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Hitting time for the continuous quantum walk

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We define the hitting (or absorbing) time for the case of continuous quantum walks by measuring the walk at random times, according to a Poisson process with measurement rate λ. From this definition we derive an explicit formula for the hitting time, and explore its dependence on the measurement rate. As the measurement rate goes to either 0 or infinity the hitting time diverges; the first divergence reflects the weakness of the measurement, while the second limit results from the quantum zeno effect. Continuous-time quantum walks, like discrete-time quantum walks but unlike classical random walks, can have infinite hitting times. We present several conditions for existence of infinite hitting times, and discuss the connection between infinite hitting times and graph symmetry.

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I. INTRODUCTION

There are two main types of quantum walks: continuous-time and discrete-time quantum walks. Discrete-time quantum walks evolve by the application of a unitary evolution operator at discrete time intervals, and continuous-time walks evolve under a (usually time-independent) Hamiltonian. Continuous-time quantum walks have been defined by Farhi and Gutmann in [1] as a quantized version of continuous-time classical random walks. Classical random walks are used in computer science to design probabilistic algorithms for computational problems most notably for 3-satisfiability (3-SAT) [2]. In a similar vein, quantum walks provide a framework for the design of quantum algorithms. Quantum walks have been used in many quantum algorithms such as element distinctness [3], matrix product verification [4], triangle finding [5], and group commutativity testing [6]. Recently, a quantum algorithm for evaluating NAND trees has been proposed which uses a quantum walk as a part of the algorithm [7]. To better understand how to use quantum walks for algorithms we need to study the properties of these walks. Many papers have studied the behavior of quantum walks for particular graphs. For example, quantum walks on the line have been examined for the continuous-time case in Refs. [1,8,9] and for the discrete-time case in [10–14]. The N cycle is treated in [15,16], and the hypercube in [17–21]. Quantum walks on general undirected graphs are defined in [22,23], and on directed graphs in [24]. Kendon [25] has a recent review of the work done in this field so far, focusing mainly on decoherence. Other reviews include an introductory review by Kempe in [26], and a review from the perspective of algorithms by Ambainis in [23].

Different quantitative characterizations of quantum walks have been defined by analogy to classical walks, such as mixing times, hitting (or absorbing) times, correlation times, etc. [15]. Often for this purpose the evolution of the quantum walk must be modified to include not only the unitary evolution, but also a measurement process to extract information about the current state of the walk. There is a natural way to introduce such a measurement process in the discrete case: Namely, a measurement is made after each step of unitary evolution. The interval between measurements is the same as the characteristic time scale for the walk in question. In the case of the continuous-time walk, such a natural definition of a measured walk does not exist. There is no intrinsic time step after which we can perform the measurement. Classically this is not a difficulty, because measurements do not disturb the state of the system. The quantum case is quite different. If we choose the measurement times arbitrarily, they can either be too long or too short with respect to the unitary evolution of the quantum walk. We can either miss important details in the evolution by measuring too infrequently, or overly distort the unitary evolution by measuring too often. In the limiting case, we can completely freeze the evolution by the quantum zeno effect [27].

Hitting times for discrete-time quantum walks have been defined and analyzed in [19,20]. The effect of making random measurements on mixing times, and its possible algorithmic applications, has been studied in [28–30]. In this paper, we introduce a measurement process for the continuous-time quantum walk which gives rise to a definition and an analytical formula for the hitting time as a function of the measurement rate (or equivalently, measurement strength). We explore the limits of measuring too weakly or too strongly, and show that the hitting time diverges in either case. This suggests the existence of an optimum rate of measurement, which depends on the unitary dynamics of the particular walk.

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We also show another difference from hitting times for classical random walks. In the classical case, a random walk on a finite connected graph always leads to finite hitting time for any vertex. This is not true for the quantum case. The existence of infinite hitting times has been argued for discrete-time and continuous-time quantum walks in [20]; in this paper we show this explicitly for the continuous-time quantum walks based on the definition of hitting time that we give, and derive conditions for the existence of infinite hitting times. Another sufficient condition that we prove is that if the complementary graph is not connected, this automatically leads to infinite hitting times for the continuous-time quantum walk on the original graph.

The paper is organized as follows. In Sec. II, we describe how to introduce the measurement process, and derive formulas for the hitting time and probability. In Sec. III, we give a condition for existence of infinite hitting times and prove that the hitting time diverges when the measurement rate goes to zero or infinity. In Sec. IV, we give examples for the hitting times for certain graphs as a function of the measurement rate. In Sec. V, we give another sufficient condition for infinite hitting times. A discussion follows in Sec. VI.

II. DEFINITION OF THE HITTING TIME FOR THE CONTINUOUS-TIME QUANTUM WALK

A. Continuous-time measured walks

We want to define hitting time for the continuous unitary evolution on undirected graph $\Gamma(V,E)$, where V is the set of vertices and E is the set of edges. Two vertices $v_1, v_2 \in V$ are connected if there exists an edge $e=\{v_1,v_2\} \in E$ (here $\{v_1,v_2\}$ should be taken as the unordered pair or set of the two vertices v_1 and v_2). Corresponding to the graph Γ, we assign the Hilbert space $\mathcal{H}_\Gamma=\ell^2(V)$. The vertex states in that Hilbert space are just labeled by the vertices of the graph—for $v \in V$, $|v\rangle \in \mathcal{H}$. They form an orthonormal basis for $\mathcal{H}_\Gamma$, $\langle v_n|v_m\rangle=\delta_{nm}$.

The hitting time for classical random walks is defined naturally as the average time to find the walk in a specific vertex. When we turn to the quantum case, the walk on the graph is defined not as a stochastic process on the vertices of the graph but as the unitary evolution of a closed quantum system with the Hilbert space $\mathcal{H}_\Gamma$ defined above. To determine when the quantum walk has reached a vertex, we need to measure the system to gain information about its current state. There are several reasonable ways to do that in the continuous-time case. We could perform strong measurements periodically with some fixed but arbitrary period T. This is not unlike the discrete case, in which the period T is given naturally by the walk itself: A measurement is performed after each unitary evolution step. This way to perform a measurement is not satisfactory in our case. We have no general way to know how to choose T just from the graph. If we choose it too small we could introduce too much decoherence, effectively masking the unitary evolution of the walk, or even worse, freezing it. If T is too large then we can miss the moment when the walk actually reaches the final vertex. And in general, the unitary transformation between measurements can be complicated and difficult to work out (unlike the discrete-time case), which makes performance harder to analyze.

Another way to measure the system is through strong measurements performed at random times. The measurement times are chosen according to a probability distribution with some measurement rate. The advantage is that we do not introduce an artificial periodicity into the dynamics, and it allows one to calculate averaged effects over different measurement patterns. The disadvantage is that it is still necessary to introduce a time scale for the measurements, this time given by the rate at which measurements are performed. The simplest and most natural way to distribute these measurements is as a Poisson process; this is equivalent to having a small constant rate λ to do a measurement. We will see that using a Poisson process allows us to find an exact analytical expression for the hitting time and hitting probability.

A third way to measure the system is using "weak" measurements (analogous to the way photodetection is described). In a small time period δt, we perform a measurement which either allows the system to evolve unitarily with a probability $1-\epsilon$, or performs a measurement to determine whether it has reached the final state with a probability ϵ. In this case, the evolution is unitary for most of the time, with "jumps" at the random times when a measurement is performed. This case and the previous one are actually equivalent—the values of δt and ϵ determine the measurement rate λ—but they give a somewhat different intuition about how to look at the measurement procedure.

In [30], it was argued that the qualitative and even quantitative behavior of the system is not too sensitive to the exact details of the measurement scheme. This suggests that the first choice above (periodic measurement) might be as good as the other two in practice, but it still introduces a discrete structure which is not desirable in dealing with continuous evolution. For this reason, in the following we explore the measurement scheme described by the second and third cases.

