle n\rangle^{\text{cl}}$ when the number of distinct energy levels is L [see point (iv) below].

(iii) The exceptional sampling times τ are given by the rule

$$\Delta E\tau=2\pi n,\tag{58}$$

where n is an integer, and $\Delta E=E_i-E_j>0$ is the energy difference between pairs of eigenenergies of the underlying Hamiltonian H. For example, the stationary energies of the benzene ring are $\{-2\gamma,-\gamma,\gamma,2\gamma\}$ as mentioned, and hence Eq. (58) predicts the exceptional sampling times $0,\pi/2\gamma,2\pi/3\gamma,\pi/\gamma,\ldots$. The condition (58) implies a partial revival of the wave packet free of measurement, namely, two modes of the system behave identically when strobed at the period τ. On these exceptional points, the solution exhibits nonanalytical behavior. This is manifested in discontinuities or diverging behavior of $\langle n\rangle$ or the fluctuations of n and also slow critical-like convergence to the asymptotic theory. The exact nature of the nonanalytical behavior depends on the initial condition as we have demonstrated for the benzene ring.

(iv) For a particle starting on $|0\rangle$, every time the condition (58) is satisfied by a pair of energy levels, the value of $\langle n\rangle$ is reduced by unity. Thus, Eq. (58) is the upper limit of $\langle n\rangle$ for a system of fixed size L. More specifically, we find that

$$\langle n\rangle=\text{number of distinct phases }\exp(-iE_k\tau),\tag{59}$$

where E_k are the energy levels of the system (see also [25]). For nearly any τ, this is the same as the number of distinct energy levels, but of course for special sampling times, this integer is less than that.

C. Bose-Einstein distribution

A curiosity is the fact that we may express the solution for the 0 (starting point) to 0 (measurement point) problem for a general ring with L sites, in terms of a Bose-Einstein distribution. The latter is defined as [48]

$$\bar{n}_k = \frac{1}{e^{-\beta\mu+\beta E_k} - 1}, \tag{60}$$

where β is the inverse temperature and μ the chemical potential. In our case, $z^{-1} = \exp(-\beta\mu)$ and $\beta E_k = i\tau E_k$ with the energy spectrum $E_k = -2\gamma\cos(2\pi k/L)$. The generating function for a ring system with L sites is

$$\hat{\phi}(z) = \frac{\sum_{k=0}^{L-1} \bar{n}_k/L}{1 + \sum_{k=0}^{L-1} \bar{n}_k/L}. \tag{61}$$

The mathematical relation of the problem at hand to the Bose-Einstein distribution is not limited to the specific energy spectrum under investigation (see also [25]). If the Hamiltonian is symmetric in the sense that all lattice points are equivalent, such that $|C_k|^2 = 1/L$, the above result is valid. In the Bose-Einstein language, the sum $\sum_{k=0}^{L-1} \bar{n}_k/L$ is the spatially averaged density. Thus, the problem of finding the generating function is mathematically equivalent to finding the relation between chemical potential, temperature, and the average number of particles, for a given energy spectrum of a system. The main conditions are that all sites are equivalent and that the initial and detection states are both on the same single ring site.

D. Revivals

The amplitude of detection at the first measurement ϕ_1 is now investigated for a particle on a ring of size L starting on the origin which is also the detection site

$$\phi_1 = \frac{1}{L}\sum_{k=0}^{L-1} e^{2i\gamma\tau\cos(2\pi k/L)}. \tag{62}$$

In the limit $L \to \infty$, the sum becomes an integral and we find $\phi_1 = J_0(2\gamma\tau)$ and $J_0(\ldots)$ is a Bessel function of the first kind [49]. Unlike the benzene, $L = 6$, case, for an infinite system with $\gamma\tau \neq 0$, the probability of detecting the particle at first measurement $F_1 = |\phi_1|^2$ is always less than unity since $|J_0(2\gamma\tau)|^2 < 1$. This is to be expected, as the wave function in an infinite system does not revive at the origin. The following question remains: Does a finite sized system always exhibit a special choice or choices of $\gamma\tau \neq 0$ such that $F_1 = 1$ (and then all F_n for $n > 1$ are zero)? This corresponds to a deterministic outcome of certainly detecting at a single detection attempt. This question put differently is the well-studied question of full revivals. Namely, does there exist some τ such that a particle, in the absence of measurement, will fully return to its initial state. If that is the case, the first measurement detects the particle with probability one if the measurement time is τ. As mentioned, for $L = 6$, this effect is found for $\gamma\tau = 2\pi k$ for $k = 0,1,2,\ldots$.

According to [12], full revivals take place for $L = 1,2,3,4,6$ only. This can be verified using our formalism. We checked this for $L = 5,7,8,9,10$ finding that the absolute value squared of the sum (62) is never equal 1 unless $\tau = 0$. For example, for $L = 10$,

$$\phi_1 = \frac{1}{5}\left[\cos(2\gamma\tau) + 4\cos\left(\frac{\gamma\tau}{2}\right)\cos\left(\frac{\sqrt{5}\gamma\tau}{2}\right)\right], \tag{63}$$

an expression which shows that $|\phi_1| < 1$ beyond the trivial case $\gamma\tau = 0$.

Remark. For a ring with four sites and sampling rate of $\gamma\tau = \pi$ one finds $\hat{\phi}(z) = z^2$, namely, the quantum walker is detected in the second measurement with probability one. Such a behavior is found when the initial wave packet is localized at the place of detection. In this example, the first measurement is performed when the wave function at the origin is zero, and hence this measurement does not alter the wave function, while in the second measurement we have full revival of the wave function at the origin.

VI. FIRST DETECTION TIME FOR AN UNBOUNDED QUANTUM WALKER

In this section, we consider the first detection problem for a free particle in an infinite lattice. We use the tight-binding Hamiltonian

$$H = -\gamma\sum_{x=-\infty}^{\infty}(|x\rangle\langle x+1| + |x+1\rangle\langle x|) \tag{64}$$

for a particle launched from the origin $|\psi(0)\rangle = |0\rangle$ and investigate the probability of first detection F_n with projective measurements performed at the origin.

Previously, Bach *et al.* [17] investigated a Hadamard quantum walk introduced in Ref. [9], showing that the survival probability of a one-dimensional walker exhibits a power-law decay, $F_n \propto n^{-3}$ in our terminology, namely, a scaling exponent 3 which is twice the classical one, i.e., $\frac{3}{2}$. This was the topic of further analytical [25], numerical [38,39], and perturbative approaches [21,22]. In this sense, it is known already that quantum walks modify the known classical exponents of classical random walk theory, where the first passage time PDF decays like $t^{-3/2}$ for large times. What seems to be missed in previous literature is that even in an infinite system there is a critical sampling effect. On a more technical level, we show how to use the generating function formalism to find the large-n behavior of the first detection probability. We then discuss S_∞, showing its nontrivial behavior.

A. Generating function

The solution of the Schrödinger equation (64) is $|\psi_f(t)\rangle = \sum_{x=-\infty}^{\infty} B_x|x\rangle$ and the amplitudes satisfy $i\dot{B}_x = -\gamma(B_{x+1} + B_{x-1})$. Using the Bessel function identity [49] $2J'_\nu(z) = J_{\nu-1}(z) - J_{\nu+1}(z)$ and the initial condition $B_x = \delta_{x,0}$, one finds

$$|\psi_f(t)\rangle = \sum_{x=-\infty}^{\infty} i^x J_x(2\gamma t)|x\rangle. \tag{65}$$

This is of course the same as $|\psi_f(t)\rangle = \exp(-iHt)|0\rangle$. To obtain the generating function we use Eq. (36), we have

$\langle 0|\hat{\psi}_f(z)\rangle = \sum_{n=0}^{\infty} z^n J_0(2\gamma\tau n)$ so

$$\hat{\phi}(z) = 1 - \frac{1}{\langle 0|\hat{\psi}_f(z)\rangle} = 1 - \frac{1}{\sum_{n=0}^{\infty} z^n J_0(2\gamma\tau n)}. \quad (66)$$

Since $J_0(0) = 1$, this can be rewritten as

$$\hat{\phi}(z) = \frac{\sum_{n=1}^{\infty} z^n J_0(2\gamma n\tau)}{1 + \sum_{n=1}^{\infty} z^n J_0(2\gamma n\tau)}. \quad (67)$$

Before analyzing Eq. (67), we derive it again using the energy spectrum. The energy levels of a tight-binding ring system (periodic boundary conditions) determined from the time independent Schrödinger equation are $E_k = -2\gamma\cos(2\pi k/L)$ and the system size L tends to infinity. As we have seen, $|C_k|^2 = 1/L$ in Eq. (42) since all lattice sites are equivalent with respect to the Hamiltonian. Using Eq. (24) or (61) with minor rearrangement,

$$\hat{\phi}(z) = \frac{\frac{1}{L}\sum_{k=0}^{L-1} \frac{z\exp\left[i2\gamma\tau\cos\left(\frac{2\pi k}{L}\right)\right]}{1 - z\exp\left[i2\gamma\tau\cos\left(\frac{2\pi k}{L}\right)\right]}}{1 + \frac{1}{L}\sum_{k=0}^{L-1} \frac{z\exp\left[i2\gamma\tau\cos\left(\frac{2\pi k}{L}\right)\right]}{1 - z\exp\left[i2\gamma\tau\cos\left(\frac{2\pi k}{L}\right)\right]}}. \quad (68)$$

This is exact for all L and reduces to Eq. (44) when $L = 6$. Let

$$I(z) \equiv \lim_{L\to\infty} \frac{1}{L}\sum_{k=0}^{L-1} \frac{z\exp\left[i2\gamma\tau\cos\left(\frac{2\pi k}{L}\right)\right]}{1 - z\exp\left[i2\gamma\tau\cos\left(\frac{2\pi k}{L}\right)\right]}, \quad (69)$$

where the sum is an integral in the limit. Changing variables $2\pi k/L = y$,

$$I(z) = \frac{1}{2\pi}\int_0^{2\pi} \frac{ze^{2i\gamma\tau\cos(y)}dy}{1 - ze^{2i\gamma\tau\cos(y)}} \quad (70)$$

and expanding to get a geometric series gives

$$I(z) = \frac{z}{2\pi}\int_0^{2\pi} e^{2i\gamma\tau\cos(y)} \sum_{k=0}^{\infty}[ze^{2i\gamma\tau\cos(y)}]^k dy. \quad (71)$$

Integrating over y using the identity $\int_0^{2\pi}\exp[iz\cos(y)]dy = 2\pi J_0(z)$ and shifting the summation by unity, we get

$$I(z) = \sum_{k=1}^{\infty} z^k J_0(2\gamma k\tau). \quad (72)$$

Using

$$\hat{\phi}(z) = \frac{I(z)}{1 + I(z)} \quad (73)$$

we find the generating function (67). Note that $1 + I(z) = \langle 0|\hat{\psi}_f(z)\rangle$, and we use it as a matter of convenience.

