Discrete-time quantum walk approach to state transfer

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We show that a quantum-state transfer, previously studied as a continuous-time process in networks of interacting spins, can be achieved within the model of discrete-time quantum walks with a position-dependent coin. We argue that, due to additional degrees of freedom, discrete-time quantum walks allow one to observe effects which cannot be observed in the corresponding continuous-time case. First, we study a discrete-time version of the engineered coupling protocol due to Christandl *et al.* [Phys. Rev. Lett. **92**, 187902 (2004)] and then we discuss the general idea of conversion between continuous-time quantum walks and discrete-time quantum walks.

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I. INTRODUCTION

Lattice models appear in quantum theory in various contexts. Just like most theoretical models in physics, they were first used to describe the properties of natural materials; however, nowadays we are reaching the stage when we are no longer bounded by nature, since our ability to engineer our own new systems with the desired physical properties is developing very rapidly. This allows testing of abstract theoretical lattice models in the laboratory with the help of new extraordinary systems like graphene [1], cold atoms in optical lattices [2], photons in arrays of linear optical elements [3], or compounds of thin layers of different materials known as heterostructures [4]. The new field of quantum information, which strongly relies on the capability of engineering and manipulation of quantum systems, has also rekindled interest in lattice models. In particular, it has been shown that lattice models offer the possibility of universal quantum computation [5,6].

In this work we consider two related fields of research: quantum walks on graphs [7,8] and quantum information transfer in spin systems [9,10]. In particular we are interested in the discrete-time quantum walk realization of a quantum-state transfer on a spin chain with position-dependent couplings [11]. It is known that special cases of spin lattice models with one magnetic excitation can be interpreted as continuous-time quantum walks [7]. Also, it has been shown that the relation between the two types of quantum walks is not trivial [12,13], because discrete-time quantum walks require an additional degree of freedom known as a coin. We show how one can convert the position dependence of couplings into the position dependence of coins. We also argue that discrete-time quantum walks provide a more general framework for the description of quantum diffusion on regular lattices, since due to the extra degree of freedom one gains more control over the walk than is allowed in a standard continuous-time scenario. Moreover, the evolution of discrete-time quantum walks is much easier to simulate on a classical computer. Our approach is based on the relation between discrete-time quantum walks and the Dirac-like equation to which the underlying quantum walk is transformed in the continuous limit of both time and space [14–16].

II. BASIC CONCEPTS

A. State transfer in spin networks

Consider a network for which every vertex corresponds to a spin-1/2. We say that there is an edge between vertex i and j if the corresponding spins interact. Most authors choose to consider an XX model of spin-spin interactions [9,10]; we follow them and set the Hamiltonian of the network to be of the form

$$H = \sum_{\{i,j\}\in E} J_{ij}\left(\sigma_x^i\sigma_x^j + \sigma_y^i\sigma_y^j\right), \tag{1}$$

where E denotes the set of edges and σ_x^i is a Pauli X matrix for the ith spin. The above Hamiltonian conserves the total spin number along the Z axis, $\sum_i \sigma_z^i$; therefore, one may restrict studies to a subspace with a fixed number of excitations, where by excitation we mean a spin pointing up along the Z axis. In particular, we are interested in an evolution restricted to a subspace with no excitations, which is invariant under the evolution generated by the Hamiltonian, and to a subspace with only one excitation. In the second case, the single excitation can be considered a single particle walking on an underlying network.

Next, imagine that there are two marked spins, a sender and a receiver, and that the whole network is in a ground state, i.e., in a subspace with no excitations. Then, the sender prepares his spin in a superposition $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$, so that the whole network is in the state

$$(\alpha|\uparrow\rangle + \beta|\downarrow\rangle)_s \otimes |\downarrow\downarrow\cdots\downarrow\rangle_{\text{net}} \otimes |\downarrow\rangle_r. \tag{2}$$

The goal is to employ the evolution generated by the Hamiltonian to transfer the quantum state from s to r in finite time T,

$$|\downarrow\rangle_s \otimes |\downarrow\downarrow\cdots\downarrow\rangle_{\text{net}} \otimes (\alpha|\uparrow\rangle + \beta|\downarrow\rangle)_r, \tag{3}$$

which is equivalent to transporting the excitation from spin s to spin r.

There are many protocols which allow for a perfect, or a nearly perfect state transfer over spin chains. The basic techniques are engineered couplings, wave packet encoding,

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and active control (see Refs. [9,10]). Here we concentrate on engineered couplings. In particular, we consider two protocols, namely the protocol of Christandl *et al.* [11] and a weakly coupled spin protocol [17,18].