B. Poisson-distributed measurements

We perform a measurement to check whether the system is in the final state $|v_f\rangle$, given by the measurement operators $\{P_f, Q_f\}$ where $P_f=|v_f\rangle\langle v_f|$, $Q_f=I-P_f$. We measure the system at random times, distributed according to a Poisson process X_t with rate $\lambda > 0$. Each time we observe a jump in the Poisson process we measure the system. Between the moments at which we perform the measurements the system evolves unitarily with a Hamiltonian $H=-\gamma L$, where L is the discrete version of the continuous Laplacian ∇^2. In our case it is given by $L=A-D$, where D is a diagonal matrix in the basis spanned by the vertex states with the degree of each vertex along the diagonal, and A is the adjacency matrix of the graph [1,31]. In this paper we take $\gamma=1$. If the degree of the vertex v_n is d_n then we have the following representation of D and A:

$$D = \sum_n d_n |v_n\rangle\langle v_n|, \tag{1}$$

$$A = \sum_{n,m} a_{nm} |v_n\rangle\langle v_m|, \tag{2}$$

where

$$a_{nm} = \begin{cases} 1 & \text{if } \{v_n, v_m\} \in E, \\ 0 & \text{if } \{v_n, v_m\} \notin E. \end{cases} \tag{3}$$

is the adjacency matrix of the graph $\Gamma(V,E)$.

This choice of Hamiltonian is not special—any similar Hamiltonian will lead to qualitatively similar behavior. As we see below, the important property is that the symmetries of the graph be reflected in the Hamiltonian; automorphisms of the graph produce permutations of the basis vectors $|v\rangle$, which should in turn be symmetries of the Hamiltonian.

Let $\omega = (t_1, t_2, \ldots)$ be a sequence of random times when the jumps of the Poisson process are observed, with $(t_n \in \mathbb{R}, 0 < t_1 < t_2 < \cdots)$. For convenience we will take $t_0 = 0$. The sequences ω belong to a probability space $(\Omega, \mathfrak{F}, \mathbb{P})$ on which the Poisson process X_t is defined,

$$X: \mathbb{R} \times \Omega \to \{0, 1, 2, \ldots\},$$

$$X_t(\omega) = n \quad \text{if } t \in [t_n, t_{n+1}). \tag{4}$$

Here Ω is the set of all sequences of random times ω, $\mathfrak{F}$ is the σ-algebra, generated by the Poisson process. The probability measure $\mathbb{P}$ on Ω is the one induced by the Poisson process. (For reference, see [32,33].)

For each sequence $\omega \in \Omega$ we define the hitting time as

$$\tau_\omega = \sum_{n=1}^{\infty} t_n p_n, \tag{5}$$

where p_n is the probability to find the system in the final state at time t_n given that the system was not measured to be in the final state in any of the previous times $t_{n-1}, \ldots, t_1$. (For reference, see [20,34].) Define the intervals between jumps t_{j-1} and t_j as $\bar{t}_j = t_j - t_{j-1}$. We want to average τ_ω over all possible trajectories ω of the Poisson process, and take this as our definition for the hitting time,

$$\tau_h = \mathbb{E}_{\mathbb{P}}(\tau_\omega) = \int_\Omega \tau_\omega d\mathbb{P}(\omega). \tag{6}$$

We would like to find an analytical formula for τ_h. From the definition of p_n, we have

$$p_n = \mathrm{Tr}\left(P_f \overleftarrow{\prod_{m=1}^{n-1}} (e^{-i(t_{m+1}-t_m)H} Q_f) e^{-it_1 H} \rho_i e^{it_1 H} \times \overrightarrow{\prod_{m=1}^{n-1}} (Q_f e^{i(t_{m+1}-t_m)H}) \right). \tag{7}$$

The arrow above the products signify whether the operators entering the products are ordered from left to right or vice versa, in other words $\overleftarrow{\prod_{m=1}^{n}} U_i = U_n U_{n-1} \cdots U_1$ and $\overrightarrow{\prod_{m=1}^{n}} U_i = U_1 U_2 \cdots U_n$.

We now introduce superoperators $\mathcal{U}_{\bar{t}}$ and $\mathcal{Q}_f$, defined by

$$\mathcal{U}_{\bar{t}}(X) = e^{-i\bar{t}H} X e^{i\bar{t}H}, \tag{8}$$

$$\mathcal{Q}_f(X) = Q_f X Q_f, \tag{9}$$

and use them to rewrite (7) as

$$p_n = \mathrm{Tr}\{P_f \mathcal{U}_{\bar{t}_n} \circ \mathcal{Q}_f \circ \mathcal{U}_{\bar{t}_{n-1}} \circ \mathcal{Q}_f \circ \cdots \circ \mathcal{U}_{\bar{t}_1}(\rho_i)\}. \tag{10}$$

We want to express the sum in Eq. (5), as a function of the $\{\bar{t}_n\}$. We do that by adding, subtracting, and rearranging terms in the sum. We discuss convergence issues of the series in the equations below in the Appendix.

$$\begin{aligned} \tau_\omega &= t_1 p_1 + t_2 p_2 + t_3 p_3 + t_4 p_4 + \cdots \\ &= t_1 p_1 + t_2 p_2 - t_1 p_2 + t_1 p_2 + t_3 p_3 - t_2 p_3 + t_2 p_3 - t_1 p_3 + t_1 p_3 \\ &\quad + t_4 p_4 - \cdots \\ &= t_1 (p_1 + p_2 + p_3 + \cdots) + (t_2 - t_1)(p_2 + p_3 + \cdots) + (t_3 - t_2) \\ &\quad \times (p_3 + p_4 + \cdots) + \cdots = \sum_{k=1}^{\infty} \bar{t}_k \sum_{n=k}^{\infty} p_n. \end{aligned} \tag{11}$$

Because the $\{t_n\}$ are the event times of a Poisson process, the interval times $\{\bar{t}_n\}$ are independent and identical random variables, exponentially distributed with parameter λ and a probability density function given by

$$f_{\bar{t}_n}(\bar{t}) = \begin{cases} \lambda e^{-\lambda \bar{t}}, & \bar{t} \geq 0, \\ 0, & \bar{t} < 0. \end{cases} \tag{12}$$

Knowing that, we reexpress formula (6),

$$\tau_h = \left(\prod_{l=1}^{\infty} \int_0^\infty d\bar{t}_l \lambda e^{-\lambda \bar{t}_l} \right) (\tau_\omega). \tag{13}$$

Then

$$\tau_h = \sum_{k=1}^{\infty} \sum_{n=k}^{\infty} \left(\prod_{l=1}^{\infty} \int_0^\infty d\bar{t}_l \lambda e^{-\lambda \bar{t}_l} \right) (\bar{t}_k p_n). \tag{14}$$

In the above expression there are two types of integrals,

$$A(X) = \int_0^\infty d\bar{t} \lambda e^{-\lambda \bar{t}} \mathcal{U}_{\bar{t}}(X), \tag{15}$$

$$B(X) = \int_0^\infty d\bar{t} \lambda e^{-\lambda \bar{t}} \bar{t} \mathcal{U}_{\bar{t}}(X). \tag{16}$$

Integrating by parts we obtain the following equations for the operators A and B,

$$A + \frac{i}{\lambda}[H, A] = X, \tag{17}$$

$$B + \frac{i}{\lambda}[H, B] = \frac{1}{\lambda} A(X), \tag{18}$$

where $A(X)$ is the solution to the first equation. (We will prove that this solution exists below.) Defining the superoperator

$$\mathcal{L}_\lambda(X) = X + \frac{i}{\lambda}[H,X],$$

we rewrite these equations as

$$\mathcal{L}_\lambda(A) = X, \tag{19}$$

$$\mathcal{L}_\lambda(B) = \lambda^{-1}A(X). \tag{20}$$

We want to prove that the superoperator $\mathcal{L}_\lambda$ is invertible when λ is a real number. For this we need to know how the adjoint of a superoperator is defined with respect to the Hilbert-Schmidt inner product for operators,

$$\langle X,Y\rangle_{\mathrm{HS}} = \mathrm{Tr}(X^\dagger Y). \tag{21}$$

Using this inner product, we see that if

$$\mathcal{C}(X) = \sum_n c_n C_n X D_n^\dagger,$$

the adjoint of $\mathcal{C}(X)$ is given by

$$\mathcal{C}^\dagger(X) = \sum_n c_n^* C_n^\dagger X D_n.$$

From that it follows that $\mathcal{L}$ is a normal superoperator,

$$\mathcal{L}_\lambda^\dagger \circ \mathcal{L}_\lambda - \mathcal{L}_\lambda \circ \mathcal{L}_\lambda^\dagger = 0. \tag{22}$$