B. Small-*n* behavior

To analyze the small-n behavior of ϕ_n, we expand the generating function as a power series of z using Eqs. (20) and (67). Such an expansion is easy to perform with a symbolic program like *Mathematica*, which provides Table II giving explicit expressions for ϕ_n when $n = 1,\dots,7$. If we set $\gamma\tau$ to a fixed value, the expansion can be carried out for relatively large n, and in this sense we may find numerically exact results which are later presented in the figures. Of course, this information is the same as that found from the exact solutions (18) and (19).

From Table II, we see that when $\gamma\tau \to 0$ we have $\phi_n = \delta_{n1}$ since then the particle is detected in the first attempt. The table also gives the leading order corrections to this expected behavior

$$\phi_n \sim \begin{cases} 1 - (\gamma\tau)^2, & n = 1 \\ -2(\gamma\tau)^2, & n \geqslant 2. \end{cases} \quad (74)$$

This can be derived from Eq. (67) using $J_0(x) \simeq 1 - x^2/4$ for $x \ll 1$. Equation (74) exhibits equal probability of detection for $n > 1$ which is merely an outcome of the Taylor expansion. Clearly, the range of validity of Eq. (74) as a small-τ approximation shrinks to smaller τ as n increases.

When $\gamma\tau \to \infty$, the amplitudes ϕ_n are zero for $n = 1,2,3,\dots$ since the wave packet spreads in an infinite system, hence, its probability of being detected on the origin is zero in this limit. A close look at Table II shows that in this limit $\phi_n \simeq J_0(2n\gamma\tau)$. Using $F_n = |\phi_n|^2$ and the asymptotic behavior of the Bessel function

$$F_n \sim \frac{\cos^2(2\gamma\tau n - \pi/4)}{\pi\gamma\tau n} \quad (75)$$

when $\gamma\tau \gg 1$. Thus, the probability of first detection decays like a $1/n$ power law, when $\gamma\tau$ is large and n is fixed and finite. This approximation breaks down for sufficiently large n. For

TABLE II. Amplitudes of ϕ_n for an infinite system, the quantum walker dispatched and detected at the origin.

n	ϕ_n
1	$J_0(2\gamma\tau)$
2	$J_0(4\gamma\tau) - J_0(2\gamma\tau)^2$
3	$J_0(2\gamma\tau)^3 - 2J_0(4\gamma\tau)J_0(2\gamma\tau) + J_0(6\gamma\tau)$
4	$-J_0(2\gamma\tau)^4 + 3J_0(4\gamma\tau)J_0(2\gamma\tau)^2 - 2J_0(6\gamma\tau)J_0(2\gamma\tau) - J_0(4\gamma\tau)^2 + J_0(8\gamma\tau)$
5	$J_0(2\gamma\tau)^5 - 4J_0(4\gamma\tau)J_0(2\gamma\tau)^3 + 3J_0(6\gamma\tau)J_0(2\gamma\tau)^2 + 3J_0(4\gamma\tau)^2J_0(2\gamma\tau) - 2J_0(8\gamma\tau)J_0(2\gamma\tau) - 2J_0(4\gamma\tau)J_0(6\gamma\tau) + J_0(10\gamma\tau)$
6	$-J_0(2\gamma\tau)^6 + 5J_0(4\gamma\tau)J_0(2\gamma\tau)^4 - 4J_0(6\gamma\tau)J_0(2\gamma\tau)^3 - 6J_0(4\gamma\tau)^2J_0(2\gamma\tau)^2 + 3J_0(8\gamma\tau)J_0(2\gamma\tau)^2 + 6J_0(4\gamma\tau)J_0(6\gamma\tau)J_0(2\gamma\tau)$ $-2J_0(10\gamma\tau)J_0(2\gamma\tau) + J_0(4\gamma\tau)^3 - J_0(6\gamma\tau)^2 - 2J_0(4\gamma\tau)J_0(8\gamma\tau) + J_0(12\gamma\tau)$
7	$J_0(2\gamma\tau)^7 - 6J_0(4\gamma\tau)J_0(2\gamma\tau)^5 + 5J_0(6\gamma\tau)J_0(2\gamma\tau)^4 + 10J_0(4\gamma\tau)^2J_0(2\gamma\tau)^3 - 4J_0(8\gamma\tau)J_0(2\gamma\tau)^3 - 12J_0(4\gamma\tau)J_0(6\gamma\tau)J_0(2\gamma\tau)^2$ $+3J_0(10\gamma\tau)J_0(2\gamma\tau)^2 - 4J_0(4\gamma\tau)^3J_0(2\gamma\tau) + 3J_0(6\gamma\tau)^2J_0(2\gamma\tau) + 6J_0(4\gamma\tau)J_0(8\gamma\tau)J_0(2\gamma\tau) - 2J_0(12\gamma\tau)J_0(2\gamma\tau)$ $+3J_0(4\gamma\tau)^2J_0(6\gamma\tau) - 2J_0(6\gamma\tau)J_0(8\gamma\tau) - 2J_0(4\gamma\tau)J_0(10\gamma\tau) + J_0(14\gamma\tau)$

example, using $\gamma\tau = 80$, by comparison with the numerically exact solution, we observe roughly 30% deviation from theory already for $n = 10$.

C. Large-n behavior

The large-n behavior of ϕ_n is of particular theoretical interest since it is expected to exhibit universal features. For ordinary random walks the transformation from z back to large n is performed with machinery called the Tauberian and Abelian theorems [1,50]. While the technique is widely applicable, the transformation method for the quantum problem is slightly more involved as compared with the corresponding classical problems, the reason being that ϕ_n turns out to exhibit a decay superimposed with oscillations, while in classical random walks the first passage probability decays monotonically to zero for large n.

The large-n analysis of ϕ_n is performed by integration in the complex plane using Eqs. (26), (72), and (73). The behavior at large n is governed by the singularity structure of $I(z)$ [Eq. (72)], which in turn is generated by the summation of the large k terms in the infinite sum since each individual summand is analytic. For large k, the asymptotic behavior of the Bessel function [49] is

$$J_0(2\gamma\tau k) \sim \frac{\cos(2\gamma\tau k - \pi/4)}{\sqrt{\pi\gamma\tau k}}. \tag{76}$$

To capture the singular behavior of $I(z)$, it is sufficient to replace the Bessel function in Eq. (72) with its asymptotic behavior, hence, we define

$$I_{\gamma\tau}(z) = \sum_{k=1}^{\infty} z^k \frac{\cos(2\gamma\tau k - \pi/4)}{\sqrt{\pi\gamma\tau k}}. \tag{77}$$

The advantage of this is that $I_{\gamma\tau}(z)$ can be explicitly calculated in terms of the polylogarithm function. As we shall see, $I_{\gamma\tau}(z)$, and so also $I(z)$, has a $(z - z_0)^{-1/2}$ singularity at some set of points z_0 on the unit circle. The large-n behavior of ϕ_n [Eq. (73)] is then determined by the behavior of $\hat{\phi}(z)$ near z_0:

$$\hat{\phi}(z) = \frac{I(z)}{1 + I(z)} \approx 1 - \frac{1}{I(z)} = 1 - c(z - z_0)^{1/2} \tag{78}$$

for some constant c, near the singular points z_0 of $I(z)$ (see below). This behavior is independent of the finite corrections to the singular behavior of $I(z)$, and thus using $I_{\gamma\tau}$ gives the exact same result as using the original $I(z)$. We start with an example.

1. Infinite system: $\gamma\tau = \pi/2$

We consider the case $\gamma\tau = \pi/2$ and find

$$I_{\pi/2}(z) = \frac{1}{\pi}\mathrm{Li}_{1/2}(-z), \tag{79}$$

where $\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} z^k/k^s$ is the polylogarithm function. Using Eq. (26),

$$\phi_n \sim \frac{1}{2\pi i}\oint_C z^{-n-1}\frac{\frac{1}{\pi}\mathrm{Li}_{1/2}(-z)}{1 + \frac{1}{\pi}\mathrm{Li}_{1/2}(-z)}dz \tag{80}$$

in the large-n limit. The integration path is shown in Fig. 5. A branch cut is found in the complex plane of integration

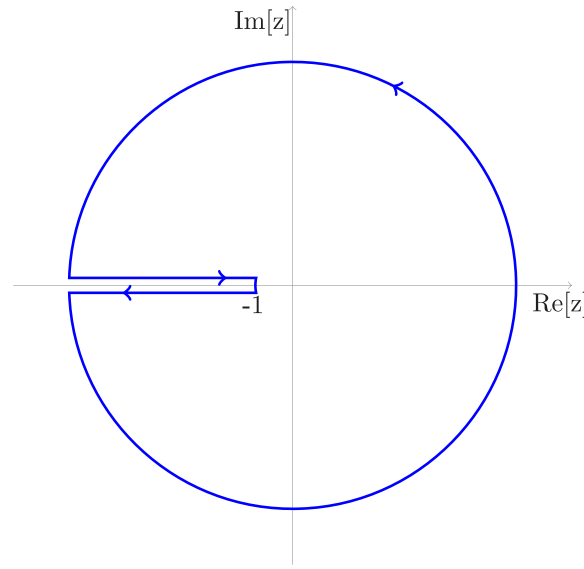

FIG. 5. Counterclockwise integration path C in Eq. (26) for evaluation of ϕ_n for an unbounded lattice with the sampling rate $\gamma\tau = \pi/2$. Equation (80) avoids the branch cut along the negative real axis when $|z| > 1$. The outer radius approaches infinity.

