Green-function approach for scattering quantum walks

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In this work a Green-function approach for scattering quantum walks is developed. The exact formula has the form of a sum over paths and always can be cast into a closed analytic expression for arbitrary topologies and position-dependent quantum amplitudes. By introducing the step and path operators, it is shown how to extract any information about the system from the Green function. The method's relevant features are demonstrated by discussing in detail an example, a general diamond-shaped graph.

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I. INTRODUCTION

Generally speaking, quantum walks (QW) represent unitary evolutions taking place in discrete spaces—graphs—for which typical basis states are localized. There are several ways to formulate QW, either considering time as a continuous (CTQW) [1,2] or a discrete variable. In the latter case, the two major formulations are the (a) coined QW (CQW), based on inner "coin" states (see, e.g., [3]), and (b) scattering QW (SQW), relying on the idea of multiport interferometers [4,5]. The continuous time and coined QW are directly related as a limit process [6], whereas the CQW and SQW have been shown to be unitarily equivalent in arbitrary topologies [7].

Quantum walks originally emerged [8] from the interest to construct and understand quantum analogs of classical random walks (CW). But soon it was realized they also would constitute powerful tools in quantum computation [9], especially given that QW can represent universal quantum computation primitives [10]. In fact, for a long time CW have been used to solve different computational problems [11]. Thus, the connections between the quantum and classical walks [12–14], allied to the particular features of the former [15], actually point to the potential usefulness of QW in building algorithms which are much faster and robuster [16,17] than their classical counterparts. As representative examples we can cite the Grover algorithm [18] (simulated through QW [19]) for searching of unsorted database, the element distinctness algorithm [20], the detection of marked elements [21], the computation of orders of solvable groups [22], and the quantum Fourier transform [23]. Moreover, even problems like the energy transport in biological systems can be analyzed by means of QW [24].

A key aspect in such a class of systems is the quantum interference between the possible "paths" (see next section) along the evolution [25–28]. It leads to a dynamics that generally spreads much faster than CW [15] (although in certain situations anomalous subdiffusive behavior may also emerge [29]). As a consequence, one gets exponentially faster hitting times from QW [1,30,31], one of the reasons why QW are particularly suitable [32] to solve searching problems [27,33]. Also, different diffusion processes, from ballistic to Anderson localization [34,35], are possible when decoherence is included.

Since interference is fundamental to explain different phenomena observed in QW [36] (including many of the applications mentioned above) it is desirable to have a description emphasizing the pathlike character of QW. In this respect Green-function methods are particularly useful [37–39]. Then, here we develop a full Green-function approach for QW in arbitrary topology and for position-dependent quantum amplitudes. For this, we assume the very appropriate discrete scattering formulation, SQW. We should observe there are few interesting works (e.g., Refs. [40–42]) addressing the classification of trajectories in QW. They, nevertheless, are based mostly on combinatorial analysis to compute all the possible final states at a time $t = n$. Our proposed construction thus is much closer to the idea of "history" of trajectories in the Feynman sense [43].

The paper is organized as follows. In Sec. II we review the scattering formulation for quantum walks, also making few useful parallels with the classical case. By direct mapping one-dimensional (1D) QW to a related type of problem, 1D point interaction lattices, in Sec. III we are able to write the exact Green function G in the form of a sum over paths. Moreover, we discuss how such a formula can be summed as a closed analytical expression. In Sec. IV the 1D construction is extended to complete arbitrary topologies. By defining the step and path operators, we show in Sec. V how to extract any system's relevant information from the exact expression for G. In Sec. VI we illustrate the features of the present approach analyzing in detail a particular example, the diamond-shaped graph. Finally, we present the conclusion in Sec. VII.

II. A BRIEF REVIEW ON THE SCATTERING FORMULATION FOR QUANTUM WALKS

To better understand the main ideas underlying the definition of quantum walk models, and thus to develop a Green-function approach, here we review QW scattering formulation [4] on the line (1D). The case of more general topologies will be discussed in the next sections.

So, consider a helpful framework for SQW: View their evolution as a dynamics defined on a 1D "Hilbert lattice," depicted in Fig. 1. Notice, however, it does not necessarily represent a spatial structure since the states (assumed on the bonds) do not need to be position eigenvectors. Under this

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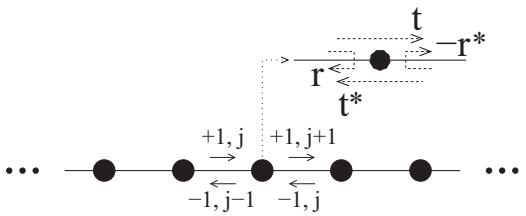

FIG. 1. The "Hilbert lattice" associate to SQW in 1D. For each site it is defined an appropriate scattering quantum amplitudes (here illustrating the phase convention in [4]).

picture, the lattice characteristic parameter is $L = \Delta j = 1$, just the spacing between two consecutive sites of the Hilbert lattice. Along each bond, joining the sites j and $j+1$ (Fig. 1), we have two possible states, $|+1, j+1\rangle$ and $|-1, j\rangle$. Then, each basis element, $|\sigma, j\rangle$, is labeled by two quantum numbers. The first, σ, sets the "direction" (± 1) along the lattice. We mention that although fully equivalent, the present is slightly different than the common SQW construction in the literature.

The discrete time evolution is given by the one-step unitary operator U, such that $|\Psi(n+1)\rangle = U|\Psi(n)\rangle$. For U, we consider the translation (S_T) and reversion-translation (S_{RT}) operators,

$$\begin{aligned} S_T|\sigma, j\rangle = |\sigma, j+\sigma\rangle, \quad {S_T}^\dagger|\sigma, j\rangle = |\sigma, j-\sigma\rangle, \\ S_{RT}|\sigma, j\rangle = {S_{RT}}^\dagger|\sigma, j\rangle = |-\sigma, j-\sigma\rangle, \end{aligned} \tag{1}$$

with both unitary and ${S_{RT}}^2 = \mathbf{1}$. We also define T and R, for which the basis states $|\sigma, j\rangle$ are eigenstates, or

$$T|\sigma, j\rangle = t_{\sigma,j}|\sigma, j\rangle, \qquad R|\sigma, j\rangle = r_{\sigma,j}|\sigma, j\rangle. \tag{2}$$

If we impose, now,

$$\begin{aligned} r_{+1,j}\, t^*_{+1,j} + r^*_{-1,j}\, t_{-1,j} = r_{+1,j}\, t^*_{-1,j} + r^*_{-1,j}\, t_{+1,j} = 0, \\ |t_{\pm,j}|^2 + |r_{\pm,j}|^2 = |t_{\pm,j}|^2 + |r_{\mp,j}|^2 = 1, \end{aligned} \tag{3}$$

then, the unitary time evolution reads ($0 \leqslant \gamma < 2\pi$),

$$U(\gamma) = \exp[i\gamma]\,(S_T\, T + S_{RT}\, R). \tag{4}$$

The term $\exp[i\gamma]$ is associated with the translation between neighbor sites ($\Delta j = L = 1$), relevant to properly describe stationary scattering solutions [44].

Provided Eq. (3) holds, there is a freedom to choose the coefficients r_j and t_j. For instance, by setting ($0 \leqslant \rho_j \leqslant 1$ and $0 \leqslant \phi_j, \varphi_j < 2\pi$ for any j)

$$t_{\sigma,j} = \rho_j \exp[i\sigma\phi_j], \qquad r_{\sigma,j} = \sigma\sqrt{1-\rho_j^2}\exp[i\sigma\varphi_j], \tag{5}$$

one gets $r_{-1,j} = -r^*_{+1,j}$ and $t_{-1,j} = t^*_{+1,j}$, just the convention used in [4] (Fig. 1).

The dynamics in Eqs. (1)–(4), in fact, represents an extended quantum version of a more simple classical random walk. Each time the classical walk needs to choose a new direction, it uses the same probabilities (P and $1-P$) to decide between right and left. By allowing in Eq. (5) ρ and the phases to depend on j, we are implicitly assuming position-dependent distribution functions for the direction choices. Obviously, by setting the same ρ, φ, and ϕ for any j we recover the usual case.

Finally, as it stands, the above model is deterministic in the quantum mechanical sense: Any initial state $|\Psi(0)\rangle$, after n time steps, is uniquely determined by the always well-defined state $U^n|\Psi(0)\rangle$. Thus, stochasticity (i.e., classical randomness) can enter into the problem only through measurements, when we determine the system location along the Hilbert lattice. In fact,

$$P_{\sigma,j}(n) = |\langle j,\sigma|\Psi(n)\rangle|^2 \tag{6}$$

is the probability to be in the quantum state (or in the present lattice language "position and direction") j,σ at time n. So, projection is an essential ingredient in QW.