This means that $\mathcal{L}_\lambda$ is diagonalizable. If X_n is an eigenvector of $\mathcal{L}_\lambda$, then X_n is an eigenvector of the Hermitian and anti-Hermitian parts of $\mathcal{L}_\lambda$ separately, which are given by

$$\mathcal{L}_\lambda^H(X) = \frac{1}{2}(\mathcal{L}_\lambda + \mathcal{L}_\lambda^\dagger)(X) = \mathcal{I}(X) = X$$

and

$$\mathcal{L}_\lambda^A(X) = \frac{1}{2}(\mathcal{L}_\lambda - \mathcal{L}_\lambda^\dagger)(X) = \frac{i}{\lambda}[H,X],$$

respectively. Let us denote the eigenvalue of $\mathcal{L}_\lambda^A$ corresponding to X_n by ix_n ($x_n \in \mathbb{R}$ because $\mathcal{L}_\lambda^A$ is anti-Hermitian). Then $\mathcal{L}_\lambda(X_n) = (1+ix_n)X_n \neq 0$. This proves that each eigenvalue of $\mathcal{L}_\lambda$ is nonzero, and that $\mathcal{L}_\lambda$ is invertible.

The solutions to Eqs (17) and (18) are

$$A = \mathcal{L}_\lambda^{-1}(X), \tag{23}$$

$$B = \lambda^{-1}\mathcal{L}_\lambda^{-2}(X). \tag{24}$$

Substituting these in (14) we obtain

$$\begin{aligned}\tau_h &= \sum_{k=1}^{\infty}\sum_{n=k}^{\infty} \lambda^{-1}\,\mathrm{Tr}[P_f(\mathcal{L}_\lambda^{-1}\circ \mathcal{Q}_f)^{n-k}\circ \mathcal{L}_\lambda^{-2}\circ(\mathcal{Q}_f\circ \mathcal{L}_\lambda^{-1})^{k-1}(\rho_i)] \\ &= \sum_{k=1}^{\infty}\sum_{n=k}^{\infty} \lambda^{-1}\,\mathrm{Tr}[P_f\mathcal{L}_\lambda^{-1}\circ(\mathcal{Q}_f\circ \mathcal{L}_\lambda^{-1})^{n-k}\circ \mathcal{L}_\lambda^{-1}\circ(\mathcal{Q}_f \\ &\quad \circ \mathcal{L}_\lambda^{-1})^{k-1}(\rho_i)] = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \lambda^{-1}\,\mathrm{Tr}[P_f\mathcal{L}_\lambda^{-1}\circ(\mathcal{Q}_f\circ \mathcal{L}_\lambda^{-1})^{l}\circ \mathcal{L}_\lambda^{-1} \\ &\quad \circ(\mathcal{Q}_f\circ \mathcal{L}_\lambda^{-1})^{k}(\rho_i)].\end{aligned} \tag{25}$$

Note that the eigenvalues of $\mathcal{L}_\lambda$ are always greater than or equal to 1 in absolute value, from which it follows that the eigenvalues of $\mathcal{Q}_f\circ\mathcal{L}_\lambda^{-1}$ are all less than or equal to 1 in absolute value. If all the eigenvalues are strictly less than 1 in absolute value, the following sum exists:

$$\sum_{k=0}^{\infty}(\mathcal{Q}_f\circ\mathcal{L}_\lambda^{-1})^l = (\mathcal{I}-\mathcal{Q}_f\circ\mathcal{L}_\lambda^{-1})^{-1}.$$

Substituting this into (25) and denoting $\mathcal{N}_\lambda = \mathcal{L}_\lambda - \mathcal{Q}_f$, we obtain the following formula for the hitting time:

$$\tau_h = \lambda^{-1}\,\mathrm{Tr}[P_f\mathcal{N}_\lambda^{-2}(\rho_i)]. \tag{26}$$

This formula is closely analogous to the formula for the hitting time derived in [21,20] for the case of a discrete-time quantum walk. If $\mathcal{Q}_f\circ\mathcal{L}_\lambda^{-1}$ has any eigenvalues equal to 1, the inverse in the above formula should be thought of as a pseudoinverse.

Another quantity that may be defined is the total probability to ever hit the final vertex [21,34],

$$p_h = \sum_{n=1}^{\infty} p_n. \tag{27}$$

We can derive a formula similar to (26) for p_h,

$$p_h = \mathrm{Tr}[P_f\mathcal{N}_\lambda^{-1}(\rho_i)]. \tag{28}$$

If this quantity is not unity, then it means that there is a nonzero probability for the particle to never reach the final vertex. This is when the quantum walk is said to have an infinite hitting time [21]. It is shown in the next section that this happens when the superoperator $\mathcal{L}_\lambda - \mathcal{Q}_f$ is not invertible, then the walk will have an infinite hitting time for some starting vertex (or superposition of vertices). In this case, we can replace the inverse with a pseudoinverse. When the hitting time is not infinite, or equivalently when the superoperator $\mathcal{L}_\lambda - \mathcal{Q}_f$ is invertible, $p_h = 1$.

C. Jumplike weak measurements

There is another way to derive formulas (26) and (28): By looking at this procedure as an iterated weak measurement (case 3 that we discussed above). Weak measurements have been considered in the literature [35,36] and one can think of them as measurements that disturb the state of the system by a small amount on average, and thus give little information on average about the state of the system. There are two types of weak measurement. The first one leaves the system in a state close to the initial one no matter what outcome is observed. The second type could change the state of system dramatically for some outcomes but these outcomes are observed with a very small probability. Below we consider a measurement of the second type. Instead of summing over all trajectories of the Poisson process at each time period δt, we perform a generalized measurement with measurement operators,

$$M_0 = \sqrt{1-\varepsilon^2}e^{-i\delta t H},$$

$$M_1 = \varepsilon P_f,$$

$$M_2 = \varepsilon Q_f. \tag{29}$$

These operators form a complete measurement as $\Sigma_{i=0}^{2} M_i^\dagger M_i = I$. The measurement is weak (in the sense of giving little information on average, as noted above) when $\varepsilon \ll 1$. Let us define a positive matrix ρ^c describing the state of the system at time t conditioned on the assumption that outcome "2" has not occurred up to this time. We measure the system repeatedly at intervals of time δt, using the same measurement operators, and if we do not observe outcome "2" the state of the system is described by the following matrix:

$$\rho^c(t+\delta t) = \sum_{i=0}^{1} M_i \rho^c(t) M_i^\dagger. \tag{30}$$

We expand in powers of the small parameter ε and take the limit $\varepsilon \to 0$ and $\delta t \to 0$, keeping the ratio $\varepsilon^2/\delta t$ constant, and obtain a master equation for $\rho^c(t)$. This gives the connection between the strength of the measurement ε and the measurement rate $\lambda = \lim_{\delta t \to 0} \varepsilon^2/\delta t$. After we expand to second order of ε we obtain

$$\begin{aligned}\rho^c(t+\delta t) &= (1-\varepsilon^2)(1-i\delta t H)\rho^c(1+i\delta t H) + \varepsilon^2 Q_f \rho^c Q_f \\ &\quad + O(\varepsilon^3) = \rho^c(t) - i\delta t[H,\rho^c] - \varepsilon^2[\rho^c(t) - Q_f\rho^c Q_f] \\ &\quad + O(\varepsilon^3).\end{aligned} \tag{31}$$