along the negative real axis when $|z| > 1$, with the singularity at $z_0 = -1$, since there $-z = 1$ and $\mathrm{Li}_{1/2}(-z) = \sum_{k=1}^{\infty} 1/\sqrt{k}$ does not converge. The radius of the outer path of integration is taken to be large ($r \to \infty$ in Fig. 5) and then

$$\phi_n \sim \frac{\mathcal{I}_+ + \mathcal{I}_-}{2\pi i}. \tag{81}$$

The integration in the complex plane reduces to two integrals running parallel to the branch cut (see Fig. 5). The first line integral $\mathcal{I}_+$ to be evaluated is slightly above the negative real axis along $z = x + i\epsilon$ with $-\infty < x < -1$ and $0 < \epsilon \to 0$. The second integral follows in the opposite direction with $z = x - i\epsilon$ (see Fig. 5). We consider $\mathcal{I}_+$ using $z^{-(n+1)} = \exp[-(n+1)\ln z]$ and Eq. (80):

$$\mathcal{I}_+ = \int_{-\infty}^{-1} \exp\left[-(1+n)\ln(x+i\epsilon)\right]\frac{\mathrm{Li}_{1/2}(-x-i\epsilon)}{\pi + \mathrm{Li}_{1/2}(-x-i\epsilon)}dx. \tag{82}$$

$\mathcal{I}_-$ is similarly defined with a change of sign in ϵ and the lower and upper integration limits switched. Changing variables to y with $x \equiv -1 - y$,

$$\mathcal{I}_+ = \int_0^{\infty} \exp\left[-(1+n)\ln(-1-y+i\epsilon)\right] \times \frac{\mathrm{Li}_{1/2}(1+y-i\epsilon)}{\pi + \mathrm{Li}_{1/2}(1+y-i\epsilon)}dy. \tag{83}$$

When $n \to \infty$ clearly the small-y limit of the integration dominates. Close to the singularity at $z = 1$ [51],

$$\mathrm{Li}_{1/2}(z) \simeq \sqrt{\frac{\pi}{1-z}} + \zeta(1/2) + \cdots, \tag{84}$$

where $\zeta(\dots)$ is the Riemann zeta function. Indeed, to obtain the leading term (which will eventually give the large-n limit of ϕ_n), we replace the summation with integration in the definition of $\mathrm{Li}_{1/2}(z)$, using

$$\sum_{k=1}^{\infty}\frac{z^k}{\sqrt{k}} \simeq \int_0^\infty \frac{dk}{\sqrt{k}} e^{k\ln(z)} = \sqrt{\pi}[-\ln(z)]^{-1/2} \simeq \sqrt{\frac{\pi}{1-z}}, \tag{85}$$

where $z<1$. We write $z = 1 + y \pm i\epsilon$, where the choice of sign depends on the path evaluated, namely $\mathcal{I}_\pm$. In the limit of small y, corresponding to large n, we find, using Eq. (84),

$$\mathrm{Li}_{1/2}(1+y\pm i\epsilon) \simeq \sqrt{\frac{\pi}{-y\mp i\epsilon}} \sim \sqrt{\frac{\pi}{ye^{\mp i\pi}}} = \pm i\sqrt{\frac{\pi}{y}}. \tag{86}$$

Given that $\ln(-1-y+i\epsilon) = \ln(1+y)+i\pi$ when $\epsilon\to 0$,

$$\mathcal{I}_+ = \int_0^\infty \exp\{-(1+n)[\ln(1+y)+i\pi]\}\frac{-i\sqrt{\pi/y}}{\pi - i\sqrt{\pi/y}}dy. \tag{87}$$

Clearly, $\exp[-(1+n)i\pi] = (-1)^{n+1}$, and approximating $(1+n)\ln(1+y)\sim ny$ in the exponential in the integrand in Eq. (87), an approximation valid in the limit of large n since then only small y contributes to the integration, and finally Taylor expanding $-i\sqrt{\pi/y}/[\pi - i\sqrt{\pi/y}] \sim 1 - i\sqrt{\pi y}$, we find

$$\mathcal{I}_+ \sim (-1)^{n+1}\int_0^\infty \exp(-ny)(1-i\sqrt{\pi y}+\cdots)dy. \tag{88}$$

The integral yields

$$\mathcal{I}_+ \sim (-1)^{n+1}\left(\frac{1}{n} - i\frac{\pi}{2n^{3/2}}\right). \tag{89}$$

The calculation of $\mathcal{I}_-$ follows the same steps

$$\mathcal{I}_- \sim (-1)^{n+1}\left(-\frac{1}{n} - i\frac{\pi}{2n^{3/2}}\right). \tag{90}$$

Finally, using Eq. (81),

$$\phi_n \sim \frac{(-1)^n}{2n^{3/2}}. \tag{91}$$

This solution exhibits an odd/even sign oscillation with an overall decay of a power law. The probability of finding the particle after n attempts goes like $F_n \sim 4^{-1}n^{-3}$. Hence, it does not exhibit oscillations, but that is merely due to our choice of sampling rate $\gamma\tau = \pi/2$ as we now show. In Fig. 6, a very nice agreement between Eq. (91) and the exact solution is seen already for not too large n.

2. *Infinite system: General τ*

We now investigate ϕ_n for sampling time $0<\gamma\tau<\pi$ with $\gamma\tau \neq \pi/2$, sticking to the case where the origin of the quantum walk is also the location where the particle is detected. We find the large-n limit of ϕ_n using

$$\phi_n \sim \frac{1}{2\pi i}\oint_C z^{-n-1}\frac{I_{\gamma\tau}(z)}{1+I_{\gamma\tau}(z)}dz \tag{92}$$

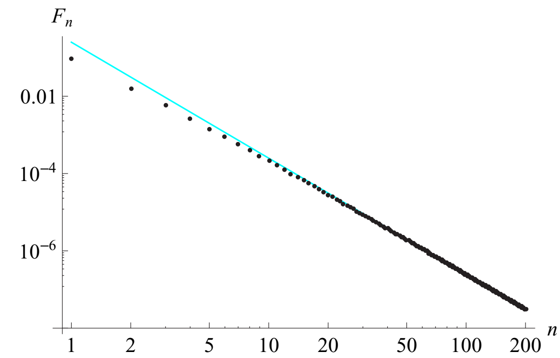

FIG. 6. First detection probability F_n versus n on a log-log plot, for an open system, detection is at the starting point and the sampling rate is $\gamma\tau = \pi/2$. For large n, the exact result (dots) converges to the asymptotic power-law behavior (91), $F_n = |\phi_n|^2 \sim 0.25n^{-3}$ (straight line).

and similar to the previous subsection, the large argument limit of the Bessel function (76) gives

$$\begin{aligned} I_{\gamma\tau}(z) &= \sum_{n=1}^{\infty} z^n \frac{\cos(2\gamma\tau n - \pi/4)}{\sqrt{\pi\gamma\tau n}} \\ &= \frac{1}{2\sqrt{\pi\gamma\tau}}\left[e^{-i\pi/4}\sum_{n=1}\frac{(ze^{2i\gamma\tau})^n}{\sqrt{n}}\right. \\ &\quad \left. + e^{i\pi/4}\sum_{n=1}^{\infty}\frac{(ze^{-2i\gamma\tau})^n}{\sqrt{n}}\right]. \end{aligned} \tag{93}$$

Clearly, for $z = r\exp(i\theta)$ with $\theta = 2\gamma\tau$ or $\theta = -2\gamma\tau$ and $r \geqslant 1$ either the second or first sums diverge, respectively. Thus, for $0 < 2\gamma\tau < 2\pi$ we find two branch cuts which are shown in Fig. 7, with two singular points $z_0 = \exp(\pm 2i\gamma\tau)$. The exception is the case treated in the previous subsection, $2\gamma\tau = \pi$, where the two branch cuts merge. The integration path in the

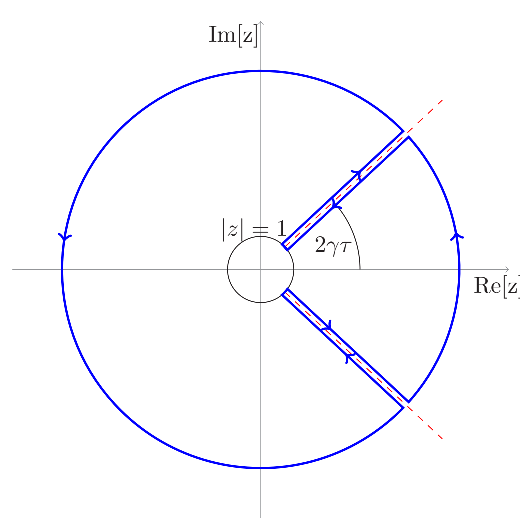

FIG. 7. Integration path for the calculation of ϕ_n in the complex plane bypasses two branch cuts (dashed lines). Integration along four lines just above and below the two dashed lines is explained in the text, while the integration around the outer circle does not contribute in the limit of an infinite radius. When $2\gamma\tau = k\pi$ the two branch cuts merge ($k = 0,1,\ldots$).