As a simple example, consider the initial state $|\Psi(0)\rangle = |+1,0\rangle$. Under U one has after $n = 3$ time steps,

$$\begin{aligned} |\Psi(3)\rangle = \exp[3i\gamma]\{&t_{+1,0}t_{+1,1}t_{+1,2}\,|+1,3\rangle + (r_{+1,0}r_{-1,-1}t_{+1,0} \\ &+ t_{+1,0}r_{+1,1}r_{-1,0})|+1,1\rangle \\ &+ r_{+1,0}t_{-1,-1}r_{-1,-2}\,|+1,-1\rangle \\ &+ r_{+1,0}t_{-1,-1}t_{-1,-2}|-1,-3\rangle + (r_{+1,0}r_{-1,-1}r_{+1,0} \\ &+ t_{+1,0}r_{+1,1}t_{-1,0})|-1,-1\rangle \\ &+ t_{+1,0}t_{+1,1}r_{+1,2}|-1,1\rangle\}. \end{aligned} \tag{7}$$

Thus, the system probability to be found, say, in $|+1,3\rangle$ is $|t_{+1,0}t_{+1,1}t_{+1,2}|^2$. Note that for three time steps, there is only one possible "path" ending up in $|+1,3\rangle$. Hence, the modulus square of the quantum amplitude associated with such a path yields the sough probability. On the other hand, there are two possible paths leading to $|-1,-1\rangle$. They correspond to the amplitudes $r_{+1,0}r_{-1,-1}r_{+1,0}$ and $t_{+1,0}r_{+1,1}t_{-1,0}$ [cf. Eq. (7)]. But contrary to CW, where the total probability is the sum of the individual probabilities of each trajectory, here the quantum interference character of the walk demands that $P_{-1,-1}(3) = |r_{+1,0}r_{-1,-1}r_{+1,0} + t_{+1,0}r_{+1,1}t_{-1,0}|^2$.

III. A GREEN-FUNCTION APPROACH FOR QUANTUM RANDOM WALKS

Here we develop a Green-function approach for the SQW in the previous section, proceeding in three steps. (a) First, we construct a mapping from our QW to a 1D generalized Kronig-Penney lattice [38], for which we can calculate the exact energy-dependent Green function G. (b) Then, we discuss which are the mapped system appropriate configurations in order to match the original problem. (c) Finally, we show how the obtained G gives the quantum walk sought dynamics. We leave to the next section the extension of the 1D results to the case of more general topologies, namely, QW on arbitrary graph structures.

A. The mapping

As already emphasized, the quantum walk does not necessarily represent any dynamics on a concrete physical lattice. Nevertheless, for our purposes it is very useful to associate the quantum walk Hilbert (space) lattice—and its underlying "kinematics" [45]—to that of a usual continuous 1D quantum scattering problem.

In Fig. 2 we show schematically the correspondence between the model of Fig. 1 with a generalized Kronig-Penney lattice of equally spaced arbitrary point interactions [38] (i.e., zero-range potentials which extend the usual delta function [46]). Each point interaction (at $x = \pm jL,\ j = 0,1,\ldots$) is entirely characterized by the quantum amplitudes $r_j^{(\pm)}(k)$ and $t_j^{(\pm)}(k)$. The superscript $+$ $(-)$ stands for the reflection or transmission of a plane wave of wave number k incoming from the left (right) of the point interaction location. Hereafter, subscripts (superscripts) for direction quantum numbers indicate that the corresponding r's and t's are those for QW (continuous scattering) systems. For the most general zero-range potential, we have (see, e.g., Ref. [47] for a full discussion)

$$r_j^{(\pm)}(k) = \frac{c_j \pm ik(d_j - a_j) + b_j k^2}{-c_j + ik(d_j + a_j) + b_j k^2}\ \exp[\pm ike_j],$$
$$t_j^{(\pm)}(k) = \frac{2ik\exp[\pm i\theta_j]}{-c_j + ik(d_j + a_j) + b_j k^2}, \tag{8}$$

where $a_j\, d_j - b_j\, c_j = 1$, with a_j,b_j,c_j,d_j,e_j real and $\theta_j \in [0,2\pi)$ [48]. Equation (8) satisfies the relations in Eq. (3) and also to

$$r_j^{(\pm)}(k) = r_j^{(\pm)*}(-k), \qquad t_j^{(\pm)}(k) = t_j^{(\mp)*}(-k). \tag{9}$$

Furthermore, for $b_j = c_j = 0$, they become independent on k (up to the phases for the r's) and Eq. (8) assumes the same form as Eq. (5).

Now, let us set $m = \hbar = 1$ (so $p = k$), define $\tau = L/v_{\text{phase}}$ with $v_{\text{phase}} = p/2$, and for convenience take $L = 1$. Then, we can make a direct association between the quantum walk one-step evolution operator U and the continuous system propagator $\mathcal{U}(\tau)$, mapping $U|\Psi(0)\rangle = |\Psi(1)\rangle$ to $\mathcal{U}(\tau)|\Phi(0)\rangle = |\Phi(\tau)\rangle$.

To concretely establish the correspondence, we start with the simplest situation of a fully biased quantum walk (i.e., one which always evolves to a same direction). We thus assume $\rho_j = 1$ and $\phi_j = 0$ for any j, from Eq. (4) leading to $U = \exp[i\gamma]\, S_T$. Such case presents a close parallel with a quantum particle propagating freely along the line. In our generalized Kronig-Penney lattice, a free particle is trivially obtained by setting all the reflection (transmission) amplitudes equal to 0 (1), so that the time evolution is $\mathcal{U}(t) = \exp[-i(\hat{p}^2/2)t]$, with $\hat{p}|p\rangle = p|p\rangle$ for $|p\rangle$ the moment eigenstate. Hence, we have a direct mapping between the complete biased quantum walk dynamics and the evolution of a free particle on the line for $t = \tau$. The equivalent quantities are listed in Table I.

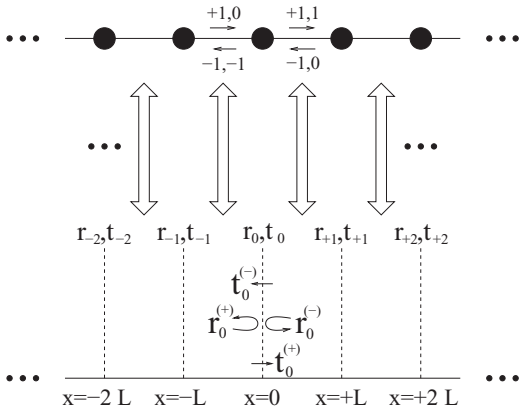

FIG. 2. Schematic association between QW Hilbert (space) lattice and a generalized Kronig-Penney configuration lattice. Each site j corresponds to a point interaction at $x = jL$ (of reflection and transmission amplitudes $r_j^{(\pm)}$ and $t_j^{(\pm)}$).

Next, we consider that in Eq. (5) for any $j \neq 0$ we have $\rho_j = 1$ and $\phi_j = 0$, and for $j = 0$ we have arbitrary ρ and phases. Also, we assume as the quantum walk initial state,

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{j=0} \exp[ij\gamma]|+1,j\rangle, \tag{10}$$

so that $P_j(n = 0) = 0$ for $j > 0$. Then, applying n times the evolution operator, Eq. (4), to $|\Psi(0)\rangle$ we get (with $r = r_{+1,0}$ and $t = t_{+1,0}$)

$$|\Psi(n)\rangle = U^n|\Psi(0)\rangle = \frac{1}{\sqrt{2\pi}} \left\{ \sum_{j=-\infty}^{j=0} \exp[ij\gamma]|+1,j\rangle + r\sum_{j=-n}^{j=-1} \exp[-ij\gamma]|-1,j\rangle + t\sum_{j=1}^{j=n} \exp[ij\gamma]|+1,j\rangle \right\}. \tag{11}$$

TABLE I. The correspondence between quantities in the complete biased quantum walk and in the 1D free propagation.

Fully biased 1D quantum walk	Free quantum propagation on the line
$U = \exp[i\gamma]\, S_T$	$\mathcal{U}(\tau) = \exp[-i(\hat{p}^2/2)\tau]$, $\tau = L/v_{\text{phase}} = L/(p/2)$, $p = k$, $L = 1$
$\lvert\Psi(0)\rangle = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{j=+\infty} \exp[ij\gamma]\lvert+1,j\rangle$	$\lvert\Phi(0)\rangle = \lvert p\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx\, \exp[ipx]\lvert x\rangle$
$\lvert\Psi(1)\rangle = U\lvert\Psi(0)\rangle = \lvert\Psi(0)\rangle$[a]	$\lvert\Phi(\tau)\rangle = \mathcal{U}(\tau)\lvert\Phi(0)\rangle = \exp[-ip^2\tau/2]\lvert\Phi(0)\rangle = \exp[-ip]\lvert\Phi(0)\rangle$
γ	p

[a]Strictly speaking, $\exp[i\gamma]$ in the definition of U in Eq. (4) is not necessary and then the equivalence would be complete (here, in each step it is up to such global phase). Nevertheless, if we take as an initial state $|\Psi(0)\rangle = |\sigma,j\rangle$, instead of states like Eq. (10), $\exp[i\gamma]$ becomes useful to study interference in more general topologies, as in Sec. VI. The important point, therefore, is that we have just a phase difference, so not compromising any parallel between the systems time evolutions.