Taking the limit $\delta t \to 0$ and using the fact that

$$\lim_{\delta t\to 0} \frac{\rho^c(t+\delta t) - \rho^c(t)}{\delta t} = \frac{d\rho^c}{dt},$$

$$\lim_{\delta t \to 0} \frac{\varepsilon^2}{\delta t} = \lambda,$$

we arrive at the master equation for ρ^c,

$$\frac{d\rho^c}{dt} = -i[H,\rho^c] - \lambda(\rho^c - Q_f\rho^c Q_f) = -\lambda \mathcal{N}_\lambda(\rho^c). \tag{32}$$

Note that ρ^c is positive but not normalized; $\mathrm{Tr}\{\rho^c\}$ is the probability that measurement result "2" has not been seen up until time t. The total probability to hit the final vertex p_h and the hitting time τ_h are given by

$$p_h = \lambda \int_0^\infty \mathrm{Tr}[P_f \rho^c(t)]dt, \tag{33}$$

$$\tau_h = \lambda \int_0^\infty t\, \mathrm{Tr}[P_f \rho^c(t)]dt. \tag{34}$$

Substituting the solution of (32),

$$\rho^c(t) = e^{-\lambda t \mathcal{N}_\lambda}[\rho^c(0)],$$

in (33) and (34) and integrating by parts, we obtain formulas (26) and (28) for the total probability to hit and the hitting time.

D. Physical implementation

The above discussion has been made very abstractly, without reference to the physical system which embodies the quantum walk in question, or how the measurements are done. This abstraction is deliberate, since our conclusions are largely independent of the details of physical implementation.

For relatively small graphs it is possible to build a quantum walk from, e.g., a network of mirrors and beam splitters [37]. This type of construction can demonstrate qualitative features of quantum walks. Quantum walks can also be used to describe the evolution of solid-state systems with "hopping" Hamiltonians, at least for small planar graphs [38]. Measurements in this case will most easily be done at particular points in space, to detect the presence or absence of the walker.

For algorithmic purposes this type of implementation is too limited. Graphs representing computationally challenging problems will typically include an exponentially large number of vertices. They will also in general not be possible to lay out neatly in three-dimensional space. For quantum walks on these more general graphs the most likely implementation is simulation by a quantum computer—either a general purpose computer [39] or one specifically designed to simulate quantum walks. Because the Hilbert space grows exponentially with the number of qubits of the quantum computer, it can efficiently simulate exponentially large graphs. Such a simulation also allows more general kinds of measurements, not necessarily localized at particular vertices of the graph, though such localized measurements may still be the most useful.

The physical realization of the quantum walk is not important for the properties described in this paper. However, it can make a significant difference in understanding the type of noise or decoherence that can arise in the system. We do not address decoherence in this paper, but in general it will tend to erode the interference effects that give quantum walks their distinctive properties.

III. CONDITIONS FOR EXISTENCE OF INFINITE HITTING TIMES

In [20,21], it was shown that quantum walks on some graphs have infinite hitting times for some initial states. This occurs when, starting from the initial state, the total probability to ever find the walk at the final vertex is less than 1. It was shown in [20,21] that infinite hitting times occur when the unitary evolution operator (for the discrete-time case) or the Hamiltonian (for the continuous-time case) has nontrivial symmetry. Since the Hamiltonian is obtained from the graph, if the graph has symmetry (i.e., a nontrivial automorphism group), then the Hamiltonian will inherit this symmetry group. This symmetry causes the Hamiltonian to be confined to certain invariant subspaces of the Hilbert space, assuming it begins in the subspace. This means that if the final vertex is not in this subspace, then the walk will never reach it and will have an infinite hitting time.

Infinite hitting times are also related to the spectrum (or more precisely, the degeneracy) of the Hamiltonian. If the

Hamiltonian is degenerate, then one can construct an invariant subspace that will confine the walk. This can be related to the symmetry group through the use of irreducible representations. Every irreducible representation of the symmetry group must lie inside an eigenspace of the Hamiltonian. If the symmetry group has an irreducible representation of dimension greater than one, then the Hamiltonian is degenerate. Therefore, for the continuous-time quantum walk a sufficient condition for the existence of infinite hitting times is the presence of an irreducible representation in the symmetry group of the graph with dimension larger than one.

As Abelian groups have only one-dimensional representations, we might expect that a symmetry group must be non-Abelian to have infinite hitting times. However, this is not always true: Having a non-Abelian symmetry group is a sufficient, but not a necessary condition. In the next section we provide examples where graphs with Abelian symmetry groups have infinite hitting times (though in these examples symmetry still plays a crucial role).

In this section, we will prove that the existence of infinite hitting times is equivalent to the noninvertibility of the superoperator $\mathcal{L}_\lambda - \mathcal{Q}_f$. We will need the following definitions [40,41].

Definition 1. A matrix pencil $A+\mu B$ (where A and B are $n\times n$ matrices and μ is a complex number) is said to be regular if there exists at least one complex μ for which the pencil is nonsingular.

Definition 2. A complex number $\bar{\mu}$ is a finite eigenvalue of the regular matrix pencil $A+\mu B$ if $\det(A+\bar{\mu}B)=0$.

Definition 3. The regular matrix pencil $A+\mu B$ is said to have an infinite eigenvalue if B is a singular matrix.

Consider all operators X such that $[H,X]=0$ and $P_f X = XP_f=0$, and denote the projector on the linear subspace of all such operators by $\mathcal{P}$. We will prove that $\mathcal{P}\neq 0$ if and only if $\mathcal{N}_\lambda = \mathcal{L}_\lambda - \mathcal{Q}_f$ is not regular. If $\mathcal{P}\neq 0$ then choose $\bar{X}$ such that $\mathcal{P}(\bar{X})=\bar{X}\neq 0$. Then $[H,\bar{X}]=0$ and from $P_f\bar{X}=\bar{X}P_f=0$ follows that $\mathcal{Q}_f(\bar{X})=\bar{X}$. Thus $\mathcal{N}_\lambda(\bar{X})=0$ which means that $\mathcal{N}_\lambda$ is singular for every λ and thus not regular. If $\mathcal{N}_\lambda$ is not regular then it is noninvertible for any λ. Let us fix λ to be real and different from 0. There exists $\bar{X}\neq 0$ such that $\mathcal{N}_\lambda(\bar{X})=0$. We have already proved that $\mathcal{L}_\lambda$ is invertible for real λ. Then

$$\mathcal{N}_\lambda(\bar{X}) = \mathcal{L}_\lambda \circ (\mathcal{I} - \mathcal{L}_\lambda^{-1} \circ \mathcal{Q}_f)(\bar{X}) = 0 \tag{35}$$

and thus

$$\mathcal{L}_\lambda^{-1} \circ \mathcal{Q}_f(\bar{X}) = \bar{X}. \tag{36}$$

Taking into account that all eigenvalues of $\mathcal{L}_\lambda$ are greater or equal to 1 in absolute value the above equality is true only if

$$\mathcal{L}_\lambda^{-1}(\bar{X}) = \bar{X}, \tag{37}$$

$$\mathcal{Q}_f(\bar{X}) = \bar{X}, \tag{38}$$

which are equivalent to

$$[H,\bar{X}] = 0, \tag{39}$$

$$P_f\bar{X} = \bar{X}P_f = 0. \tag{40}$$

This means that $\mathcal{P}$ is nonzero.

Let us explicitly give the form of the projective superoperator $\mathcal{P}$ in terms of the projectors on the eigenspaces of the Hamiltonian H. For this purpose we define the intersection operation $\cap$ for orthogonal projections. For any two orthogonal projection operators P_1 and P_2, $P_1 \cap P_2$ will denote the orthogonal projector on the subspace which is the intersection of the subspaces onto which P_1 and P_2 project. Let the Hamiltonian H have the following decomposition:

$$H = \sum_{i=1}^{r} E_i P_i,$$

where E_i are the eigenvalues of H ($E_i \neq E_j$ for $i\neq j$), P_i are the projectors onto the eigenspaces of H corresponding to eigenvalues E_i. Since H is Hermitian, $P_iP_j=\delta_{ij}P_i$, and $\mathrm{Tr}\,P_i = d_i$ is the multiplicity of the E_i eigenvalue. The projector $\mathcal{P}$ is then

$$\mathcal{P}(X) = \sum_{i=1}^{r} (P_i \cap Q_f) X (P_i \cap Q_f). \tag{41}$$

From this form it is easy to see that $\mathcal{P}$ is a completely positive superoperator. As such, if it is different from 0, then there must exist a density matrix ρ such that $\mathcal{P}(\rho)=\rho$. If the walk begins in such a state ρ, it will never arrive at the final vertex.