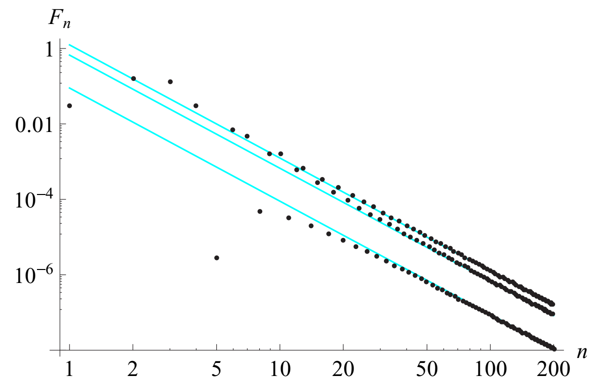

FIG. 8. F_n versus n for the rational sampling time $\gamma\tau/\pi = \frac{1}{3}$. Now, the detection probability F_n decays monotonically like n^{-3} with a superimposed periodic oscillation. The lines are the asymptotic theory (95) which for large n nicely match the exact expression (dots).

complex plane now avoids two branch cuts, but otherwise the calculation is similar to the one we performed in the previous section. In Appendix C, we find one of our main results

$$\phi_n \sim 2\sqrt{\frac{\gamma\tau}{\pi n^3}}\cos\left(2\gamma\tau n + \frac{\pi}{4}\right). \tag{94}$$

Thus, the probability of measuring the quantum walker returning to its origin for the first time is

$$F_n \sim \frac{4\gamma\tau}{\pi n^3}\cos^2\left(2\gamma\tau n + \frac{\pi}{4}\right). \tag{95}$$

This formula predicts that when $\gamma\tau/\pi$ is a rational number, the probability F_n multiplied by n^3 is periodic. Such a behavior is shown in Fig. 8. In contrast, if $\gamma\tau/\pi$ is not rational, the asymptotic behavior is quasiperiodic and appears noisy, the theory (95) perfectly matching the exact solution. This we demonstrate in Fig. 9 for the choice of irrational $\gamma\tau/\pi = 0.8/\pi$.

3. *Critical sampling*

A strange aspect of Eq. (95) is that in the limit of $2\gamma\tau \to \pi$ it does not recover the result found for $2\gamma\tau = \pi$, $F_n \sim 0.25n^{-3}$

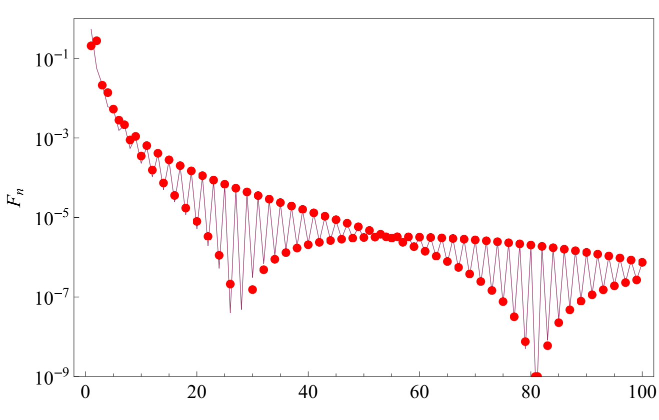

FIG. 9. F_n versus n for the choice of an irrational sampling rate $\gamma\tau/\pi = 0.8/\pi$, for a quantum walk on a one-dimensional lattice (note the log linear scale). The numerically exact solution (red circles) nicely matches the theory (the curve) already for moderate values of n.

found in Eq. (91). Instead, $\lim_{2\gamma\tau\to\pi} F_n \sim n^{-3}$, so a factor 4 mismatch is found. This surprising result is no doubt due to the presence of two branch cuts for the case under study, while for $2\gamma\tau = \pi$ we have only one. This implies that the convergence to formula (95) when $2\gamma\tau \simeq \pi$ is very slow, and is reminiscent of the behavior at the exceptional sampling times we saw for finite L.

These calculations can be extended for $\gamma\tau > 2\pi$ and critical behavior is found for $\gamma\tau = k\pi/2$ with $k = 1,2,\dots$ since then the two branch cuts merge, and one finds $F_n \sim k/(4n^3)$. Otherwise, Eq. (95) is valid for all sampling periods $0 < \gamma\tau$. Note that the energies on a finite tight-binding ring are given by $E_k = -2\gamma\cos(2\pi k/L)$, as mentioned. Hence, in the limit of large L we find a band of energies of size $\Delta E = 4\gamma$. If we use this width in Eq. (58), we find the exceptional sampling time $2\gamma\tau = k\pi$. This argument leads us to speculate that the width of the band, in an infinite system, will determine the exceptional points that survive the $L \to \infty$ limit.

Critical sampling implies that the convergence of the generic formula for $2\gamma\tau$ close to π must be a little funny. Thus, for $2\gamma\tau = 0.95\pi$, we have that at $n = 40$ the ratio of prediction to exact is -2.72 (i.e., even the sign is wrong), whereas for $n = 60$ the ratio is 0.705, for $n = 80$, the ratio is 1.03, at $n = 100$, the ratio is 0.947, and at $n = 120$, the ratio is 0.968, so things are converging, even though even intermediate n's are way off.

D. One-dimensional quantum walks are not recurrent, the survival probability is highly irregular

The probability that the quantum walker will eventually be detected on its origin is given by $1 - S_\infty = \sum_{n=1}^{\infty} F_n$. Here, S_∞ is the probability that the particle survived, namely, the probability that it was not detected. For a one-dimensional (1D) classical random walk on the integers, i.e., the binomial random walk, where the particle has probability $\frac{1}{2}$ to jump left or right, the survival probability is zero, so eventually the particle is detected at its origin. The quantum walk in one dimension is generally nonrecurrent as previously pointed out [9,17]. The spreading is ballistic, not diffusive, and hence the return to the origin is not guaranteed in an open system.

We focus therefore on the nontrivial value of the survival probability S_∞. Using the exact expressions for F_n we have used *Mathematica* to obtain estimation for $1 - S_\infty$ using two methods. The first is summing F_n for a large value of n using the exact expression for F_n. More precisely, we expand the generating function $\hat{\phi}(z)$ in z the coefficients giving ϕ_n up to some large value of n, and hence also F_n. Then, we estimate the reminder using our asymptotic large-n formulas. In the second method we numerically perform the integration in Eq. (27), using Eq. (67). Both methods yield the same results.

In Fig. 10, we show $1 - S_\infty$ versus $\gamma\tau$. For $\gamma\tau \to 0$, we get $S_\infty = 0$ since the particle starting at the origin is detected with probability one if the measurement is made immediately after the release of the particle. Not surprisingly, when $\gamma\tau \to \infty$, $S_\infty \to 0$ (though it remains small though finite for $\gamma\tau \simeq 10$). An unforeseen property is the cusps in $1 - S_\infty$, presented in the figure, found for $\gamma\tau = \pi k/2$ with $k = 1,2,\dots$. Mathematically, these cusps must be related to the appearance of two branch cuts in the complex plane.

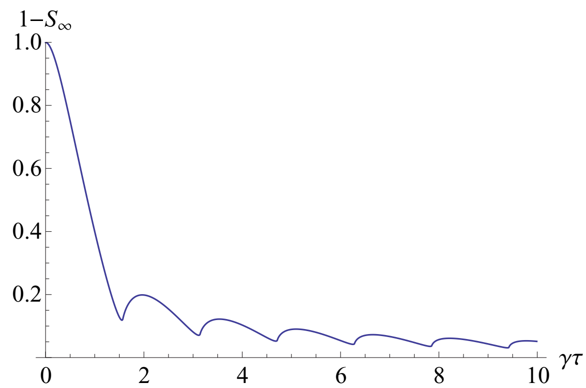

FIG. 10. For the one-dimensional tight-binding quantum walk, the probability that the particle is eventually detected $1 - S_\infty = \sum_{n=1}^{\infty} F_n$ versus the sampling rate $\gamma\tau$ exhibits a nonmonotonic behavior. Unlike its classical random walk counterpart, the quantum walk is not recurrent, unless $\gamma\tau \to 0$, which is the trivial case.

The nonmonotonic behavior of the probability of eventual measurement is not something we could have anticipated.

For large $\gamma\tau$, we find $F_n \propto 1/n$ for finite n and $F_n \propto n^{-3}$ for large n [Eqs. (75) and (95)]. Matching these solutions indicates a transition occurs when $n_{tr} = c(\gamma\tau)$ where c is a constant of order unity. We may estimate the probability of detection as $\sum_{n=1}^{n_{tr}} F_n$. Here, we do not sum in the interval (n_{tr},∞) since here F_n decays like n^{-3} and hence is negligible. Using Eq. (75), switching from summation to integration, we find

$$1 - S_\infty \simeq \frac{\ln \gamma\tau}{2\pi\gamma\tau} \tag{96}$$

when $\gamma\tau \gg 1$. In this rough estimation, we used $\ln\gamma\tau \gg \ln c$. Further discussion on S_∞ and a far better approximation is provided in Appendix D.

E. Transition to large system

For a large but finite ring of size L we expect to see, for intermediate times, a behavior similar to the infinite system, where on the one hand the asymptotic limit (95) is reached, but the particle still does not sense the finiteness of the system. This behavior is presented in Fig. 11 for a ring with $L = 100$ sites. At first F_n decays as for the infinite system with the same sampling rate (see Fig. 12). However, at least in this example, roughly at $n \simeq 70$ we see a sudden increase in F_n. This is a nonclassical behavior; for a classical random walk on a large ring the survival probability has a power-law decay for intermediate times, crossing over to an exponential decay for long times. The significant increase in F_n is due to a partial revival at the origin, a nonclassical effect, and is obviously related to the ballistic nature of the quantum walk. The precise nature of this transition merits further study.

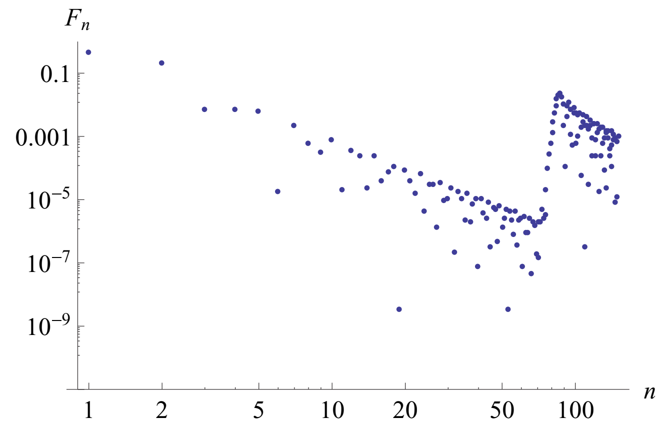

FIG. 11. Quantum walk on a ring with $L = 100$ sites for a sampling rate $\gamma\tau = 0.6$ with detection at the origin of the walk. For small n, the system exhibits a behavior similar to that of an infinite system (see Fig. 12). Roughly at $n = 70$, there is a sudden increase in F_n, probably due to a partial revival of the packet at the origin.