Now, defining $|\Psi_{\text{scat.}}\rangle = \lim_{n\to+\infty}|\Psi(n)\rangle$, one finds

$$|\Psi_{\text{scat.}}\rangle = \frac{1}{\sqrt{2\pi}}\left\{\sum_{j=-\infty}^{j=0}\exp[ij\gamma]|+1,j\rangle + r\sum_{j=-\infty}^{j=-1}\exp[-ij\gamma]|-1,j\rangle + t\sum_{j=+1}^{j=+\infty}\exp[ij\gamma]|+1,j\rangle\right\}. \tag{12}$$

Note that $U|\Psi_{\text{scat.}}\rangle = |\Psi_{\text{scat.}}\rangle$, so it is a stationary state.

An equivalent situation for the generalized Kronig-Penney lattice is to assume that all r's but one (the reflection amplitude for the point interaction at the origin) are identically null, namely, $r_j^{(+)} = 0$ and $t_j^{(+)} = 1$ $(j \neq 0)$ and $r_0^{(+)}(p) = r(p)$, $t_0^{(+)}(p) = t(p)$. In this case, the scattering solution for a particle incident from the left reads

$$|\Phi_{\text{scat.}}\rangle = \frac{1}{\sqrt{2\pi}}\left\{\int_{-\infty}^{0} dx\ \exp[ipx]|x\rangle + r(p)\int_{-\infty}^{0} dx\ \exp[-ipx]|x\rangle + t(p)\int_{0}^{+\infty} dx\ \exp[ipx]|x\rangle\right\}. \tag{13}$$

Comparing Eqs. (12) and (13), it is evident the correspondence between the two situations.

We can go further, considering that only at two sites the walk can "choose" (from $r_{\pm1,j}$ and $t_{\pm1,j}$, $j = 0, 1$) a direction to proceed, whereas at the other sites the direction is always maintained, with $\rho_j = 1$ and $\phi_j = 0$ for any $j \neq 0, 1$. Thus, repeating the same calculations for the initial state $|\Psi(0)\rangle$ of Eq. (10), we get

$$|\Psi_{\text{scat.}}\rangle = \frac{1}{\sqrt{2\pi}}\left\{\sum_{j=-\infty}^{j=0}\exp[ij\gamma]|+1,j\rangle + r\sum_{j=-\infty}^{j=-1}\exp[-ij\gamma]|-1,j\rangle + t\sum_{j=+2}^{j=+\infty}\exp[ij\gamma]\times|+1,j\rangle + a|-1,0\rangle + b\exp[i\gamma]|+1,1\rangle\right\}, \tag{14}$$

where

$$r = r_{+1,0} + t_{-1,0}\,a, \qquad t = t_{+1,1}\,b,$$
$$a = \frac{t_{+1,0}\,r_{+1,1}\exp[2i\gamma]}{1 - r_{+1,1}r_{-1,0}\exp[2i\gamma]}, \tag{15}$$
$$b = \frac{t_{+1,0}}{1 - r_{+1,1}r_{-1,0}\exp[2i\gamma]}.$$

This expression should be compared with that for the associated problem of two general point interactions located at $x = 0$ and $x = 1$, whose scattering state (incoming from the left) is given by

$$|\Phi_{\text{scat.}}\rangle = \frac{1}{\sqrt{2\pi}}\left\{\int_{-\infty}^{0} dx\exp[ipx]|x\rangle + r(p)\int_{-\infty}^{0} dx \times \exp[-ipx]|x\rangle + t(p)\int_{1}^{+\infty} dx\ \exp[ipx]|x\rangle + a(p)\int_{0}^{1} dx\exp[-ipx]|x\rangle + b(p)\int_{0}^{1} dx\exp[ipx]|x\rangle\right\}, \tag{16}$$

for the coefficients $r(p)$, $t(p)$, $a(p)$, and $b(p)$ obtained from Eq. (15) through the substitutions $r_{\pm1,j} \to r_j^{(\pm)}(p)$, $t_{\pm1,j} \to t_j^{(\pm)}(p)$, and $\gamma \to p$. Once more we find a direct association between the two cases.

By repeating this procedure of "turning on" more and more sites in the quantum walk and zero-range potentials in the Kronig-Penney lattice, one realizes that their relation is indeed direct. The one-to-one mapping is a simple identification of quantities in the two cases. The direction coefficients $r_{\sigma,j}$ and $t_{\sigma,j}$ at each site in the quantum walk corresponds to the scattering amplitudes $r_j^{(\pm)}$ and $t_j^{(\pm)}$ of a point interaction in the Kronig-Penney model. The quantum number j is associated with the appropriate position eigenvalues x/L, likewise for σ with respect to the signal of p. Lastly, the SQW single-step evolution U (up to the phase $\exp[i\gamma]$) is akin to $\mathcal{U}(t = \tau)$ for the continuous scattering system.

We finally note that we have discussed the mapping assuming a scattering scenario, with the QW initial state given by Eq. (10). However, we also could start with an initial state localized in some region of the quantum walk lattice and an initial wave packet localized in an equivalent region of the generalized Kronig-Penney lattice. Then, by applying the respective time evolution operators, again we would find a direct association between their dynamics: The multiple scattering of the wave packet in the Kronig-Penney lattice resembling the proliferation of paths (e.g., see the example in Sec. II) in the quantum walk. So, the correspondence between the two systems is complete and not restricted to the type of initial state assumed. This fact becomes more evident from the Green-function approach next.

B. Quantum walks and finite lattices

To calculate the exact Green function in the case of an infinite generalized Kronig-Penney lattice is a difficult task [38]. However, a key aspect in solving QW through the proposed mapping is that in almost all situations of interest, the original system can be mapped to a finite lattice—a limited number of point scatters along the line—and not to an infinite comb of zero-range potentials.

For example, let us assume that the quantum walk initial state $|\Psi(0)\rangle$ is, say, either $|-1,-1\rangle$ or $|+1,+1\rangle$, thus localized about and leaving from the origin. Now, suppose we shall discuss any quantity for times no longer than $n = N$, or for contexts where the dynamics never takes the system beyond

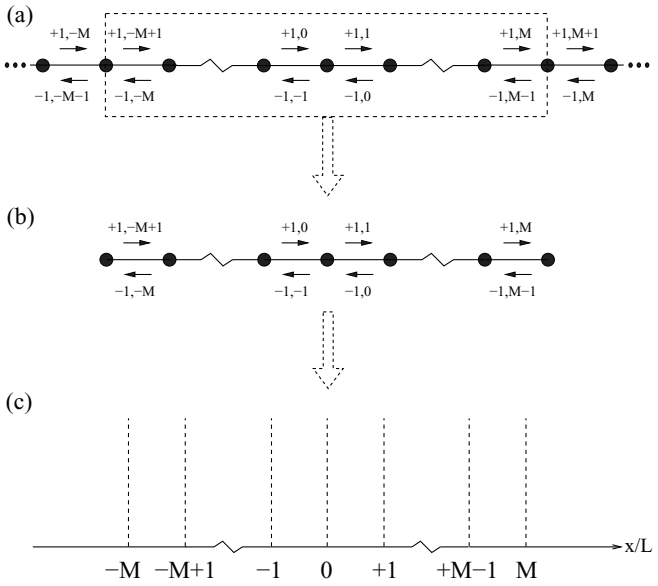

FIG. 3. (a) If under a particular instance, the QW relevant dynamics is restricted to the states $|j| \leqslant M$, (b) then, effectively the system can be described by a finite Hilbert space "lattice", (c) whose mapping leads to a finite set of general point interactions on the line.

the sites $j = \pm J$, $J > 0$. Examples are as follows: (a) to determine the probability to be at the state j (i.e., to calculate $|\langle j,\sigma|\Psi(n)\rangle|^2$) for n up to $n = N$; and (b) to obtain the probability for the walk to reach for the very first time a "distance" $j = J$ from the origin ($j = 0$) at times $n = 1,2,\ldots$, known as the first passage time problem in classical random walk theory [49].

For (b), any evolution leading to $\langle j,\sigma\,|U^n\,|\Psi(0)\rangle \neq 0$ ($|j| > J$, arbitrary n) has no interest for the problem solution [15]. In (a), after N steps the initial state has spread at most a distance $|j| = N$ from the origin. Hence, as illustrated in Fig. 3, in both situations the relevant dynamics for the QW is related just to a segment of the infinite generalized Kronig-Penney lattice, encompassing $2M + 1$ (for M equal to J or N) point interactions. So, in such instances, effectively one needs to deal only with finite lattices.