Now we will prove that if $\mathcal{N}_\lambda$ is regular as a matrix pencil then all its eigenvalues lie on the imaginary axis. Let us assume that $\mathcal{N}_\lambda$ is invertible for some $\lambda\neq 0$ and $\mathcal{N}_{\lambda_0}$ is noninvertible for some $\lambda_0\neq 0$, $\lambda_0\neq\lambda$. Then $\mathcal{N}_\lambda(X)\neq 0$ for all $X\neq 0$ and there exists $X_0\neq 0$ such that $\mathcal{N}_{\lambda_0}(X_0)=0$. Then $(\mathcal{N}_\lambda - \mathcal{N}_{\lambda_0})(X_0) = i(1/\lambda - 1/\lambda_0)[H,X_0]\neq 0$ and therefore $[H,X_0]\neq 0$. Analogously $(\lambda\mathcal{N}_\lambda - \lambda_0\mathcal{N}_{\lambda_0})(X_0) = (\lambda-\lambda_0)(\mathcal{I} - \mathcal{Q}_f)(X_0)\neq 0$ therefore $(\mathcal{I}-\mathcal{Q}_f)(X_0)\neq 0$. As $\mathcal{I}-\mathcal{Q}_f$ is a projector, it follows that

$$\langle X_0, (\mathcal{I} - \mathcal{Q}_f)(X_0)\rangle_{\mathrm{HS}} \neq 0. \tag{42}$$

Taking into account that $\mathcal{I}-\mathcal{Q}_f$ and $\mathcal{H}(\cdot)=[H,\cdot]$ are both Hermitian superoperators, $\langle X_0,(\mathcal{I}-\mathcal{Q}_f)(X_0)\rangle_{\mathrm{HS}}$ and $\langle X_0, \mathcal{H}(X_0)\rangle_{\mathrm{HS}}$ are both real numbers. Denoting $\bar{\lambda}_0^r = \mathrm{Re}(1/\lambda_0)$ and $\bar{\lambda}_0^i = \mathrm{Im}(1/\lambda_0)$ we have

$$\langle X_0, (\mathcal{I} - \mathcal{Q}_f - \bar{\lambda}_0^i \mathcal{H})(X_0)\rangle_{\mathrm{HS}} + i\bar{\lambda}_0^r \langle X_0, \mathcal{H}(X_0)\rangle_{\mathrm{HS}} = 0. \tag{43}$$

This equality is only possible if both the real and imaginary parts vanish, implying that $\bar{\lambda}_0^r=0$ and hence $\mathrm{Re}(\lambda_0)=0$.

Using this result, we will now prove that if $\mathcal{N}_\lambda$ is a regular matrix pencil, and thus does not have infinite eigenvalues, then the hitting time τ_h behaves regularly as a function of λ on the real line: it does not diverge for any real λ except when λ goes to 0 or infinity. Physically, this means that when we measure either very weakly or very strongly we never find the particle in the final vertex. The first limit is easy to understand since it expresses the fact that if we never measure, we will never find the particle anywhere. The second limit, $\lambda \to \infty$, corresponds to the quantum zeno effect: The evolution of the system is restricted to a subspace orthogonal to the final vertex.

To prove this conclusion, we represent superoperators as matrices using the following isomorphism:

$$\phi:\mathcal{C}(\cdot) = \sum_n c_n C_n(\cdot) D_n^\dagger \to \phi(\mathcal{C}) = \mathbf{C} = \sum_n c_n C_n \otimes D_n^* . \tag{44}$$

Now we represent the superoperator pencil $\mathcal{N}_\lambda$ by the matrix pencil

$$\mathbf{N}_\lambda = \phi(\mathcal{N}_\lambda) = I \otimes I - Q_f \otimes Q_f^* - \frac{i}{\lambda}(H \otimes I - I \otimes H^*). \tag{45}$$

By assumption this matrix pencil is regular. Every regular matrix pencil $A+\mu B$ has the following canonical form:

$$A + \mu B = T \,\mathrm{diag}[N^{(m_1)}, \ldots, N^{(m_p)}, J^{(n_1)}(\mu_{n_1}), \ldots, J^{(n_q)}(\mu_{n_q})]S, \tag{46}$$

where T and S are invertible matrices, constant with respect to μ, and $\mathrm{diag}(N^{(m_1)}, \ldots, N^{(m_p)}, J^{(n_1)}, \ldots, J^{(n_q)})$ is a block-diagonal matrix with the matrices $N^{(m_1)}, \ldots, N^{(m_p)}, J^{(n_1)}, \ldots, J^{(n_q)}$ on the diagonal and zeros everywhere else. The blocks $N^{(m)}$ and $J^{(n)}$ are square matrices of order m and n, respectively, of the form

$$N^{(m)} = \begin{pmatrix} 1 & \mu & 0 & \cdots & 0 & 0 \\ 0 & 1 & \mu & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & \mu \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}, \tag{47}$$

$$J^{(n)}(\mu_l) = \begin{pmatrix} \mu+\mu_l & 1 & 0 & \cdots & 0 & 0 \\ 0 & \mu+\mu_l & 1 & \cdots & 0 & 0 \\ 0 & 0 & \mu+\mu_l & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mu+\mu_l & 1 \\ 0 & 0 & 0 & \cdots & 0 & \mu+\mu_l \end{pmatrix}, \tag{48}$$

or more succinctly $N^{(m)} = I^{(k)} + \mu K^{(m)}$ and $J^{(n)}(\mu_0) = (\mu + \mu_0) I^{(n)} + K^{(n)}$, where $I^{(m)}$ is the identity matrix of order m and $K^{(m)}$ is a $m \times m$ matrix with "1" immediately above the diagonal and "0" everywhere else. The $N^{(m)}$ blocks are present when the matrix pencil has infinite eigenvalues and the $J^{(n)}$ blocks correspond to finite eigenvalues.

We want to examine the behavior of the inverse of a regular matrix pencil when μ approaches one of its eigenvalues. Assume that μ_0 is a finite eigenvalue of the pencil and the corresponding $n \times n$ block to that eigenvalue is $J(\mu_0)$. The inverse of this block is given by

$$J^{-1}(\mu_0) = \sum_{j=0}^{n-1} \frac{(-K)^j}{(\mu+\mu_0)^{j+1}}. \tag{49}$$

In the above $K^0 = I$ and $K = K^{(n)}$. The inverses of all blocks that do not correspond to the eigenvalue μ_0 will have regular behavior when μ approaches $-\mu_0$. We similarly examine the behavior of $N^{(n)}$ when μ goes to infinity. The inverse of this block is given by

$$N^{-1} = \sum_{j=0}^{n-1} (-\mu K)^j. \tag{50}$$

The inverses of the blocks corresponding to finite eigenvalues will have regular behavior when μ approaches infinity.

As the matrix pencil

$$\bar{\mathbf{N}}_\mu \equiv \mathbf{N}_{1/\mu} = I \otimes I - Q_f \otimes Q_f^* + i\mu(H \otimes I - I \otimes H^*) \tag{51}$$

is regular and has both finite ($\mu=0$) and infinite eigenvalues [because both matrices $I \otimes I - Q_f \otimes Q_f^*$ and $i(H \otimes I - I \otimes H^*)$ are singular], both types of blocks $N^{(k)}$ and $J^{(l)}$ are present in its normal form. If we express formula (26) in terms of matrices and vectors with $\mu = 1/\lambda$ we obtain an analogous expression

$$\tau_h = \mu P_f^v \cdot \bar{\mathbf{N}}_\mu^{-2} \rho_i^v, \tag{52}$$

where P_f^v and ρ_i^v are the vectorized versions of the matrices P_f and ρ_i.