VII. OTHER APPROACHES AND SOME CONNECTIONS

Krovi and Brun [18,19] derived a general expression for the average hitting time $\langle n\rangle$ for discrete quantum walks. Their formalism is based on a trace formula for a density matrix, while we relate the statistics of the first detection event to the wave function free of measurements. They also point out the possibility of infinite average hitting times on finite graphs. This theme is important in the context of the efficiency of search. A classical random walker, on a finite graph, always finds the target (assuming the walk is ergodic). In that sense, a classical walk is very efficient since it will always reach its target. On the other hand, a classical walk tends to explore territory previously visited, so the time it takes to reach the target is relatively long. Quantum walks are considered faster, if compared to classical walks, in the sense that they scale ballistically. However, as we showed for the simple benzene ring geometry, the average hitting time (for specific initial conditions) may diverge. It implies that one cannot categorically say that quantum search, in the average hitting time sense, is more efficient than the classical counterpart. Further, we have found the so called half dark states, namely, certain initial conditions where the particle is eventually detected only with probability $\frac{1}{2}$ even on a small graph like a benzene ring. For the ring geometry, and for initial condition on the origin, Eq. (57) shows that the average $\langle n\rangle$ scales with the size of system, which is the same as the classical search, as mentioned. It should be noted that

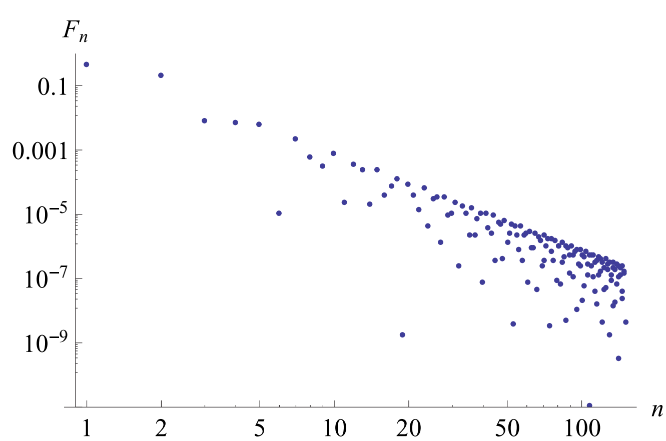

FIG. 12. Same as Fig. 11 for an infinite system.

diverging $\langle n \rangle$ for finite systems and half dark states are found here for the stroboscopic measurement under investigation. The latter has many advantages, for example, in revealing quantum periodicities, but if the goal is to detect the particle with probability one, measurements on random times drawn from a Poisson process could be more efficient [20].

As mentioned in the Introduction, the quantum first passage time question has been controversial in the sense that many conflicting approaches to the problem have been suggested. One way to treat the quantum first passage time problem is by adding a non-Hermitian term to the Hamiltonian [36]. Briefly, the non-Hermitian approach leads to the nonconservation of the normalization of the wave function, which can be interpreted as the survival probability of the particle. This approach was shown to be related to the projective measurement method in the limit of small finite τ [21,22]. It is an interesting question, however, as to whether the non-Hermitian approach can predict the behaviors found in this paper, for example, Eq. (95). Especially important is whether the limits of large n and small τ commute, an issue left to future research.

Dhar *et al.* [21,22], after laying the general framework to the problem, including introducing the fundamental concept of the wave function ϕ_n, investigated the limit of small τ. In this sense, the problem is investigated close to the Zeno limit. The stroboscopic sampling for finite τ investigated herein allows for revivals, critical sampling, and other special quantum effects which are clearly missed in this Zeno limit. They [21,22] use a perturbation theory and derive an effective Hamiltonian where the effects of the failed prior detections are included as a non-Hermitian part of the Hamiltonian. That method together with numerical simulations predicts, for a specific initial condition and a finite sized system, with infinite walls at the edges, that the survival probability has a power-law decay of $-\frac{1}{2}$ or $-\frac{3}{2}$. This is an interesting observation since it shows that in some cases half integer exponents control the decay of the survival probability, while so far we have found only integer values. We have verified the main qualitative findings of Dhar *et al.* using both the generating function and, alternatively, the recursion relation (17) (not shown), in particular the $n^{-3/2}$ of $1 - S_n$ when the initial and measurement sites are at opposite ends of the system and a $n^{-1/2}$ decay when the initial site is at the center of the system and the measurements are performed at one end. We find oscillations to be superimposed on these decays. The presence of these new exponents which are not reflected in the 0-0 infinite chain case we studied herein clearly merits further study, but indicates that the geometry plays a crucial role.

Another approach suggests the use of the classical renewal equation, derived by Schrödinger [6] long before the appearance of wave mechanics in the context of the first passage time of a Brownian motion, to investigate also the quantum first passage time problem [32,37]. This approach seems very different than ours since it does not take into consideration the effect of measurement, and it uses probabilities instead of amplitudes to describe the quantum statistical aspects of the first passage problem.

In [34], a discarding system method was used for the problem of recurrence of quantum walks. These authors investigated an ensemble of identically prepared systems and suggested the following measurement procedure. After one time step measure the occupancy of the particle at the origin (the outcome is a binary yes or no answer) and then discard the system. Take a second identically prepared second system and let it evolve for two time steps, measure at the origin, and again discard the system. Continue similarly for a long time. One then constructs the probability of measurement at the origin, for times $t = 1,2,\dots$. In this way, one may define a Pôlya number, which in classical random walks gives the criterion whether a random walk is transient or recurrent. This approach is of course very different than ours. As pointed out in Ref. [34], one can imagine several approaches to the problem of recurrence of a quantum random walker.

Historical remark. Equation (10) in Ref. [15] is the renewal equation for classical random walks after which the author writes: "The equation was proposed by Schrödinger in terms of cumulative probabilities." A minor historical remark is that a close look at the original publication [6] does not reveal an explicit equation. However, translating the original work to English reveals that indeed the origin of the renewal equation is in that classic paper. In Appendix B of [15], Muga and Leavens mention a quantum renewal equation; their conclusion is that this equation (which is not at all related to ours) is not valid.

VIII. SUMMARY

The quantum first detected passage time problem rests on two fundamental postulates of quantum reality. The first is the Schrödinger equation and the second is the projective measurement postulate. The latter is the fifth postulate listed in [13] which states that immediately after the measurement, the state of the system is a normalized projection of $|\psi\rangle$, where $|\psi\rangle$ is the state function of the system just prior to the measurement. Without these assumptions, the first tested in many experiments but the second in far fewer, quantum theory is not complete. Our goal, following [21], was not to question basic physical assumptions, but rather to show how these postulates lead to the solution of the first detection problem.

The quantum renewal equation (17) and the Z transforms equations (23), (36), and (37) give a rather general relation between the amplitude of first detection ϕ_n and the wave function of the system free of measurement $|\psi_f\rangle$. In that sense, the problem of first detection reduces to the solution of the Schrödinger equation, e.g., the determination of the energy spectrum. In particular, similar to the corresponding classical first passage problems, the generating function is a powerful tool with which we can attain many insights.

We have illustrated several surprising features, both for closed systems, i.e., rings, and for open systems. Generally, the quantum first detection problem exhibits behaviors very different than classical, but still some relations remain. For example, for a classical random walk on an infinite line, the first passage PDF decays like $n^{-3/2}$, similarly the corresponding quantum amplitude (neglecting the oscillations) gives $\phi_n \sim n^{-3/2}$ [see Eqs. (91) and (94)]. However, the quantum problem exhibits rich behaviors, which are related to the sampling rate $\gamma\tau$, including oscillations of F_n superimposed on the power-law decay, the Zeno effect when $\tau \to 0$ and a surprising critical behavior when $\gamma\tau = k\pi/2$. Critical slowing down, namely ultraslow convergence, is found when the sampling time τ times the energy band is equal to multiples of 2π. Thus, the first detection problem is critically sensitive to the sampling rate even for an infinite system and even in the large-n limit. Of course, for real systems this conclusion can be reached only if the coherence is maintained for long times. Another notable result is the nonanalytical behavior of the survival probability S_∞ as we tune $\gamma\tau$ (see Fig. 10). This should be compared with the classical result where the final probability of detecting the particle in one dimension is unity.

For a finite system like a ring, we find strong sensitivity to the initial condition: for an initial condition starting on the origin $x = 0$, which is also the detected site, the average number of measurements until detection $\langle n\rangle$ increases linearly with the system size L [see Eq. (57)]. Furthermore, $\langle n\rangle$ does not depend on the sampling time τ, aside from ever present exceptional sampling [see Eq. (58)]. Since $\langle n\rangle \propto L$, we find essentially classical behavior for the average and for this particular initial condition [the quantum effects are observed in the variance (50)].

However, when starting at other sites, $\langle n\rangle$ depends crucially on the sampling time τ, and in fact $\langle n\rangle$ may diverge as τ is tuned. The revivals, optimal detection times, exceptional points given by the simple formula (58), half dark states, quantization of $\langle n\rangle$ for the $|0\rangle \to |0\rangle$ transition [25], unbounded fluctuation of $\bar{n}$ (Fig. 3) describe rich behaviors even in small systems. They also point out the advantage of stroboscopic observation of the system since this captures underlying quantum features. Even for a finite sized system, the probability of being eventually detected is not always unity. However, we showed that at least when starting on the origin which is also the location of the detection, the particle is detected with probability unity for any sampling time τ, and in that sense the quantum walk on a finite ring or more generally a graph [25] is recurrent. Finally, the tools developed in this paper can serve as a starting point for many other first detection problems and the advance of single particle first detection theory.

ACKNOWLEDGMENTS

We thank the Israel Science Foundation, Grant No. 376/12, for funding and J. Asboth for pointing out Ref. [25]. E.B. thanks A. Dhar for discussions and hospitality at the ICTS Campus in Bangalore.

APPENDIX A: ITERATIONS, GENERAL MEASUREMENTS

In this Appendix, we present the details of the derivation of our general formulation.