C. The finite lattice Green function and its relation to the original quantum walk problem

Once the quantum walk dynamics one shall study is mapped to an appropriate (finite) generalized Kronig-Penney lattice, the next step is to calculate the Green function for the latter. Based on certain techniques [50,51], the way to do so has been developed in [38]. Here we just summarize the main steps (for details, see [38]).

Suppose a particle of energy $E = k^2/2$, for which $G(x_f,x_i;k)$ denotes its energy-dependent Green function. The initial and final positions, respectively, x_i and x_f, are arbitrary points along the 1D lattice (e.g., Fig. 4). Then, the exact G [up to a factor $(ik)^{-1}$, unnecessary for our purposes] reads [38,50]

$$G(x_f,x_i;k) = \sum_{\text{s.p.}} W_{\text{s.p.}} \exp[i\,S_{\text{s.p.}}(x_f,x_i;k)]. \qquad (17)$$

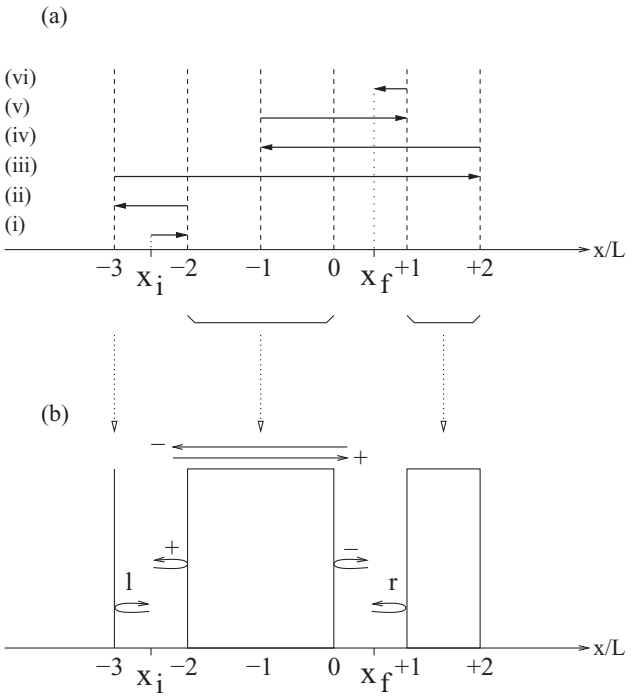

FIG. 4. (a) For a finite Kronig-Penney lattice of six general point interactions, and specific end points x_i and x_f, a representative "scattering path" composed by stretches, (i)–(vi), of straight trajectories. It has a total length of $L_{\text{s.p.}} = 11 + (-2 - x_i) + (1 - x_f)$, ($L = 1$). (b) The $\mathcal{R}$'s and $\mathcal{T}$'s in Eq. (18) are the resulting composite reflection and transmission amplitudes for sets of point interaction potentials, as illustrated.

The sum is performed over all possible infinite "scattering paths" (s.p.) starting and ending at the points x_i and x_f. For each s.p., the classical action is written as $S_{\text{s.p.}} = k\,L_{\text{s.p.}}$, with $L_{\text{s.p.}}$ the s.p. total length. The prefactor amplitude (or weight) $W_{\text{s.p.}}$ is given by the product of the quantum coefficients gained each time the particle is scattered off by a given contact potential along the way.

To illustrate a typical term in Eq. (17), we consider a lattice with six point interactions equally spaced by $L = 1$. Taking as the end points $-3 < x_i < -2$ and $0 < x_f < 1$, a representative scattering path is depicted in Fig. 4. For such s.p., the particle starts at x_i, goes to the right, reflects from $x = -2$, moves to the left, reflects from $x = -3$, and then goes to the right, tunneling all the potentials until reflecting from $x = 2$. In this part of the trajectory—stretches (i), (ii), and (iii) in Fig. 4(a)—the partial weight is $W_{(i)+(ii)+(iii)} = r_{-2}^{(+)}\,r_{-3}^{(-)}\,t_{-2}^{(+)}\,t_{-1}^{(+)}\,t_{0}^{(+)}\,t_{+1}^{(+)}\,r_{+2}^{(+)}$. From $x = 2$, the particle travels to the left, is transmitted through the potentials at $x = 1$ and $x = 0$, and then is reflected by the point interaction at $x = -1$. Next, it travels to $x = 1$ (tunneling the potential at the origin), suffers another reflection, and finally gets to the end point x_f. In this part of the trajectory—(iv), (v), and (vi) in Fig. 4(a)—the amplitude is $W_{(iv)+(v)+(vi)} = t_{+1}^{(-)}\,t_{0}^{(-)}\,r_{-1}^{(-)}\,t_{0}^{(+)}\,r_{+1}^{(+)}$. Hence, the total prefactor weight for this particular s.p. is $W_{\text{s.p.}} = W_{(i)+(ii)+(iii)} \times W_{(iv)+(v)+(vi)}$. The scattering path length is

simply $L_{\text{s.p.}} = 11 + (-2 - x_i) + (1 - x_f)$, as readily seen from Fig. 4(a).

To obtain G in a closed form, one should classify and to sum up [cf. Eq. (17)] all the infinitely many possible trajectories of the kind exemplified above. Fortunately, it always can be done by regrouping the infinite sets of trajectories into a finite number of classes [38,52]. Furthermore, as proved in [50], these classes form geometric series, allowing their exact summation. For instance, from such a procedure the correct Green function for the system in Fig. 4 can be calculated, leading to [38,50]

$$\begin{aligned} G(x_f,x_i;k) = {} & \frac{\mathcal{T}_+}{[1-\mathcal{R}_{\rm l}\mathcal{R}_+][1-\mathcal{R}_-\mathcal{R}_{\rm r}]-\mathcal{T}_+\mathcal{T}_-\mathcal{R}_{\rm l}\mathcal{R}_{\rm r}} \\ & \times (\exp[-ikx_i]+\mathcal{R}_{\rm l}\exp[ikx_i]) \\ & \times (\exp[ikx_f]+\mathcal{R}_{\rm r}\exp[-ikx_f]). \end{aligned} \tag{18}$$

In the above expression, the $\mathcal{R}$'s and $\mathcal{T}$'s are effective reflection and transmission amplitudes, resulting from groups of zero-range potentials as depicted in Fig. 4(b). They are explicitly given by

$$\begin{aligned} \mathcal{R}_{\rm l} &= r_{-3}^{(-)}\exp[6ik], \quad \mathcal{R}_{\rm r} = r_{+1}^{(+)}\exp[2ik] + \frac{t_{+1}^{(-)}t_{+1}^{(+)}r_{+2}^{(+)}\exp[4ik]}{1-r_{+1}^{(-)}r_{+2}^{(+)}\exp[2ik]}, \\ \mathcal{R}_+ &= r_{-2}^{(+)}\exp[-4ik] + \frac{\left[r_{-1}^{(+)} - \left(r_{-1}^{(-)}r_{-1}^{(+)} - t_{-1}^{(-)}t_{-1}^{(+)}\right)r_0^{(+)}\exp[2ik]\right]t_{-2}^{(-)}t_{-2}^{(+)}\exp[-2ik]}{1-\left(r_{-2}^{(-)}r_{-1}^{(+)}+r_{-1}^{(-)}r_0^{(+)}\right)\exp[2ik]+\left(r_{-1}^{(-)}r_{-1}^{(+)}-t_{-1}^{(-)}t_{-1}^{(+)}\right)r_{-2}^{(-)}r_0^{(+)}\exp[4ik]}, \\ \mathcal{T}_+ &= \frac{t_{-2}^{(+)}t_{-1}^{(+)}t_0^{(+)}}{1-\left(r_{-2}^{(-)}r_{-1}^{(+)}+r_{-1}^{(-)}r_0^{(+)}\right)\exp[2ik]+\left(r_{-1}^{(-)}r_{-1}^{(+)}-t_{-1}^{(-)}t_{-1}^{(+)}\right)r_{-2}^{(-)}r_0^{(+)}\exp[4ik]}, \\ \mathcal{R}_- &= \mathcal{R}_+\exp[4ik], \text{ where in } \mathcal{R}_+ \text{ we exchange } (+)\longleftrightarrow(-) \text{ and } j=-2\longleftrightarrow j=0, \\ \mathcal{T}_- &= \mathcal{T}_+, \text{ where in } \mathcal{T}_+ \text{ we exchange } (+)\longleftrightarrow(-) \text{ and } j=-2\longleftrightarrow j=0. \end{aligned} \tag{19}$$

Here, two points should be emphasized: (a) The energy domain G is given by a sum over all the possible multiple scattering processes suffered by the particle; (b) each s.p. in the series Eq. (17) represents a trajectory in which the particle spends a time of roughly $t \sim n\tau$, for n the number of scattering along the path (e.g., $n = 12$ in the example of Fig. 4).