When μ goes to 0 we can see from formula (49) with $\mu_0 = 0$ that the asymptotic behavior of τ_h is given by

$$\tau_h = \tau_h^r(\mu) + \frac{1}{\mu} P_f^v (S^{-1} P_0 T^{-1})^2 \rho_i^v + O\left(\frac{1}{\mu^2}\right), \tag{53}$$

where $\tau_h^r(\mu)$ is a function which is regular in a neighborhood of $\mu=0$, T and S are the invertible matrices in the canonical form (46) of the matrix pencil $\bar{\mathbf{N}}_\mu$, and P_0 is the projector on the eigenspace with eigenvalue $\mu=0$. Now as long as $P_f^v (S^{-1} P_0 T^{-1})^2 \rho_i^v \neq 0$, τ_h will go to infinity when μ goes to 0 (λ going to infinity) no matter whether terms of higher order, $O(\frac{1}{\mu^2})$, are present or not.

Analogously, when μ goes to infinity, τ_h has the asymptotic behavior

$$\tau_h = \mu P_f^v (S^{-1} P_\infty T^{-1})^2 \rho_i^v + O(\mu^2), \tag{54}$$

where P_∞ is the projector on the eigenspace with infinite eigenvalue. Here again as long as $P_f^v (S^{-1} P_\infty T^{-1})^2 \rho_i^v \neq 0$, τ_h will go to infinity when μ goes to infinity (λ going to 0) no matter whether terms of higher order, $O(\mu^2)$, are present or not.

As we shall see in the next section, the hitting time in the examples that we will give below has the following form as a function of λ:

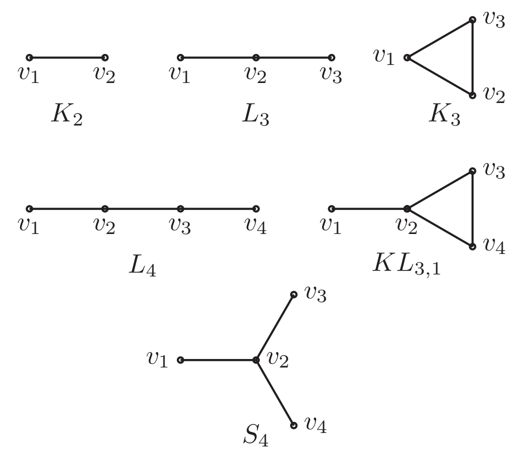

FIG. 1. Graph examples (with assigned vertex labels).

$$\tau_h = \tau_{(1)}\lambda + \frac{\tau_{(-1)}}{\lambda}, \tag{55}$$

where the constants $\tau_{(1)}$ and $\tau_{(-1)}$ depend on the particular graph. The divergence as $\lambda \to 0$ and $\lambda \to \infty$ are thus immediately apparent.

IV. EXAMPLES

In this section, we will consider as examples the graphs in Fig. 1, using the labeling of the vertices given in the figure when necessary. Infinite hitting times ($p_h \neq 0$) exist for the graphs L_3, K_3, L_4, $KL_{3,1}$, and S_4 for certain choices of initial and final vertices.

We can describe the probability to hit p_h and the hitting time τ_h in another way, by specifying two operators $\mathfrak{P}_\lambda(\Gamma, v_f)$ and $\mathfrak{H}_\lambda(\Gamma, v_f)$, and calculating their expectations in the initial state,

$$p_h = \mathrm{Tr}[\mathfrak{P}_\lambda(\Gamma, v_f)\rho_i], \tag{56}$$

$$\tau_h = \mathrm{Tr}[\mathfrak{H}_\lambda(\Gamma, v_f)\rho_i], \tag{57}$$

where

$$\mathfrak{P}_\lambda(\Gamma, v_f) = [(\mathcal{L}_\lambda - \mathcal{Q}_f)^{-1}]^\dagger(P_f), \tag{58}$$

$$\mathfrak{H}_\lambda(\Gamma, v_f) = \frac{1}{\lambda}[(\mathcal{L}_\lambda - \mathcal{Q}_f)^{-2}]^\dagger(P_f). \tag{59}$$

Here ρ_i is the density matrix describing the initial state of the system, and P_f is the projector onto the final vertex. These equations follow from formulas (26) and (28), respectively, by using the definition of the Hilbert-Schmidt inner product.

In the following, we will show the operators $\mathfrak{P}_\lambda(\Gamma, v_f)$ and $\mathfrak{H}_\lambda(\Gamma, v_f)$ in the vertex state basis for the graphs in Fig. 1 and briefly discuss properties of quantum walks on each graph. It is useful to describe the hitting probability and time in terms of these matrices, because they give the result for any starting state.

A. Example 1

The graph K_2 has the reflection symmetry group C_2. As this group is Abelian, the Hamiltonian of K_2 is nondegenerate. The two eigenvectors have nonzero overlap with both vertex states, and therefore there can be no infinite hitting times. We can see this from the matrices $\mathfrak{P}$ and $\mathfrak{H}$,

$$\mathfrak{P}_\lambda(K_2, v_1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{60}$$

$$\mathfrak{H}_\lambda(K_2, v_1) = \begin{pmatrix} \frac{2}{\lambda} & \frac{i}{\lambda} \\ -\frac{i}{\lambda} & \frac{2}{\lambda} + \frac{\lambda}{2} \end{pmatrix}. \tag{61}$$

The dependence of the hitting time for vertex v_1 can include two terms: The $2/\lambda$ term diverges as $\lambda \to 0$, which simply represents the increasing time it takes to find the particle as the measurement rate goes to zero; if the system starts at vertex v_2 there is also a $\lambda/2$ term, which diverges as $\lambda \to \infty$ because of the quantum zeno effect: As the measurement rate increases, we can "freeze" the system's evolution.

B. Example 2

The situation is different in the case of the L_3 graph. The graph again has symmetry group C_2, and the Hamiltonian has no degeneracies. Despite that, however, one of the three energy eigenstates has zero overlap with the v_2 vertex, $(1/\sqrt{2}, 0, -1/\sqrt{2})$. This means that even without degeneracy, there is an infinite hitting time if the final vertex is v_2. This is not accidental—the symmetry of the graph is still responsible for the existence of this infinite hitting time. Under the action of C_2 each energy eigenstate $|e_i\rangle$ will have to be either symmetric or antisymmetric. The Hilbert space thus splits into symmetric and antisymmetric subspaces which are orthogonal to each other. As the vertex state $|v_2\rangle$ is obviously symmetric under the action of the group, it will be orthogonal to the antisymmetric subspace, leading to an infinite hitting time for v_2 starting from either v_1 or v_3. This is a general observation for any graph that has C_2 as a symmetry group: Any vertices that are left invariant under the action of the group will have infinite hitting times. By contrast, there are no infinite hitting times to reach vertices v_1 and v_3. We can see all of these properties by examining the matrices $\mathfrak{P}_\lambda$ and $\mathfrak{H}_\lambda$,

$$\mathfrak{P}_\lambda(L_3, v_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{62}$$

$$\mathfrak{H}_\lambda(L_3, v_1) = \begin{pmatrix} \frac{3}{\lambda} & -\frac{1}{2\lambda} + i & \frac{1}{2\lambda} - \frac{i}{2} \\ -\frac{1}{2\lambda} - i & \lambda + \frac{4}{\lambda} & \frac{\lambda}{2} - \frac{1}{2\lambda} + \frac{i}{2} \\ \frac{1}{2\lambda} + \frac{i}{2} & \frac{\lambda}{2} - \frac{1}{2\lambda} - \frac{i}{2} & \frac{3\lambda}{2} + \frac{3}{\lambda} \end{pmatrix}. \tag{63}$$

The existence of infinite hitting time for reaching v_2 can easily be seen from the $\mathfrak{P}$ matrix for v_2;

$$\mathfrak{P}_\lambda(L_3,v_2)=\begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{2}\\ 0 & 1 & 0\\ \frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}, \tag{64}$$

$$\mathfrak{H}_\lambda(L_3,v_2)=\begin{pmatrix}\frac{\lambda}{8}+\frac{9}{8\lambda} & \frac{1}{4\lambda}-\frac{i}{4} & \frac{\lambda}{8}+\frac{9}{8\lambda}\\ \frac{1}{4\lambda}+\frac{i}{4} & \frac{2}{\lambda} & \frac{1}{4\lambda}+\frac{i}{4}\\ \frac{\lambda}{8}+\frac{9}{8\lambda} & \frac{1}{4\lambda}-\frac{i}{4} & \frac{\lambda}{8}+\frac{9}{8\lambda}\end{pmatrix}. \tag{65}$$

As $\mathfrak{P}_\lambda(L_3,v_2)$ is not the identity, there must be initial states that will result in a probability less than 1 to hit v_2. For example, this will be true for any initial state which is a superposition of states $|v_1\rangle$ and $|v_3\rangle$.