1. Derivation of ϕ_n, $\hat{\phi}(z)$

We here show by induction that

$$|\theta_n\rangle = [U(\tau)(1-\hat{D})]^{n-1}U(\tau)|\psi(0)\rangle \tag{A1}$$

is identical to

$$|\theta_n\rangle = U(n\tau)|\psi(0)\rangle - \sum_{k=1}^{n-1} U[(n-k)\tau]\hat{D}|\theta_k\rangle. \tag{A2}$$

The case $n = 1$ can be easily verified since both equations give $|\theta_1\rangle = U(\tau)|\psi(0)\rangle$. We now argue by induction, assuming the validity of Eq. (A2) for some n, and proving it for $n + 1$. As can be seen from Eq. (A1), the effective waveform is propagated between measurements

$$\begin{aligned}|\theta_{n+1}\rangle &= U(\tau)(1-\hat{D})|\theta_n\rangle \\ &= U(\tau)U(n\tau)|\psi(0)\rangle \\ &\quad - \sum_{k=1}^{n-1} U[(n+1-k)\tau]\hat{D}|\theta_k\rangle - U(\tau)\hat{D}|\theta_n\rangle \\ &= U[(n+1)\tau]|\psi(0)\rangle - \sum_{k=1}^{n+1-1} U[(n+1-k)\tau]\hat{D}|\theta_k\rangle.\end{aligned} \tag{A3}$$

This is of course the same as Eq. (A2) but for $n + 1$, hence, the proof is completed.

The Z transform of Eq. (A2) gives a closed formula for $|\theta(z)\rangle = \sum_{n=1}^{\infty} z^n|\theta_n\rangle$. Using the convolution theorem, we find

$$|\theta(z)\rangle = [1 + U(z)\hat{D}]^{-1}U(z)|\psi(0)\rangle. \tag{A4}$$

For a single detected site at 0 ($\hat{D} = |0\rangle\langle 0|$) and denoting $\phi_n = \langle 0|\theta_n\rangle$, Eqs. (A2) and (A4) can be represented as

$$\begin{aligned}\phi_n &= \langle 0|U(n\tau)|\psi(0)\rangle - \sum_{k=1}^{n-1}\langle 0|U[(n-k)\tau]|0\rangle\phi_k, \\ \hat{\phi}(z) &= \frac{\langle 0|U(z)|\psi(0)\rangle}{1+\langle 0|U(z)|0\rangle},\end{aligned} \tag{A5}$$

respectively, as it is stated in the text.

2. General measurements

We consider the first detection measurement of an observable whose corresponding bra is $\langle\mathcal{O}|$ with the additional condition $\langle\mathcal{O}|\mathcal{O}\rangle = 1$ so $\sum_{x\in X}\langle x|$ is not such a measurement if the set X has more then one element, but $\langle x|$ or $\langle E_m|$, denoting an energy state of the system, are. For example, we select a specific energy level denoted E_m and ask what is the statistics of first detection time of that state, so here $\langle\mathcal{O}| = \langle E_m|$ (the subscript m is for measurement). The energy states are assumed to be nondegenerate for simplicity. The generating function in this case is

$$\hat{\phi}(z) = \frac{\langle\mathcal{O}|\hat{U}(z)|\text{initial}\rangle}{1+\langle\mathcal{O}|\hat{U}(z)|\mathcal{O}\rangle}. \tag{A6}$$

Here, the state $\langle\mathcal{O}|$ is not only normalized but it must be an eigenstate of a Hermitian operator, in such a way that it describes a physical measurement. For example, consider the case where the initial state is a stationary state of the Hamiltonian $|E_i\rangle$ and the observable state is $|\mathcal{O}\rangle = |E_m\rangle$. Then, the assumption that the Hamiltonian is time independent means that

$$\langle E_m|\hat{U}(z)|E_i\rangle = [z^{-1}\exp(iE_m\tau) - 1]^{-1}\delta_{mi}, \tag{A7}$$

where δ_{mi} is the delta of Kronecker, we find

$$\hat{\phi}(z) = ze^{-iE_m\tau}\delta_{mi}. \tag{A8}$$

This is the expected result, if we start with a stationary state i this state will be detected with probability one only if $m = i$. More than one measurement is actually not informative in this case, hence, $\phi_n = 0$ for $n > 1$ (this is easily understood since the generating function contains a single term linear in z when $m = i$).

It is emphasized again that the measurement is different from the standard textbook measurement that asks what is the energy of the system at a certain time (say τ). In our case, the measurement performed gives a binary answer either yes or no, and this gives a definitive answer to the question whether the system is in the mth state at times $\tau, 2\tau \ldots$.

APPENDIX B: ANALYTIC CALCULATIONS OF MOMENTS OF F_n FOR A L-SITE RING

1. 0 → 0

We start with the problem where the particle is both released from and detected at the origin. There is a simple proof that $\mathcal{F} \equiv \sum_n F_n = 1 - S_\infty = 1$. Equation (61) gives

$$\hat{\phi}(z) = \frac{\sum_{k=0}^{L-1} \bar{n}_k}{L + \sum_{k=0}^{L-1} \bar{n}_k}. \tag{B1}$$

Now, for $z = e^{i\theta}$,

$$\bar{n}_k = \frac{1}{e^{i(\tau E_k - \theta)} - 1} = \frac{\cos(\tau E_k - \theta) - 1 - i\sin(\tau E_k - \theta)}{2 - 2\cos(\tau E_k - \theta)}$$
$$= -\frac{1}{2} - \frac{i}{2}\cot\frac{\tau E_k - \theta}{2}. \tag{B2}$$

Thus, on the unit circle, $z = e^{i\theta}$, $\hat{\phi}(z)$ has the form

$$\hat{\phi}(e^{i\theta}) = \frac{-L/2 + iA}{L/2 + iA}, \tag{B3}$$

where A is real. Thus, $|\hat{\phi}(e^{i\theta})|^2 = 1$, and so, using Eq. (27),

$$\mathcal{F} = \sum_n F_n = \int_0^{2\pi} \frac{d\theta}{2\pi} |\hat{\phi}(e^{i\theta})|^2 = 1 \tag{B4}$$

and the particle is detected with probability unity.

For z off the unit circle, $\hat{\phi}(z)$ can be written as a rational function of z, that is to say, the quotient of two polynomials. In fact, we have

$$\hat{\phi}(z) = \frac{\mathcal{N}(z)}{\mathcal{D}(z)}. \tag{B5}$$

The exact forms of the numerator and denominator depend on whether L is even or odd since in the former case we have $K = L/2 + 1$ different E_j's, of which all but two are doubly degenerate, whereas in the latter case we have $K = (L+1)/2$ E_j's, all but one of which are doubly degenerate. We treat the L odd case in detail, the even case being similar.

Note that we do not need in the following the specific values of the energies for the different states, so we absorb τ into the energies for efficiency. In particular, using Eq. (B1),

$$\mathcal{N}(z) = \left[\prod_{i=0}^{K-1}(e^{iE_i} - z)\right] \sum_{j=0}^{K-1} \frac{d_j z}{e^{iE_j} - z};$$
$$\mathcal{D}(z) = \left[\prod_{i=0}^{K-1}(e^{iE_i} - z)\right]\left[L + \sum_{j=0}^{K-1} \frac{d_j z}{e^{iE_j} - z}\right]. \tag{B6}$$

Here, d_j is the degeneracy of the jth energy level, so that $d_0 = 1$ and otherwise $d_j = 2$. The denominator is a polynomial of degree $K-1$ since the z^K term cancels out, while the numerator is of degree K, and has no z^0 term. For the moment, we treat $\mathcal{N}(z)$ and $\mathcal{D}(z)$ as two order K polynomials in z defined by Eq. (B6). The two polynomials both have complex coefficients, each depending on the same set of real numbers $\{E_0, \ldots, E_{K-1}\}$. What we want to show is that the two polynomials are related, for arbitrary K, by the relation

$$\mathcal{D}_K(z) = (-1)^{K-1} e^{i\sum_j E_j} z^K \mathcal{N}_K^*(1/z), \tag{B7}$$

where we have made explicit the dependence of the polynomials on K, and have left implicit the dependence on the set of numbers $\{E_j\}$, $j = 0, \ldots, K-1$. The polynomial $\mathcal{N}^*$ is the polynomial with coefficients conjugate to those of $\mathcal{N}$. Equivalently, this is the polynomial with all the $\{E_j\}$ replaced by $\{-E_j\}$. For example, for $K = 1$,

$$\mathcal{N}_1(z) = z; \quad \mathcal{D}_1(z) = (e^{iE_0} - z) + z = e^{iE_0}, \tag{B8}$$

which clearly obey the relation (B7), for arbitrary real E_0. We will now prove Eq. (B6) by induction. We start by noting the most of the terms in $\mathcal{N}_K$ and $\mathcal{D}_K$ also appear in $\mathcal{N}_{K-1}$, $\mathcal{D}_{K-1}$ with the set of energies $\{E_j\}$, $j = 0, \ldots, K-2$. We have

$$\mathcal{N}_K(z) = (e^{iE_{K-1}} - z)\mathcal{N}_{K-1}(z) + 2z\prod_{i=0}^{K-2}(e^{iE_i} - z);$$
$$\mathcal{D}_K(z) = (e^{iE_{K-1}} - z)\mathcal{D}_{K-1}(z) + 2\prod_{j=0}^{K-1}(e^{iE_j} - z) + 2z\prod_{i=0}^{K-2}(e^{iE_i} - z)$$
$$= (e^{iE_{K-1}} - z)\mathcal{D}_{K-1}(z) + 2e^{iE_{K-1}}\prod_{j=0}^{K-2}(e^{iE_j} - z). \tag{B9}$$

We can now use the induction hypothesis, assuming Eq. (B7) is valid for $K-1$, to rewrite the first line of Eq. (B9):

$$(-1)^{K-1} z^K e^{i\sum_j E_j}\mathcal{N}_K^*(1/z) = (-1)^{K-1} z^K e^{i\sum_j E_j}\left[(e^{-iE_{K-1}} - 1/z)\mathcal{N}_{K-1}^*(z) + (2/z)\prod_{i=0}^{K-2}(e^{-iE_i} - 1/z)\right]$$
$$= -ze^{iE_{K-1}}(e^{-iE_{K-1}} - 1/z)\mathcal{D}_{K-1}(z) + 2ze^{iE_{K-1}}\prod_{i=0}^{K-2}(e^{iE_i} - z)$$
$$= (e^{iE_{K-1}} - z)\mathcal{D}_{K-1}(z) + 2e^{iE_{K-1}}\prod_{i=0}^{K-2}(e^{iE_i} - z) = \mathcal{D}_K(z), \tag{B10}$$

where we have invoked the last line of Eq. (B9) in the final step. This completes the induction proof.