In the study of QW, common questions are related to the system state, say, after evolving n steps. But from (a)–(b) above, such information is fully contained in the series representation of G. Therefore, since the correspondence between QW and generalized Kronig-Penney lattices is straightforward, we can readily associate each term in Eq. (17) to a possible evolution of a quantum walk [e.g., that in Eq. (7)]. Moreover, such terms can be viewed as a Fourier decomposition of G. Given that the Green-function Fourier transform is the time domain propagator, an individual term in Eq. (17), when properly mapped, represents then a possible path for $t = n$ time steps in the quantum walk.

Finally, depending on specific QW quantities we shall calculate, in practice a simple inspection and selection of paths in the expansion for G will suffice. However, for larger n's and more complicated topologies (Sec. IV), it may be cumbersome to deal with individual terms in Eq. (17). Fortunately, one can make the Green function a systematic protocol for QW by introducing the *path and step* operators. As we discuss in Sec. V, they are useful tools to extract any information about the system directly from an already summed closed expression for G.

IV. EXTENSION TO ARBITRARY TOPOLOGIES

QW can be defined in arbitrary topologies [15] (i.e., for general graph structures [7]). The scattering formulation is then obtained through a direct extension of the construction in Sec. II [4,5,7].

Suppose an undirected simple network [53] of sites connected by bonds (examples in Fig. 5). Its topology represents the particular Hilbert space arrangement in which the quantum walk dynamics takes place. Like the 1D lattice, each bond joining two neighbor sites—say j and j'—is associated with only two basis states, one incoming to j and the other to j'. For instance, for the bond joining (j_x-1,j_y) to (j_x,j_y) in Fig. 5(a), we have $|1,(j_x,j_y)\rangle$ and $|3,(j_x-1,j_y)\rangle$, whereas for the bond connecting j to j' (j to j'') in Fig. 5(b), we have $|3,j\rangle$ and $|1,j'\rangle$ ($|2,j\rangle$ and $|2,j''\rangle$). But contrary to the 1D case, the possible "directions" (bonds) to get to a site j from its first neighbors may depend on the specific j. Thus, the quantum number σ_j assumes the values $1,2,\ldots,K_j$, with K_j the coordination number (valence) of site j. In more regular structures $K_j = K$ regardless of j [e.g., $K = 4$ in Fig. 5(a)].

The construction of the time evolution operators is discussed e.g., in Refs. [4,5,7]. Here we just outline the main ideas following Ref. [7]. First, one needs to characterize the lattice topology, namely, to specify for any j the sets: (a) $\mathcal{S}_j = \{j^{(1)}, j^{(2)}, \ldots, j^{(K_j)}\}$ of all the K_j sites which are first neighbors of j [e.g., in Fig. 5(b), $\mathcal{S}_j = \{j', j'', j'''\}$]; (b) $\mathcal{N}_j = \{\sigma_{j^{(1)}},\sigma_{j^{(2)}},\ldots,\sigma_{j^{(K_j)}}\}$ for $\sigma_{j^{(n)}}$ the direction quantum number for the state incoming to site $j^{(n)}$ through the bond joining $j^{(n)}$ and j [in Fig. 5(b), $\mathcal{N}_j = \{\sigma_{j'}=1,\sigma_{j''}=2,\sigma_{j'''}=1\}$]; and (c) $\mathcal{B}_j = \{\tilde{\sigma}_{j^{(1)}},\tilde{\sigma}_{j^{(2)}},\ldots,\tilde{\sigma}_{j^{(K_j)}}\}$ with $\tilde{\sigma}_{j^{(n)}}$ the direction quantum number for the state $|\tilde{\sigma}_{j^{(n)}},j\rangle$ incoming to j along the bond connecting j and $j^{(n)}$ [in Fig. 5(b), $\mathcal{B}_j = \{\tilde{\sigma}_{j^{(1)}}=3:$ bond j–j', $\tilde{\sigma}_{j^{(2)}}=2:$ bond j–j'', $\tilde{\sigma}_{j^{(3)}}=1:$ bond j–$j'''\}$].

Second, one defines the one-step time evolution U in terms of its action over each basis state $|\sigma_j, j\rangle$, or (with $\sigma_j = \tilde{\sigma}_{j^{(i)}} \in$

$\mathcal{B}_j$ and $\sigma_{j^{(i)}}$ the corresponding element in $\mathcal{N}_j$)

$$U(\gamma)|\sigma_j, j\rangle = \exp[i\gamma]\Big(r_{\sigma_j\sigma_j,j}|\sigma_{j^{(i)}}, j^{(i)}\rangle + \sum_{n=1;n\neq i}^{n=K_j} t_{\sigma_j\tilde{\sigma}_{j^{(n)}},j}|\sigma_{j^{(n)}}, j^{(n)}\rangle\Big). \quad (20)$$

Finally, the r's and t's are chosen such that for any j the $K_j \times K_j$ matrix Γ_j (of elements $[\Gamma_j]_{\sigma\,\sigma} = r_{\sigma\sigma,j}$ and $[\Gamma_j]_{\sigma'\sigma} = t_{\sigma'\sigma,j}$, for both $\sigma \neq \sigma'$ in $\{1,2,\ldots,K_j\}$) is unitary. This makes U also unitary [7], establishing SQW in arbitrary topologies.

The usual (i.e., continuous in time and space) quantum mechanical dynamics on network structures (known as quantum graph systems [54]) is likewise a generalization of the evolution in a 1D lattice with zero-range potentials [38,55]. It is obtained by properly matching the solutions of a 1D free [56] Schrödinger equation in the different arms (bonds) at the vertices (sites). For this end, one assumes for each j a matrix $S_j(k)$ (see below), which describes how an incoming plane wave of wave number k is scattered off at the vertex j. So, any j can be viewed as a general point interaction, but

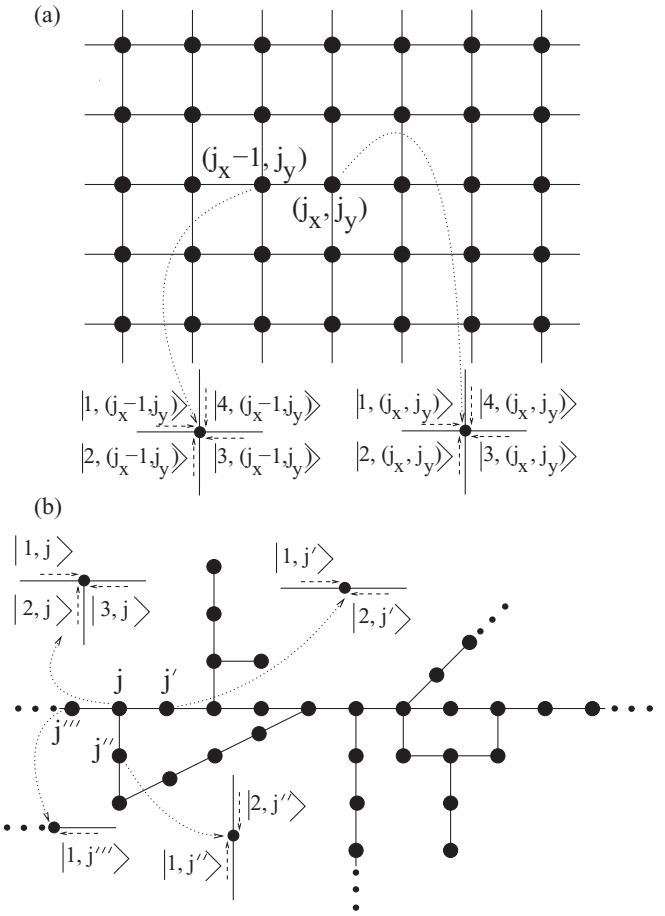

FIG. 5. Examples of graph structures, which generalize 1D QW. For SQW, the states (as illustrated) are defined on the bonds joining the different sites j. (a) All the sites have a same number of first neighbors in a regular topology. (b) For an irregular structure, such number depends on j.

connecting K_j directions instead of the common two (left and right) on the line. Furthermore, if for all j, $S_j S_j{}^\dagger = S_j{}^\dagger S_j = \mathbf{1}$, the resulting dynamics is unitary, conserving flux probability.

Quantum graphs can be solved through a Green-function approach [57]. In fact, it has been shown [39] that the exact G is also given by Eq. (17), where now the scattering paths are all the possible trajectories along the network, starting and ending at the points x_i and x_f (located in arbitrary arms of the graph). The W's are the quantum amplitudes gained along the s.p.'s due to the scattering at the different sites. Finally, the mentioned procedure of classifying and summing up different classes of s.p.'s still holds in this case [39]. So, we always can write the exact G as a closed analytical expression.