C. Example 3

The graph K_3 has symmetry group D_3, and its Hamiltonian is degenerate. It has infinite hitting times to hit any vertex. If we calculate $\mathfrak{P}$ and $\mathfrak{H}$ for this graph, we discover a new property of these matrices. The graph K_3 is not isomorphic to L_3, but its $\mathfrak{P}$ and $\mathfrak{H}$ matrices for any vertex of K_3 are also given by (64) and (65) (or their appropriate cyclic permutations), the same as for L_3. This is because the Hamiltonians of the L_3 and K_3 graphs commute. We will observe similar behavior below for other graphs with commuting Hamiltonians.

D. Example 4

The quantum walk on the graph L_4 has the same qualitative behavior as the walk on L_2. They both have the same symmetry group, C_2, as does the L_3 graph. But in the case of L_4, as in the case of L_2, there are no infinite hitting times.

E. Examples 5 and 6

We will examine the graphs $KL_{3,1}$ and S_4 together, because it turns out that their behavior is closely related. The graph $KL_{3,1}$ again has C_2 for its symmetry group, this time representing reflection about the horizontal axis. The Hamiltonian is nondegenerate, but there are infinite hitting times for the vertices v_1 and v_2, due to the existence of an eigenvector which vanishes on those two vertices: $(0,0,1/\sqrt{2},-1/\sqrt{2})$. This is quite analogous to the case of the graph L_3—graphs with C_2 symmetry have infinite hitting times for vertices that are fixed points under the action of the symmetry group.

The graph S_4 has D_3 as a symmetry group. Its Hamiltonian is degenerate, and it has infinite hitting times to hit any vertex. It turns out that the matrices $\mathfrak{P}$ and $\mathfrak{H}$ for hitting vertices v_1 and v_2 in S_4 coincide with the same matrices for $KL_{3,1}$,

$$\mathfrak{P}_\lambda(KL_{3,1},v_1)=\mathfrak{P}_\lambda(S_4,v_1)=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&\frac{1}{2}&\frac{1}{2}\\0&0&\frac{1}{2}&\frac{1}{2}\end{pmatrix}, \tag{66}$$

$$\begin{aligned}\mathfrak{H}_\lambda(KL_{3,1},v_1)&\\ =\mathfrak{H}_\lambda(S_4,v_1)&\\ =\begin{pmatrix}\frac{3}{\lambda} & -\frac{1}{\lambda}+i & \frac{3}{4\lambda}+\frac{i}{2} & \frac{3}{4\lambda}+\frac{i}{2}\\ -\frac{1}{\lambda}-i & \lambda+\frac{13}{2\lambda} & \frac{\lambda}{2}-\frac{1}{\lambda}+\frac{i}{4} & \frac{\lambda}{2}-\frac{1}{\lambda}+\frac{i}{4}\\ \frac{3}{4\lambda}-\frac{i}{2} & \frac{\lambda}{2}-\frac{1}{\lambda}-\frac{i}{4} & \lambda+\frac{15}{8\lambda} & \lambda+\frac{15}{8\lambda}\\ \frac{3}{4\lambda}-\frac{i}{2} & \frac{\lambda}{2}-\frac{1}{\lambda}-\frac{i}{4} & \lambda+\frac{15}{8\lambda} & \lambda+\frac{15}{8\lambda}\end{pmatrix}&,\end{aligned} \tag{67}$$

$$\mathfrak{P}_\lambda(KL_{3,1},v_2)=\mathfrak{P}_\lambda(S_4,v_2)=\begin{pmatrix}\frac{1}{3}&0&\frac{1}{3}&\frac{1}{3}\\0&1&0&0\\\frac{1}{3}&0&\frac{1}{3}&\frac{1}{3}\\\frac{1}{3}&0&\frac{1}{3}&\frac{1}{3}\end{pmatrix}, \tag{68}$$

$$\begin{aligned}\mathfrak{H}_\lambda(KL_{3,1},v_2)=\mathfrak{H}_\lambda(S_4,v_2)&\\ =\begin{pmatrix}\frac{\lambda}{18}+\frac{8}{9\lambda} & \frac{1}{3\lambda}-\frac{i}{6} & \frac{\lambda}{18}+\frac{8}{9\lambda} & \frac{\lambda}{18}+\frac{8}{9\lambda}\\ \frac{1}{3\lambda}+\frac{i}{6} & \frac{2}{\lambda} & \frac{1}{3\lambda}+\frac{i}{6} & \frac{1}{3\lambda}+\frac{i}{6}\\ \frac{\lambda}{18}+\frac{8}{9\lambda} & \frac{1}{3\lambda}-\frac{i}{6} & \frac{\lambda}{18}+\frac{8}{9\lambda} & \frac{\lambda}{18}+\frac{8}{9\lambda}\\ \frac{\lambda}{18}+\frac{8}{9\lambda} & \frac{1}{3\lambda}-\frac{i}{6} & \frac{\lambda}{18}+\frac{8}{9\lambda} & \frac{\lambda}{18}+\frac{8}{9\lambda}\end{pmatrix}&.\end{aligned} \tag{69}$$

Just as with graphs L_3 and K_3, $KL_{3,1}$, and S_4 have the same matrices because the Hamiltonians of the graphs commute; and, as we can see from the above, this produces similar dynamics when we measure the walk in the corresponding final vertices v_1 and v_2.

This is not the case, however, when the final vertex is v_3 or v_4 for these graphs. For S_4, the $\mathfrak{P}$ and $\mathfrak{H}$ matrices for v_3 and v_4 can be obtained from those above by interchanging v_1 with v_3 or v_4. For $KL_{3,1}$, however the matrices are

$$\mathfrak{P}_\lambda(KL_{3,1},v_3) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{70}$$

$$\mathfrak{H}_\lambda(KL_{3,1},v_3) = \begin{pmatrix} \lambda + \frac{5}{\lambda} & -\frac{\lambda}{2} - \frac{1}{\lambda} - \frac{i}{2} & 0 & -\frac{\lambda}{2} - i \\ -\frac{\lambda}{2} - \frac{1}{\lambda} + \frac{i}{2} & \frac{5}{2\lambda} + \frac{7}{\lambda} & -\frac{1}{\lambda} - \frac{3i}{2} & -\lambda - \frac{1}{\lambda} + \frac{i}{2} \\ 0 & -\frac{1}{\lambda} + \frac{3i}{2} & \frac{4}{\lambda} & \frac{1}{\lambda} \\ \frac{\lambda}{18} + \frac{8}{9\lambda} & -\lambda - \frac{1}{\lambda} - \frac{i}{2} & \frac{1}{\lambda} & \lambda + \frac{4}{\lambda} \end{pmatrix}. \tag{71}$$

The matrices $\mathfrak{P}_\lambda(KL_{3,1},v_4)$ and $\mathfrak{H}_\lambda(KL_{3,1},v_4)$ can be found by interchanging v_3 and v_4 in the matrices above.