As an immediate corollary, we obtain

$$\hat{\phi}^*(1/z)\hat{\phi}(z) = \frac{\mathcal{N}^*(1/z)}{\mathcal{D}^*(1/z)} \times \frac{\mathcal{N}(z)}{\mathcal{D}(z)} = 1, \tag{B11}$$

which implies $|\hat{\phi}(e^{i\theta})|^2 = 1$, which we previously obtained.

An alternative route to prove Eq. (B7) is to use Eq. (B6) and write

$$\mathcal{N}(z) = \sum_{j=0}^{K-1} d_j z \prod_{\substack{i=0\\ i\neq j}}^{K-1} (e^{iE_i} - z) \tag{B12}$$

and so

$$\begin{aligned}\mathcal{D}(z) &= L\prod_{i=0}^{K-1}(e^{iE_i} - z) + \mathcal{N}(z)\\ &= L\prod_{i=0}^{K-1}(e^{iE_i} - z) + \sum_{j=0}^{K-1} d_j[(z - e^{iE_j})\\ &\quad + e^{iE_j}]\prod_{\substack{i=0\\ i\neq j}}^{K-1}(e^{iE_i} - z).\end{aligned} \tag{B13}$$

Clearly,

$$\sum_{j=0}^{K-1} d_j(z - e^{iE_j})\prod_{\substack{i=0\\ i\neq j}}^{K-1}(e^{iE_i} - z) = -\left(\sum_{j=0}^{K-1} d_j\right)\prod_{i=0}^{K-1}(e^{iE_i} - z), \tag{B14}$$

and using $\sum_{j=0}^{K-1} d_j = L$ we find

$$\mathcal{D}(z) = \sum_{j=0}^{K-1} d_j e^{iE_j}\prod_{\substack{i=0\\ i\neq j}}^{K-1}(e^{iE_i} - z). \tag{B15}$$

Thus, $\mathcal{D}(z)$ is the same as $\mathcal{N}(z)$ when the replacement $d_j z \to d_j \exp(iE_j)$ is made. It is now easy to verify the theorem (B7).

This factorization of $\hat{\phi}(z)$ allows for a simple calculation of $\langle n\rangle$, the mean detection time. The one added piece of information we require is the location of the zeros of $\mathcal{D}$. It is clear that all these zeros lie outside the unit circle, as otherwise, S_∞ would diverge. For large n, ϕ_n decays geometrically as r^{-n}, where r is the absolute value of the radius of the pole nearest to the origin. For the sum of $|\phi_n|^2$ to converge, we must have $r > 1$. There is one exception to this rule. It turns out that for a discrete set of exceptional values of $\gamma\tau$, one (or in the case of even L, a complex conjugate pair) zero hits the unit circle. Given the relationship between the numerator $\mathcal{N}$ and the denominator $\mathcal{D}$, a zero of $\mathcal{N}$ must hit the unit circle and coincide with the zero of $\mathcal{D}$ at the exceptional point. In this case, there is no pole in $\hat{\phi}(z)$ at this point, and all poles of $\hat{\phi}(z)$ still lie strictly outside the unit circle. We will return to the identification of these exceptional values of $\gamma\tau$ in a moment, but let us first proceed and calculate $\langle n\rangle$ for a nonexceptional $\gamma\tau$. Given our theorem (B7) relating $\mathcal{N}$ and $\mathcal{D}$, we have

$$\hat{\phi}(z) = ze^{-i\sum_j E_j}\prod_{i=0}^{K-1}\frac{z - 1/z_i^*}{(z - z_i)/z_i}, \tag{B16}$$

where, as before $K = (L+1)/2$ for L odd and $L/2 + 1$ for K even, and the z_i are the zeros of $\mathcal{D}(z)$. Then,

$$\hat{\phi}^*(1/z)\frac{d}{dz}\hat{\phi}(z) = \frac{1}{z} + \sum_{i=1}^{K-1}\left[\frac{1}{z - 1/z_i^*} - \frac{1}{z - z_i}\right]. \tag{B17}$$

We have to integrate this over the unit circle, which by the residue theorem picks up a contribution of $2\pi i$ for each pole in the interior, which lie at 0 and $1/z_i^*$. Thus, as long as we are not dealing with an exceptional point, we have

$$\langle n\rangle = K. \tag{B18}$$

This agrees with explicit numerical calculations for $L = 5,6$. If the exceptional point is such that a single pole touches the unit circle (a real pole for even L or a complex one for odd L), then $\langle n\rangle$ is reduced by one. If the exceptional point is such that a complex conjugate pair touch the unit circle, $\langle n\rangle$ is reduced by two at this value of $\gamma\tau$.

2. Exceptional τ

For z on the unit circle, we may write $z = e^{i\theta}$. Studying the structure of $\mathcal{D}$, it is clear that one way to make $\mathcal{D}$ vanish is to require that two of the factors $e^{iE_k} - z$ are zero, in which case every individual term in $\mathcal{D}$ vanishes separately. In other words, we have, for a pair of energies $E_j < E_k$,

$$\theta = E_j\tau + 2\pi n_j = E_k\tau + 2\pi n_k, \tag{B19}$$

for two integers n_j, n_k. This gives us

$$\tau = 2\pi n_{jk}/(E_k - E_j); \quad \theta = \mathrm{mod}(E_j\tau, 2\pi) \tag{B20}$$

for an integer n_{jk}. Thus, for each pair j,k, there are an infinite number of exceptional values of τ. For $L = 6$, for example, we have $\langle n\rangle = 4$ for nonexceptional points. As the energy levels in this case are $\{-2\gamma, -\gamma, \gamma, 2\gamma\}$, we have an exceptional $\tau = \theta = 0$, with degeneracy 3, so $\langle n\rangle$ is reduced by 3. A second exceptional value is $\gamma\tau = \pi/2, \theta = \pi$, which comes from the pair $\{E_0, E_3\}$ with degeneracy 1. We also have $\gamma\tau = \pi, \theta = \pi$, coming both from the pair $\{E_0, E_3\}$ with $n_{jk} = 2$ and also from $\{E_1, E_2\}$ so that this root has degeneracy 2. In addition, we have $\gamma\tau = 2\pi/3$, with $\theta = 2\pi/3$, $4\pi/3$, coming from $\{E_0, E_2\}$ and $\{E_1, E_3\}$, respectively, so that $\langle n\rangle$ is again reduced by 2.

3. $L = 6, 3 \to 0$

Unfortunately, there does not appear to be any such miracle occurring for the $L = 6$ ring when the particle starts at 3 and we detect at 0, the $3 \to 0$ transition. Again, $\hat{\phi}(z)$ can be written as a rational polynomial, but we have not found any simple relationship between the numerator and denominator. Nevertheless, we can still compute the moments of n. We start by factoring $\mathcal{D}$,

$$\hat{\phi}(z) = i\frac{z\hat{\mathcal{N}}(z)}{\mathcal{D}(z)} = -i\frac{z\hat{\mathcal{N}}(z)}{D_0(z - z_1)(z - z_2)(z - z_3)}, \tag{B21}$$

where we have also factored out z and a phase from the numerator, such that $\hat{\mathcal{N}}$ has real coefficients. In particular,

$$\mathcal{N}(z) = 8\,\sin(\gamma\tau)\sin^2(\gamma\tau/2)[1+2z\cos(\gamma\tau)+z^2];$$
$$\mathcal{D}(z) = -2[z^3\{2\cos[\gamma\tau)+\cos(2\gamma\tau)] - 3z^2[1+\cos(\gamma\tau)+\cos(3\gamma\tau)] + z[4\cos(\gamma\tau)+5\cos(2\gamma\tau)]-3\}. \quad \text{(B22)}$$

Given this, we have

$$\mathcal{F} \equiv 1 - S_0 = \oint \frac{dz}{2\pi i z}\hat{\phi}^*(1/z)\hat{\phi}(z) = \oint \frac{dz}{2\pi i}\frac{\hat{\mathcal{N}}(1/z)\hat{\mathcal{N}}(z)}{D_0^2\prod_i[(z-z_i)(z-1/z_i)]}. \quad \text{(B23)}$$

We can formally do the contour integral, picking up the residues at the three poles inside the unit circle, namely, $1/z_i$, $i=1,\ldots,3$. The result can be written as the ratio of polynomials in the three values z_i. The key here is that both polynomials are *symmetric* under permutations of the three z_i's. Therefore, by the fundamental theorem of symmetric polynomials [52] (p. 90), each can be expressed uniquely in terms of the three elementary symmetric polynomials, $s_1 = z_1+z_2+z_3$, $s_2 = z_1z_2+z_1z_3+z_2z_3$, and $s_3 = z_1z_2z_3$. These three elementary polynomials are, however, simply related to the coefficients of the polynomial $\mathcal{D}$:

$$s_1 = 3[1+\cos(\gamma\tau)+\cos(3\gamma\tau)]/D_0;$$
$$s_2 = -[4\cos(\gamma\tau)+5\cos(2\gamma\tau)]/D_0;$$
$$s_3 = -3/D_0, \quad \text{(B24)}$$

where

$$D_0 = -2[2\cos(\gamma\tau)+\cos(2\gamma\tau)] \quad \text{(B25)}$$

is the coefficient of the z^3 term in $\mathcal{D}$. Performing these substitutions (via the command SymmetricReduction in *Mathematica*) in the numerator and denominator and, simplifying, we find $\mathcal{F}=1$ so the survival is zero $S_0=0$. This equation holds at all but the exceptional points, which do not have three poles in $\hat{\phi}(z)$ due to the collision of a pole (or pair of conjugate poles) with the zeros of $\mathcal{N}$ on the unit circle, leaving these cases to be examined individually. Since $\mathcal{D}$ does not depend on the initial condition, the set of exceptional points is the same as for the $0\to 0$ transition.