Summarizing, QW in general networks are direct extensions of QW in 1D exactly in the same way that quantum graphs are natural extensions of Kronig-Peney lattices. Therefore, it is easy to realize that our previous mapping between the two types of systems in 1D remains valid in arbitrary topologies, too.

Lastly, to define the reflection and transmission scattering amplitudes in a quantum graph—and to associate them with QW coefficients—we consider the same labeling used to characterize the lattices' topologies. Thus, for $\mathcal{B}_j = \{\tilde{\sigma}_{j^{(1)}}, \tilde{\sigma}_{j^{(2)}}, \ldots, \tilde{\sigma}_{j^{(K_j)}}\}$, the matrix elements of S_j are

$$[S_j]_{i\,i} = r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})}, \qquad [S_j]_{i\,l} = t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})}\ (i \neq l). \quad (21)$$

In Eq. (21), $r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})}$ ($t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})}$) is the reflection (transmission) coefficient for the particle incoming to site j from bond $\tilde{\sigma}_{j^{(i)}}$ to be reflected (transmitted) to bond $\tilde{\sigma}_{j^{(i)}}$ ($\tilde{\sigma}_{j^{(l)}}$). The unitarity of the S_j's plus the symmetries of the Schrödinger equation for real potentials [58] [i.e., $S_j{}^\dagger(k) = S_j(-k)$], yield (where $i,l,n = 1,2,\ldots,K^{(j)}$)

$$\begin{aligned}
r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})}(k) &= r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})^*}(-k),\\
t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})}(k) &= t_j^{(\tilde{\sigma}_{j^{(l)}}\tilde{\sigma}_{j^{(i)}})^*}(-k),\\
\sum_{l\neq i} t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})} t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})^*} + r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})} r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})^*} &= 1,\\
\sum_{n\neq i,l} t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(n)}})} t_j^{(\tilde{\sigma}_{j^{(l)}}\tilde{\sigma}_{j^{(n)}})^*} + r_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(i)}})} t_j^{(\tilde{\sigma}_{j^{(l)}}\tilde{\sigma}_{j^{(i)}})^*}&\\
+ r_j^{(\tilde{\sigma}_{j^{(l)}}\tilde{\sigma}_{j^{(l)}})^*} t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})} &= 0. \quad (22)
\end{aligned}$$

The above are natural generalizations [39,58] of the usual relations for the scattering coefficients [cf. Eqs. (3) and (9)] of a point scatterer on the line. Note also that if we impose time-reversal invariance, $t_j^{(\tilde{\sigma}_{j^{(i)}}\tilde{\sigma}_{j^{(l)}})} = t_j^{(\tilde{\sigma}_{j^{(l)}}\tilde{\sigma}_{j^{(i)}})}$.

Hence, the direction coefficients in a quantum walk, the Γ_j's, are in one-to-one correspondence with the scattering matrices S_j's in a quantum graph system.

V. EXTRACTING INFORMATION FROM G: THE STEP AND PATH OPERATORS

From the previous results, it turns out that the exact Green function, Eq. (17), is actually the *generating function* of all the possible walks leaving from and arriving at the bonds corresponding to x_i and x_f, respectively. So, any individual or

group of QW paths are obtained through proper manipulations of G.

In this way, more simple tasks like to determine all the trajectories for $|\Psi(0)\rangle = |\sigma, j\rangle$ evolving, say, only two times steps ($n = 2$), can be done by identifying particular terms directly in the G series representation, Eq. (17). However, the huge proliferation of paths in instances such as to find certain trajectories connecting two bonds very far apart, or resulting from high values of n, makes the full series expansion difficult to deal with. In such cases, a better approach is first to sum up the series [59] [using the already mentioned procedures in the literature [38,39,50,51] to get expressions like Eq. (18)] and then to extract the sought information from G with the help of the two operators described below.

The first is $\hat{S}_n$, yielding all the paths of exactly n time steps. To define $\hat{S}_n$, note that any walk state gains a factor $\exp[i\gamma]$ at each time step [see Eq. (20)]. From the mapping, such a factor is equivalent to $z = \exp[ikL]$ in the (continuous) quantum graph problem. So, let us set G_z as G in Eq. (17), but with the substitution $\exp[ikL] \to z$, and for which the scattering amplitudes are identified with the appropriate quantum walk coefficients Γ_j's (Sec. IV). Thus, one finds that if the step operator $\hat{S}_n$ acting on G_z has the form,

$$\hat{S}_n \equiv \frac{1}{n!}\frac{\partial^n}{\partial z^n}\bigg|_{z=0}, \tag{23}$$

then $\left|\hat{S}_n G_z\right|^2$ gives the total probability for the quantum walk to leave the bond x_i and to get to the bond x_f in exactly n steps. We should mention that such construction has already been proposed in [5,44] to treat scattering problems. Considering the Green-function approach, we see that $\hat{S}_n$ can be applied in more general contexts.

The second is $\hat{P}_{\mathcal{P}}$, which extracts from G all the paths with specific trajectory stretches $\mathcal{P}$. Any quantum walk s.p. can be described by the sequence of coefficients r and t it gains along the way [cf. Eq. (7)]. For instance, consider Fig. 5(b) and assume $n = 6$ applications of U to the system initially at $|1, j\rangle$. One possible sequence of successively visited states during the evolution, thus representing a possible path, is

$$|1,j\rangle \to |1,j'\rangle \to |3,j\rangle \to |1,j'\rangle \to |3,j\rangle \to |2,j''\rangle \to |2,j\rangle.$$

Here $W = t_{1\,1,j}\, r_{1\,1,j'}\, r_{3\,3,j}\, r_{1\,1,j'}\, t_{3\,2,j}\, r_{2\,2,j''}$ is its probability amplitude, which can be rewritten as $W = (r_{1\,1,j'})^2\,(r_{3\,3,j})^1\,(r_{2\,2,j''})^1\,(t_{1\,1,j})^1\,(t_{3\,2,j})^1$. Thus, any trajectory (or part of it) can be represented by $\mathcal{P} = \{(\alpha_1,n_{\alpha_1}),(\alpha_2,n_{\alpha_2}),\ldots;(\beta_1,n_{\beta_1}),(\beta_2,n_{\beta_2}),\ldots\}$, that is, by the set of indexes and exponents associated with the quantum coefficients r and t of the path stretch (with α and β standing for $\sigma'\sigma'', j$). In our example, $\alpha_1 = 1\,1, j'$; $\alpha_2 = 3\,3, j$; $\alpha_3 = 2\,2, j$; $\beta_1 = 1\,1, j'$; $\beta_2 = 3\,2, j$; $n_{\alpha_1} = 2$; $n_{\alpha_2} = n_{\alpha_3} = n_{\beta_1} = n_{\beta_2} = 1$.

Now, by properly choosing x_i and x_f (which obviously depends on $\mathcal{P}$; see Sec. VI) we get that $G_{\mathcal{P}} = \hat{P}_{\mathcal{P}} G$ is a sum—in the form of Eq. (17)—but containing only paths whose parts of their trajectories are given by $\mathcal{P}$. The explicit expression for $\hat{P}_{\mathcal{P}}$ is

$$\hat{P}_{\mathcal{P}} \equiv \prod_{\alpha\in\mathcal{P}} \frac{(r_\alpha)^{n_\alpha}}{n_\alpha!}\frac{\partial^{n_\alpha}}{\partial r_\alpha^{n_\alpha}}\bigg|_{r_\alpha=0} \prod_{\beta\in\mathcal{P}} \frac{(t_\beta)^{n_\beta}}{n_\beta!}\frac{\partial^{n_\beta}}{\partial t_\beta^{n_\beta}}\bigg|_{t_\beta=0}, \tag{24}$$

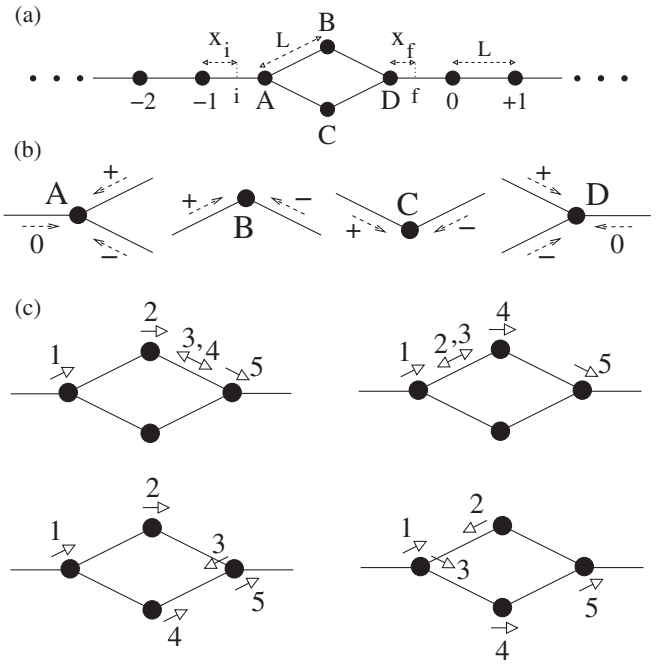

FIG. 6. (a) A graph composed by a diamond-shaped region (sites A, B, C, D) attached to semi-infinite leads (sites $j \leqslant -1$ and $j \geqslant 0$, for which $r_j = 0$ and $t_j = 1$). (b) The σ labeling for A, B, C, and D. (c) For $n = 5$ time steps, schematics of all possible s.p.'s first entering into the diamond region through the superior bond [those entering through the inferior bond are simple specular images of (c)].

which must act on the Green function as the following: First one performs all the indicated derivatives; second, one sets the coefficients r_α and t_β equal to zero; finally one multiplies the resulting expression by the coefficients $(r_\alpha)^{n_\alpha}$'s and $(t_\beta)^{n_\beta}$'s.