B. Continuous-time quantum walks

The state in continuous-time quantum walks (CTQWs) [7] is described by the position of a particle on a graph. The continuous evolution, which is governed by the Schrödinger equation, is determined by the Hamiltonian H which is an $n \times n$ Hermitian matrix proportional to the adjacency matrix of the underlying graph G which has n vertices:

$$H_{ij} \begin{cases} \neq 0, & \text{iff } (i,j) \in E(G), \\ = 0, & \text{else}, \end{cases} \tag{4}$$

where $E(G)$, as before, denotes the set of edges of G. The probability that at time t the walker, whose state is $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$, is located at vertex x is $P_x(t) = |\langle x|\psi(t)\rangle|^2$, where $\{|x\rangle\}$ is the orthonormal basis spanning the space of the vertices.

For CTQWs on a graph all of whose edges have equal weight, the corresponding Hamiltonian is simply the Laplacian of the underlying graph $L = D - A$, which is a diagonal matrix D minus the graph adjacency matrix A (whose entries A_{ij} are either 0 or 1 if vertices i and j are disconnected or connected, respectively). The diagonal entries $D_{jj} = d_j$ denote the degree of vertex j. As a result, the sum of all elements in each column and each row of the Laplacian is zero. When the Laplacian plays the role of the Hamiltonian, the diagonal entries are important only in the case of irregular graphs. For regular graphs they are all equal, and, since one can freely add or subtract from the Hamiltonian multiples of identity without changing the dynamics of the system, they can be neglected. In the case of a general CTQW on a chain, the only nonzero elements of the Hamiltonian are $H_{j,j+1}$, $H_{j,j-1}$, and H_{jj}. In the case of a single excitation subspace of a spin network, the elements of the corresponding CTQW Hamiltonian are given exactly by the strengths of spin couplings $H_{ij} = J_{ij}$.

C. Discrete-time quantum walks

In discrete-time quantum walks (DTQWs) [8], the state of the system $|x,c\rangle$ is described by the position of a walker on a graph x and by the state of an auxiliary system c which determines the direction the walker is going to take in the next step. This auxiliary system is often referred to as the coin, which for a walk on a one-dimensional graph like a chain or cycle is simply a two-level system $c = \leftarrow, \rightarrow$. In such cases, one step of the evolution is given by a unitary operator $U = SC$, which is a product of the coin operator

$$C|x, \rightarrow\rangle = \cos\theta|x, \rightarrow\rangle - \sin\theta|x, \leftarrow\rangle, \tag{5}$$

$$C|x, \leftarrow\rangle = \sin\theta|x, \rightarrow\rangle + \cos\theta|x, \leftarrow\rangle, \tag{6}$$

and the conditional shift operator

$$S|x, \rightarrow\rangle = |x+1, \rightarrow\rangle, \tag{7}$$

$$S|x, \leftarrow\rangle = |x-1, \leftarrow\rangle. \tag{8}$$

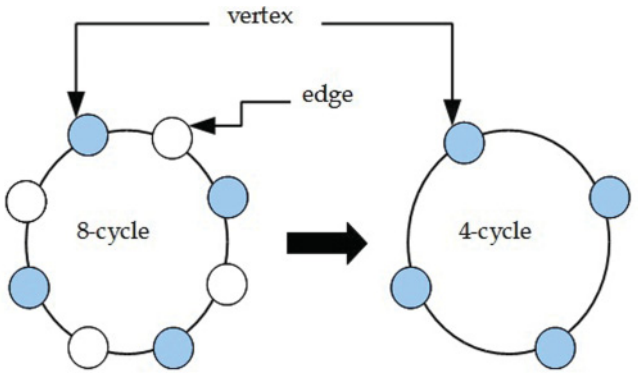

FIG. 1. (Color online) Because the interference phenomenon occurs for the second-nearest neighbors, even vertices can be interpreted as edges.

Therefore, one step is given by

$$U|x, \rightarrow\rangle = \cos\theta|x+1, \rightarrow\rangle - \sin\theta|x-1, \leftarrow\rangle, \tag{9}$$

$$U|x, \leftarrow\rangle = \sin\theta|x+1, \rightarrow\rangle + \cos\theta|x-1, \leftarrow\rangle. \tag{10}$$

The parameter θ denotes the coin flip rate. Equivalently, the unitary evolution operator of one step can be written as

$$U = e^{ip\sigma_z} e^{i\sigma_y\theta}, \tag{11}$$

where p is the momentum operator and σ_j are Pauli matrices acting on the coin space.

In DTQWs on chains and even cycles, interference occurs only between positions separated by a distance of two (second-nearest neighbors); therefore, one can consider two independent walks: one on even vertices and another on odd vertices. Because of this fact, even vertices can be treated as *edges* as in Fig. 1, which is crucial for our work. Since we are interested in the walk on *vertices*, not on edges, in our case one step of evolution is given by U^2 and the initial state is always supported on the vertex space only, as in Ref. [12]. Moreover, throughout this work we consider DTQWs on finite chains, which can be simulated by walks on cycles with a reversing coin at one vertex, i.e., a coin for which the coin flip rate is $\theta = \pi/2$ [see Eqs. (5) and (6) and Fig. 2].