This same general procedure works for the calculation of $\langle n\rangle$ as well, since again we only have the simple poles from $\mathcal{D}(1/z)$ to contend with, again giving three contributions. The result of this exercise is as given in the main text.

4. $L = 6, 1 \to 0$

The same general procedure can be applied to the calculation of $\mathcal{F}$ for the 1 to 0 or 2 to 0 transitions, and gives $\mathcal{F}=\frac{1}{2}$ at all but the exceptional points, which again have to be handled separately.

APPENDIX C: CALCULATING THE INTEGRAL (92)

The integration path in Eq. (92) is shown in Fig. 7 and since the integration along the outer zone $|z|\to\infty$ does not contribute, we need to consider four integration segments, which are at a distance ϵ above and below the two branch cuts. We distinguish these four paths with indices σ and β that get values ± 1. σ is an indicator for the branch cut, $\sigma=+1$ represents the upper branch cut (see Fig. 7), and $\sigma=-1$ the lower one. The index β is for the direction of integration, $\beta=+1$ for outward integration in the radial direction while $\beta=-1$ is for inward integration (see Fig. 7). In the complex plane, the parametrization of the four paths is

$$z(y) = (1+y+i\epsilon\beta)e^{2i\sigma\gamma\tau}, \quad 0<y<\infty \quad \epsilon\to 0^+. \quad \text{(C1)}$$

Along these paths it is easy to show that

$$I_{\gamma\tau}[z(y)] = \frac{1}{2\sqrt{\pi\gamma\tau}}\{e^{-i\sigma\pi/4}\mathrm{Li}_{1/2}[(1+y+i\epsilon\beta)e^{4i\sigma\gamma\tau}] + e^{i\pi\sigma/4}\mathrm{Li}_{1/2}(1+y+i\epsilon\beta)\}. \quad \text{(C2)}$$

In the integration we consider the small-y limit corresponding to large n using Eq. (84) along the four paths. The second term in Eq. (C2) $\mathrm{Li}_{1/2}(1+y+i\epsilon\beta)\simeq\beta i\sqrt{\pi/y}$ is the large term and we get

$$\lim_{\epsilon\to 0} I_{\gamma\tau}[z(y)] \sim \frac{i\beta e^{i\pi\sigma/4}}{2\sqrt{\gamma\tau y}}. \quad \text{(C3)}$$

The generating function is given by

$$\hat{\phi}[z(y)] \sim 1 - \frac{1}{I_{\gamma\tau}[z(y)]} \sim 1 + 2i\beta e^{-i\pi\sigma/4}\sqrt{\gamma\tau y}. \quad \text{(C4)}$$

Integrating along the four lines, taking into consideration the clockwise direction of the integration we find

$$\phi_n = \sum_{\beta=\pm,\sigma=\pm}\frac{\beta\mathcal{I}_{\sigma\beta}}{2\pi i}, \quad \text{(C5)}$$

where

$$\mathcal{I}_{\sigma\beta} \sim \int_0^\infty \underbrace{\exp\{-(1+n)\ln[(1+y+i\epsilon\beta)e^{i2\sigma\gamma\tau}]\}}_{z(y)^{-n-1}} \times \underbrace{(1+2i\beta e^{-i\sigma\pi/4}\sqrt{\gamma\tau y})}_{\sim\hat{\phi}[z(y)]}\underbrace{e^{2i\sigma\gamma\tau}dy}_{dz}. \quad \text{(C6)}$$

In the limit $\epsilon\to 0$ the integration gives

$$\mathcal{I}_{\sigma\beta} \sim e^{-2in\sigma\gamma\tau}\left(\frac{1}{n} + i\beta e^{-i\sigma\pi/4}\sqrt{\frac{\pi\gamma\tau}{n^3}}\right), \quad \text{(C7)}$$

where we used $(1+n)\ln(1+y)\sim ny$ since n is large and $\int_0^\infty\sqrt{y}\exp(-yn)\mathrm{d}y = n^{-3/2}\sqrt{\pi}/2$. Using Eq. (C5) we find Eq. (94).

APPENDIX D: SURVIVAL PROBABILITY FOR A PARTICLE ON A LINE

We presented the final detection probability $1-S_\infty$ in Fig. 10 for a particle starting on the origin of an infinite line.

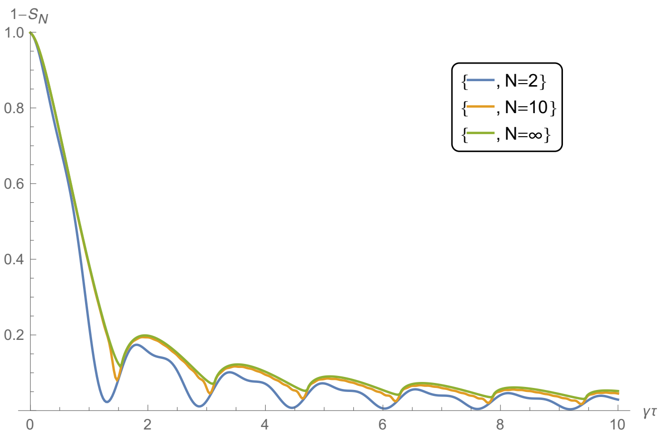

FIG. 13. $1 - S_N$ versus $\gamma\tau$ for a quantum walk on a line, the particle is launched from the origin.

Here, we discuss briefly approximations for this probability. A simple approximation is to consider the finite sum

$$1 - S_N = \sum_{n=1}^{N} F_n. \tag{D1}$$

The values of F_n are taken from Table II. As shown in Fig. 13, already for $N = 2$ the general features, i.e., nonmonotonic decay of $1 - S_\infty$ and periodic minima as τ is varied, are clearly observed. This approximation works very well already for $N = 10$. This shows that the small-n behavior of F_n controls the final survival probability.

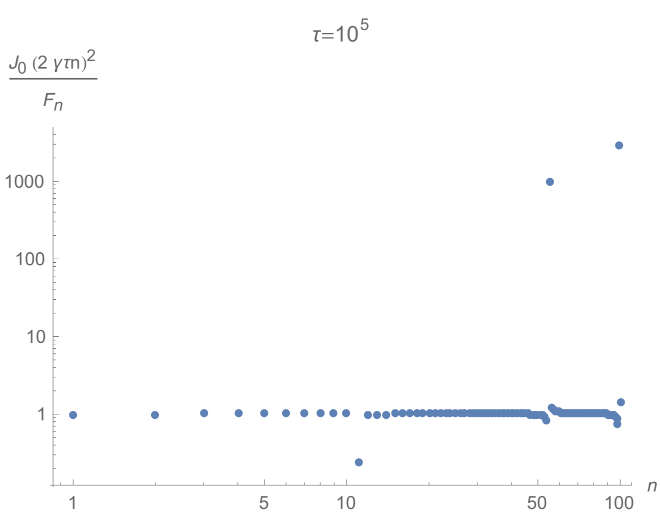

FIG. 14. The ratio $J_0(2n\gamma\tau)^2/F_n$ for $\gamma\tau = 10^5$.

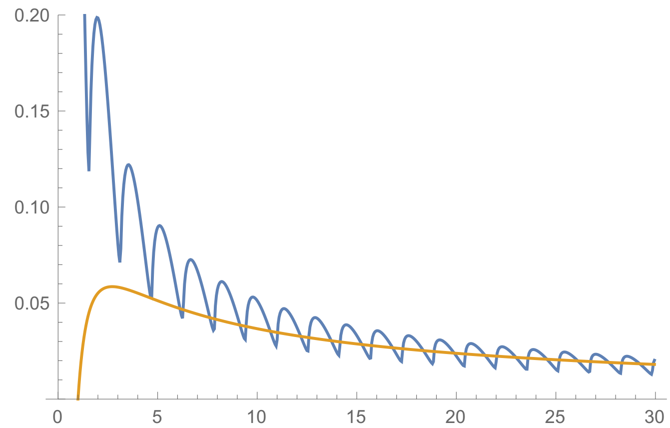

FIG. 15. $1 - S_\infty$ versus $\gamma\tau$. The approximation (96) is compared with the exact result, and it works reasonably well for large $\gamma\tau$, as expected. However, it does not predict the spiky cusps or the nonmonotonic behavior of $1 - S_\infty$.

For large $\gamma\tau$ we have $\phi_n \simeq J_0(2n\gamma\tau)$ [see discussion above Eq. (75)]. This approximation is compared with the exact result in Fig. 14. In this limit of large $\gamma\tau$, Eq. (75) holds. The approximation for $1 - S_\infty$ [Eq. (96)] which also works in the large-$\gamma\tau$ limit is tested in Fig. 15. The approximation is just qualitative. We obtained a far better approximation

$$1 - S_\infty \simeq \frac{1}{4\pi\gamma\tau}\{\ln[16\pi^2(\gamma\tau)^2\theta^*(\pi - \theta^*)] - 2\}, \tag{D2}$$

where $\theta^* = \text{modulo}(2\gamma\tau,\pi)$. This approximation is demonstrated in Fig. 16.

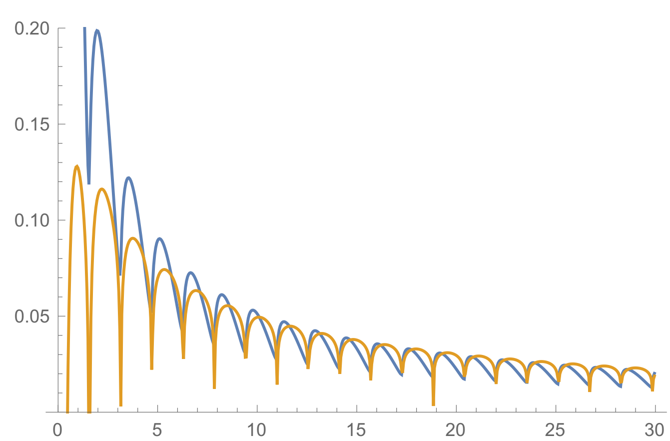

FIG. 16. $1 - S_\infty$ versus $\gamma\tau$. The approximation (D2) works well.

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