If we shall select just a path which is itself entirely represented by $\mathcal{P}$, then in the above definition we simply change $|_{r_\alpha=0}$ and $|_{t_\beta=0}$ by $|_{r=0}$ and $|_{t=0}$, with r and t *all* the quantum amplitudes in G.

Lastly, we note that for an initial state being the superposition of N basis states, $|\Psi(0)\rangle = \sum_{\sigma,j} c_{\sigma,j}|\sigma, j\rangle$, we must consider N Green functions, each with a x_i corresponding to the bond of $|\sigma, j\rangle$. So, in any calculation, the contribution of each of these G's should be weighted by the associated factor $c_{\sigma,j}$.

VI. AN EXAMPLE: A DIAMOND-SHAPED GRAPH

Finally, to illustrate some features of our Green-function approach, we discuss a quantum walk for the topology depicted in Fig. 6. We assume complete general coefficients [observing Eq. (22)], in the diamond region—sites A, B, C and D—and free evolution, $r_j = 0$ and $t_j = 1$, in the leads region—sites $j \leqslant -1$ and $j \geqslant 0$. We mention that this system, in the case of $r_A = r_D = -1/3$, $t_A = t_D = 2/3$, $r_B = r_C = 0$, and $t_B = t_C = 1$, has been studied in Ref. [44]. Such particular values represent the so-called Grover coins (see, e.g., [3]).

Consider this quantum graph for the initial and the end positions x_i and x_f, respectively, in the bonds i and f

[Fig. 6(a)]. The exact Green function reads

$$G(x_f,x_i;k) = \mathcal{T}\exp[ik(x_f - x_i)], \tag{25}$$

with $\mathcal{T}$ the global transmission amplitude resulting from the multiple s.p.'s which cross the diamond-shaped region. By using the procedures in [39], one gets

$$\mathcal{T} = \left(\frac{t_{0+,A}\,P_+ + t_{0-,A}\,P_-}{g}\right)\exp[2i\gamma]. \tag{26}$$

P_+/g (P_-/g) represents the contribution of all the s.p.'s which initially enter the diamond region through the superior (inferior) arm. They are given by ($\sigma = \pm$ and $\overline{\sigma} = -\sigma$)

$$\begin{aligned}
P_\sigma &= T_{\sigma\,0} + \{T_{\overline{\sigma}\,0}(T_{\sigma\,\overline{\sigma}}\,r_{\overline{\sigma}\,\overline{\sigma},A} + R_{\sigma\,\sigma}\,t_{\sigma\overline{\sigma},A}) - T_{\sigma\,0}(T_{\overline{\sigma}\,\sigma}\,t_{\sigma\,\overline{\sigma},A} + R_{\overline{\sigma}\,\overline{\sigma}}\,r_{\overline{\sigma}\,\overline{\sigma},A})\}\exp[2i\gamma],\\
g &= \{1 - (T_{+-}\,t_{-+,A} + R_{++}\,r_{++,A})\exp[2i\gamma]\}\{1 - (T_{-+}\,t_{+-,A} + R_{--}\,r_{--,A})\exp[2i\gamma]\}\\
&\quad -(T_{+-}\,r_{--,A} + R_{++}\,t_{+-,A})(T_{-+}\,r_{++,A} + R_{-+}\,t_{-+,A})\exp[4i\gamma],\\
T_{+0} &= t_{+-,B}\,\{t_{+0,D} + r_{--,C}\,(t_{+-,D}\,t_{-0,D} - r_{--,D}\,t_{+0,D})\exp[2i\gamma]\}\exp[i\gamma]/f,\\
T_{+-} &= t_{+-,B}\,t_{+-,D}\,t_{-+,C}\exp[2i\gamma]/f,\\
R_{+-} &= r_{++,B} + t_{+-,B}\{t_{-+,B}\,r_{++,D} + t_{-+,B}\,r_{--,C}\,(t_{-+,D}\,t_{+-,D} - r_{++,D}\,r_{--,D})\exp[2i\gamma]\}\exp[2i\gamma]/f,\\
f &= (1 - r_{--,B}\,r_{++,D}\exp[2i\gamma])(1 - r_{--,C}\,r_{--,D}\exp[2i\gamma]) - t_{+-,D}\,t_{-+,D}\,r_{--,B}\,r_{--,C}\exp[4i\gamma]\\
T_{-0} &= T_{+0}, \qquad T_{-+} = T_{+-}, \qquad R_{--} = R_{++}, \text{ where in all the right-hand side terms we must exchange } B \longleftrightarrow C.
\end{aligned} \tag{27}$$

For Eqs. (26) and (27) we have already used the mapping, writing them in terms of quantum walk quantities.

The amplitude $\mathcal{T}$ simplifies considerably if for any σ, σ', we have $t_{\sigma\,\sigma',X} = t_X$ and $r_{\sigma\,\sigma,X} = r_X$ with $X = A,B,C,D$. Furthermore, if the coefficients for the sites A and D and for the sites B and C are set equal, namely, $r_A = r_D$, $t_A = t_D$, $r_B = r_C$, and $t_B = t_C$, Eqs. (26) and (27) yields

$$\mathcal{T} = \frac{2\,t_A^2\,t_B}{1 - 2\,(t_A + r_A)\,r_B\exp[2i\gamma] - (t_A + r_A)^2\left(t_B^2 - r_B^2\right)\exp[4i\gamma]}\exp[3i\gamma]. \tag{28}$$

For the particular Grover coin values, we get from Eq. (28) $\mathcal{T} = 8\exp[3i\gamma]/(9 - \exp[4i\gamma])$, in agreement with Ref. [44] as it should be.

We emphasize that $\mathcal{T}$ is given by a sum over all the possible paths leaving i, going into the diamond region, and finally leaving to the bond f. So, the probability for $i \to f$ in exactly n steps can be obtained by applying the step operator to $\mathcal{T}_z = \mathcal{T}|_{\exp[i\gamma]\to z}$. Such a type of calculation is useful because it gives the hitting time $|h_n|^2$ [31] (i.e., the probability for the walk to reach a given state $|\sigma,j\rangle$ from $|\sigma',j'\rangle$ as function of n). The present Green-function approach allows one to obtain hitting times in a rather direct way. To exemplify this, we first consider the most general case, Eqs. (26) and (27), and select all the paths reaching the bond f in five time steps. Then, $h_5 = \hat{S}_5\mathcal{T}_z$ reads

$$\begin{aligned}
h_5 &= t_{0+,A}\{[t_{+-,B}\,r_{++,D}\,r_{--,B} + r_{++,B}\,r_{++,A}\,t_{+-,B}]t_{+0,D} + [t_{+-,B}\,t_{+-,D}\,r_{--,C} + r_{++,B}\,t_{+-,A}\,t_{+-,C}]t_{-0,D}\}\\
&\quad + t_{0-,A}\{[t_{+-,C}\,r_{--,D}\,r_{--,C} + r_{++,C}\,r_{--,A}\,t_{+-,C}]t_{-0,D} + [t_{+-,C}\,t_{-+,D}\,r_{--,B} + r_{++,C}\,t_{-+,A}\,t_{+-,B}]t_{+0,D}\},
\end{aligned} \tag{29}$$

which represents the eight possible trajectories with $n = 5$ [Fig. 6(c)].