The infinite hitting times for the L_3 and $KL_{3,1}$ graphs can be understood to arise because the Hamiltonian of those graphs commutes with the Hamiltonian of a more symmetric graph. As we shall see in the next section, this fact can lead to infinite hitting times under certain circumstances.

V. INFINITE HITTING TIMES FOR GRAPHS WITH NONCONNECTED COMPLEMENTARY GRAPH

We will now look in a little more detail at infinite hitting times, which are one of the most surprising differences between classical random walks and quantum walks. In the classical case, if the graph is finite and connected, the probability to reach any vertex starting from any other is always 1. That is not the case for quantum walks. A sufficient condition for infinite hitting times was given in [42]: If the graph's Hamiltonian is sufficiently degenerate, infinite hitting times will always exist. For continuous-time walks, any degeneracy at all is sufficient. (This is a sufficient but not a necessary condition because, as we have shown above, even graphs with nondegenerate Hamiltonians may have infinite hitting times.) We will now show that another sufficient condition for a continuous-time quantum walk to have an infinite hitting time is the nonconnectedness of the complementary graph. Consider a graph Γ with n vertices and Hamiltonian H_Γ given by the usual expressions, Eq. (1) and Eq. (2). The complete graph K_n with n vertices has the following Hamiltonian (in the basis spanned by the vertex states):

$$H_{K_n} = \begin{pmatrix} n-1 & -1 & \cdots & -1 \\ -1 & n-1 & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & n-1 \end{pmatrix}. \tag{72}$$

This can be rewritten more succinctly as

$$H_{K_n} = n(I - |\psi_0\rangle\langle\psi_0|) = n\bar{P}_0, \tag{73}$$

where $|\psi_0\rangle = \frac{1}{\sqrt{n}}\Sigma_{k=1}^n |k\rangle$ and $\bar{P}_0 = I - |\psi_0\rangle\langle\psi_0|$.

The complementary graph Γ^c of a graph Γ is obtained by connecting vertices that are not connected in the original graph Γ, and removing the edges that are present in the original graph. Then it is easy to see that the Hamiltonian of Γ^c is

$$H_{\Gamma^c} = H_{K_n} - H_\Gamma. \tag{74}$$

Another observation is that the Hamiltonian of every graph Γ commutes with the Hamiltonian of the complete graph with the same number of vertices,

$$[H_\Gamma, H_{K_n}] = 0. \tag{75}$$

This follows from the observation that $|\psi_0\rangle$ is always an eigenvector of H_Γ with eigenvalue 0. As

$$H_\Gamma = \bar{P}_0 H_\Gamma \bar{P}_0, \tag{76}$$

(75) is obvious. We can see from (74) that $[H_\Gamma, H_{\Gamma^c}]=0$.

Let us assume that the graph Γ is connected but the complementary graph Γ^c is not, and consider the quantum walk on Γ^c. Because Γ^c is not connected, there are initial states that never reach a particular final vertex if the initial state includes only vertices which are not connected to the final vertex. Let us consider an initial state $|\psi_i\rangle$ that contains only vertex states that belong to one of the connected components of Γ^c. Let us further assume that

$$\langle\psi_0|\psi_i\rangle = \frac{1}{\sqrt{n}}\sum_{k=1}^{n}\langle k|\psi_i\rangle = 0,$$

which is always possible if the connected component has more than one vertex. Since $|\psi_i\rangle$ is orthogonal to $|\psi_0\rangle$, it immediately follows that it is an eigenstate of H_{K_n} with eigenvalue n.

If the final state $|\psi_f\rangle$ contains only vertices belonging to a different connected component of Γ^c, the probability to ever reach the final state is 0,

$$\langle\psi_f|e^{-itH_{\Gamma^c}}|\psi_i\rangle = 0 \quad \forall \ t. \tag{77}$$

Setting all of this together, we can see now that

$$\langle\psi_f|e^{-itH_\Gamma}|\psi_i\rangle = \langle\psi_f|e^{-it(H_{K_n}-H_{\Gamma^c})}|\psi_i\rangle = e^{-itn}\langle\psi_f|e^{itH_{\Gamma^c}}|\psi_i\rangle = 0. \tag{78}$$

This proves the existence of infinite hitting time for the original graph Γ.

We note that similar considerations may apply in some cases if the complete graph is replaced by a symmetric graph whose Hamiltonian commutes with H_Γ. An example of this is the similarity of the dynamics of the $KL_{3,1}$ and S_4 graphs.

Finally, we note that this sufficient condition for infinite hitting times is not particularly strong. For a graph with a large number of vertices, the complementary graph is almost always connected. This condition may prove useful for particular cases, however.

VI. DISCUSSION

We have examined continuous-time quantum walks and studied natural definitions for the hitting time. After considering different possibilities for introducing a measurement scheme, one of them emerges as a natural one for the continuous case: Measuring the presence or absence of the particle at the final vertex at Poisson-distributed random times, with an adjustable rate λ. This is exactly equivalent to performing a particular type of weak measurement at frequent intervals, in the limit yielding continuous monitoring with time resolution $1/\lambda$. Using this measurement scheme, we derived an analytical formula for the hitting time which closely resembles the formula for the discrete-time case.

This formula enables us to find a necessary and sufficient condition for the existence of quantum walks with infinite hitting times, namely that a certain superoperator pencil is not regular. In the case of finite hitting times, the dependance of the hitting time on the rate of the measurement was studied, and the intuitive expectation for its behavior in the limits of weak and strong measurement rate was confirmed. In particular, as the measurement rate goes to infinity, the hitting time can diverge due to the quantum zeno effect.

As in the discrete case, the symmetry of the graph plays a very strong role in the emergence of infinite hitting times. The graph symmetry group, if large enough, causes degeneracies in the eigenspectrum of the Hamiltonian which in turn leads to the emergence of infinite hitting times for certain vertices. But this is not the only way in which symmetry can lead to infinite hitting times. Even when no degeneracy is present, symmetry can cause some eigenvectors of the Hamiltonian to have zero overlap with some vertex states, as in the case of the L_3 and $KL_{3,1}$ graphs examined in Sec. IV. This can be attributed to the fact that under the action of the group C_2, the Hilbert space splits into symmetric and antisymmetric subspaces, and some eigenvectors from the antisymmetric subspace could have zero overlap with certain vertex states. Further study exploring this idea is needed to see if similar effects occur for other symmetry groups in the absence of degeneracy.

Finally, in Sec. V we show another condition for infinite hitting times. The quantum walk on a connected graph can have infinite hitting times if the complementary graph is disconnected. This is in sharp contrast with the classical case, where every random walk on a connected graph will hit any vertex with probability 1 at long times. While this new condition is rather specific, it is possible that it can be generalized by replacing the completely connected graph with some other highly symmetric graph, such that the Hamiltonian still commutes with the Hamiltonian of the original graph. It may be possible to explain any infinite hitting times on any graph in this way, giving a unifying view of the whole subject. It is clear that many questions remain, and that hitting times for continuous-time quantum walks are a very fruitful area of research.

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APPENDIX

We will prove that Eq. (11) is valid in the absence of infinite hitting times. If there are no infinite hitting times, then formulas (26) and (28) give the values of the hitting time and probability to hit, respectively, and they are finite numbers. We used (14) and (13) to derive them, so they need to converge as well. The integral over the probability space of the Poisson process will converge only if the integrand $\tau_\omega = \sum_{k=1}^{\infty}\bar{t}_k\sum_{n=k}^{\infty}p_n$ converges for almost all sequences $\omega \in \Omega$. Thus we can consider only sequences ω for which the corresponding series converges. In this case the series is absolutely convergent because it consists of positive terms only. This permits us to rearrange them to get the series on the second line of Eq. (11). Canceling terms in that series (we can do this without endangering its convergence or the value to which it sums), we obtain the same series as in the first line of (11) but with zeros inserted between its terms. More precisely, we have one zero between the second and third term, two zeros between the third and fourth term, and so on. Obviously, if this series is convergent then the one in the first line of (11) is convergent too, and they both have the same value. This concludes the proof.

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