Certainly, in more symmetric situations analytical results are easier to obtain. Indeed, for the case of Eq. (28), $\mathcal{T}_z$ can be casted as

$$\mathcal{T}_z = \frac{-t_A^2}{(t_A + r_A)^2\left(t_B^2 - r_B^2\right)}\left\{\frac{t_B + r_B}{z^2 - z_-} + \frac{t_B - r_B}{z^2 - z_+}\right\}, \tag{30}$$

where $z_\pm = (\pm t_B - r_B)/[(t_A + r_A)(t_B^2 - r_B^2)]$. Hence, for $|h_n|^2 = |(n!)^{-1}\,(\partial^n\mathcal{T}_z/\partial z^n)_{z=0}|^2$, we find that

$$|h_n|^2 = \left|t_A^2\,(t_A + r_A)^{(n-1)/2-1}\right|^2 \times \begin{cases} |(t_B + r_B)^{(n-1)/2} - (-1)^{(n-1)/2}(t_B - r_B)^{(n-1)/2}|^2 & \text{if } n \text{ is odd},\\ 0 & \text{if } n \text{ is even}, \end{cases} \tag{31}$$

is the probability to cross the diamond region in exactly n steps. $|h_n|^2 = 0$ for $n < 3$, since at least three time steps are necessary to leave the bond i and to arrive at bond f. Also, from a direct inspection in Fig. 6 one realizes that a transmission is not possible for an even number of steps, a result explicit in Eq. (31). If $t_B = t_C = 0$, obviously the system never gets to the right lead and Eqs. (28) and (31) are identically null. Finally, if we consider $r_B = 0$ and $t_B = 1$, we find $P_n \neq 0$ only for $n \equiv 3 \pmod 4$. Furthermore, assuming $t_A = 2/3$ and $r_A = -1/3$, we recover the result in Ref. [44], namely, $|h_n|^2 = (8/9^{(n+1)/4})^2$ for $n \equiv 3 \pmod 4$ and $|h_n|^2 = 0$ otherwise.

As discussed in the previous section, specific $\mathcal{P}$'s are obtained from the Green function by means of the path operator $\hat{P}_{\mathcal{P}}$. For instance, suppose we shall select the trajectories directly crossing the diamond region (i.e., transmissions through A, then through B or C, and finally through D, with no multiple reflections). In this special case, the path operator is

$$\hat{P}_{\mathcal{P}} = \frac{t_{+-,B}}{1!}\frac{\partial}{\partial t_{+-,B}}\bigg|_{t=0\,(t\neq t_{0+,A},\,t_{+0,D}),r=0} + \frac{t_{+-,C}}{1!}\frac{\partial}{\partial t_{+-,C}}\bigg|_{t=0\,(t\neq t_{0-,A},\,t_{-0,D}),r=0}, \tag{32}$$

leading to

$$\hat{P}_{\mathcal{P}}\,\mathcal{T} = (t_{0+,A}\,t_{+-,B}\,t_{+0,D} + t_{0-,A}\,t_{+-,C}\,t_{-0,D})\exp[3i\gamma]. \tag{33}$$

Note that Eq. (32) is in a simpler form than the general definition, Eq. (24). This is so because we have used the fact that $\hat{P}_{\mathcal{P}}$ acts on a transmission Green function. Indeed, there is no need to perform derivatives as e.g., $t_{0\sigma,A}\,(\partial/\partial t_{0\sigma,A})|_{t_{0\sigma,A}=0}$. Thus, the path operator is considerably simplified if we choose suitable configurations to calculate G.

We can think of more general paths, namely, to cross the diamond region in a total of $n = n_+ + n_-$ steps, but for exactly n_+ (n_-) steps taking in the superior (inferior) arm, that is, in the bonds A–B and B–D (A–C and C–D). If for simplicity we assume that for each site X ($X = B$ or C), all the t's and r's are equal, regardless the quantum numbers σ's [as in Eq. (28)], then the mentioned operator, to be applied to $\mathcal{T}$, is written as

$$\begin{aligned}\hat{P}_{\mathcal{P}} = \sum_{n_+^{(1)}+\ldots+n_+^{(6)}=n_+-1,\; n_-^{(1)}+\ldots+n_-^{(6)}=n_--1} & \frac{(t_{-+,A})^{n_+^{(1)}}}{n_+^{(1)}!}\frac{(r_{++,A})^{n_+^{(2)}}}{n_+^{(2)}!}\frac{(t_B)^{n_+^{(3)}}}{n_+^{(3)}!}\frac{(r_B)^{n_+^{(4)}}}{n_+^{(4)}!}\frac{(t_{-+,D})^{n_+^{(5)}}}{n_+^{(5)}!}\frac{(r_{++,D})^{n_+^{(6)}}}{n_+^{(6)}!} \\ \times \frac{(t_{+-,A})^{n_-^{(1)}}}{n_-^{(1)}!}\frac{(r_{--,A})^{n_-^{(2)}}}{n_-^{(2)}!}\frac{(t_C)^{n_-^{(3)}}}{n_-^{(3)}!}\frac{(r_C)^{n_-^{(4)}}}{n_-^{(4)}!}\frac{(t_{+-,D})^{n_-^{(5)}}}{n_-^{(5)}!}\frac{(r_{--,D})^{n_-^{(6)}}}{n_-^{(6)}!} & \left[\left(\frac{\partial^{n_+^{(1)}}}{\partial t_{-+,A}^{n_+^{(1)}}}\right)\left(\frac{\partial^{n_+^{(2)}}}{\partial r_{++,A}^{n_+^{(2)}}}\right)\left(\frac{\partial^{n_+^{(3)}}}{\partial t_B^{n_+^{(3)}}}\right)\left(\frac{\partial^{n_+^{(4)}}}{\partial r_B^{n_+^{(4)}}}\right)\left(\frac{\partial^{n_+^{(5)}}}{\partial t_{-+,D}^{n_+^{(5)}}}\right)\right. \\ \times \left.\left(\frac{\partial^{n_+^{(6)}}}{\partial r_{++,D}^{n_+^{(6)}}}\right)\left(\frac{\partial^{n_-^{(1)}}}{\partial t_{+-,A}^{n_-^{(1)}}}\right)\left(\frac{\partial^{n_-^{(2)}}}{\partial r_{--,A}^{n_-^{(2)}}}\right)\left(\frac{\partial^{n_-^{(3)}}}{\partial t_B^{n_-^{(3)}}}\right)\left(\frac{\partial^{n_-^{(4)}}}{\partial r_B^{n_-^{(4)}}}\right)\left(\frac{\partial^{n_-^{(5)}}}{\partial t_{+-,D}^{n_-^{(5)}}}\right)\left(\frac{\partial^{n_-^{(6)}}}{\partial r_{--,D}^{n_-^{(6)}}}\right)\right]_{t=0\,(t\neq t_{0\pm,A},\;t_{\pm 0,D}),\;r=0}.\end{aligned} \tag{34}$$

Although the above expression may seem rather cumbersome, it is amenable to work with by using algebraic manipulation softwares (what we have tested by investigating different situations; results will be reported elsewhere). In certain instances, nevertheless, the calculations can be carried on straightforwardly. For instance, consider all the paths which get to the right lead only passing through the superior arm. Furthermore, assume that among them, we shall select those tunneling the site B exactly n times. In this case, the path operator is simply

$$\hat{P}_{\mathcal{P}} = \frac{(t_B)^n}{n!}\frac{\partial^n}{\partial t_B^n}\bigg|_{t=0\,(t\neq t_{0+,A},\;t_{+0,D}),\;r=0\,(r\neq r_{++,A},\;r_{++,D})}. \tag{35}$$

For n even its results in $\hat{P}_{\mathcal{P}}\mathcal{T} = 0$, and for n odd in

$$\hat{P}_{\mathcal{P}}\mathcal{T} = \frac{t_{0+,A}\,(r_{++,A})^{\frac{n-1}{2}}\,(t_B)^n\,(r_{++,D})^{\frac{n-1}{2}}\,t_{+0,D}\,\exp[(2n+1)i\gamma]}{(1-r_{++,A}r_B\exp[2i\gamma])^{\frac{n+1}{2}}(1-r_Br_{++,D}\exp[2i\gamma])^{\frac{n+1}{2}}}. \tag{36}$$

VII. CONCLUSION

By means of appropriate mappings to systems for which the exact G can be calculated, quantum graphs, we have obtained closed and general expressions for SQW Green functions. Furthermore, the procedure allows one to discuss complete arbitrary topologies and position-dependent quantum amplitudes [60].

By introducing two operators, namely, step and path operators, we have shown how to extract from G any relevant dynamical information about the system. For instance, one can exploit particular paths in a quantum walk as well as obtain the contribution of orbits of specific time length n. Such possibilities have been exemplified in details for a diamond-shaped graph structure.

An important fact, not explored in this contribution, is that our formulation naturally allows the introduction of energy (or equivalently, wave number k) dependent transition amplitudes. In the QW context, such k could be faced as an extra inner variable. Since different walks may have different k's, using the Green-function approach, then one could address the case of collective QW. A complete study of energy-dependent SQW will be the subject of a future work.

Finally, we have discussed G only for QW scattering formulation. Nevertheless, as already mentioned in the Introduction, the SQW and CQW are unitary equivalent. Moreover, CTQW are associated with CQW. So, the Green-function framework for SQW can be extended to such other constructions as well.

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