III. CONTINUOUS LIMIT OF QUANTUM WALKS

The continuous limit of DTQWs on a chain results in the one-dimensional Dirac equation [14–16]. The operator (11) can be rewritten as

$$U = U(t) = e^{ip\sigma_z vt} e^{i\sigma_y\omega t}, \tag{12}$$

where v is the velocity and ω is the angular frequency. The two parameters are chosen so that for a unit time step $vt = 1$ and $\omega t = \theta$, thus recovering Eq. (11). Taking infinitesimal time steps and applying the Trotter theorem, one obtains

$$\lim_{n\to\infty} U(t/n)^n = e^{i(p\sigma_z v + \sigma_y\omega)t}. \tag{13}$$

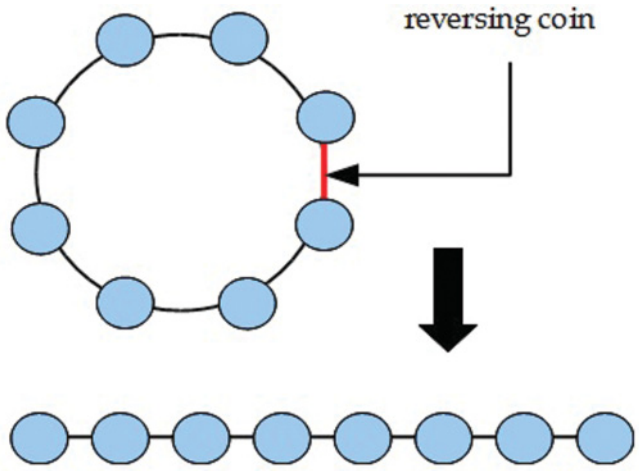

FIG. 2. (Color online) A DTQW on a finite chain is effectively simulated by a walk on a cycle. The coin operator associated to one of the vertices corresponding to edges (see Fig. 1) flips the coin state and as a result reverses the walk.

The term in parentheses above corresponds to the Hamiltonian of the system, which has exactly the form of the one-dimensional Dirac Hamiltonian,

$$H = cp\sigma_z + mc^2\sigma_y. \tag{14}$$

The correspondence between Eqs. (13) and (14) is fully established when one identifies v with the speed of light and ω with the mass of the particle. In particular, $\omega t = \theta$; however, we take $t = 1$ and therefore the mass of the quantum walker corresponds to the coin flip rate θ. However, due to the discrete nature of time and the periodicity of coin operator $e^{i\sigma_y\theta}$, one is unable to differentiate between θ and $\theta + k2\pi$. On the other hand, in the limit of infinite mass the particle should be almost immobile and the relation between the Dirac equation and the DTQW requires $\theta \to \frac{\pi}{2}$; hence, one often takes $m = \tan\theta$ (see Ref. [14]). Note that for small angles $\tan\theta \approx \theta$. It is also important to notice that, due to the structure of the conditional translation operator, the continuization of time is intrinsically combined with the continuization of space; i.e., either both space and time are continuous, or both are discrete.

The Hamiltonian of a CTQW on a chain with uniform couplings is the following: $H_{i,i+1} = H_{i+1,i} = -J$ and $H_{i,i} = 2J$; however, for regular graphs diagonal elements can be neglected and set equal to zero. The action of the Hamiltonian on a state localized at x is

$$H|x\rangle = -J\left(|x+1\rangle - 2|x\rangle + |x-1\rangle\right). \tag{15}$$

The above is a discrete version of the Laplacian. The continuization of the above leads to

$$H = -J\frac{d^2}{dx^2}. \tag{16}$$

Obviously, this Hamiltonian describes a free particle in one dimension with $J = \frac{1}{2m}$; therefore, the coupling constant J can be interpreted as an inverse of the walker's mass.

In the continuous limit, the quantum walker can be considered a relativistic (DTQW) or a nonrelativistic free particle (CTQW). The main parameters governing the dynamics of the walk, namely coins and couplings, are related to the particle's mass. Strauch [12] showed that a continuous-time quantum walk can be obtained from a discrete one in the limit $\theta \to \frac{\pi}{2}$. Heuristically, this limit corresponds to a very heavy particle, for which it is much harder to observe relativistic effects; therefore, it corresponds to a relativistic-to-nonrelativistic transition. Another important feature of quantum walks is that in both models space is discrete, but only for DTQWs is time also discrete. Once again, a heuristic explanation of this fact can be given as follows. Let the two quantum walks be discrete versions of Dirac and Schrödinger free particles, respectively. In a nonrelativistic model, time and space are treated separately; therefore, there is nothing strange in discretizing only one of them. However, in relativistic physics, time and space are combined and one has to discretize the whole space-time at once, since it would be problematic to define consistent Lorentz transformations on space-time which is only partially discrete.

IV. PERFECT-STATE TRANSFER IN DTQWS

Let us apply the analogy between mass, coins, and couplings to show that a perfect-state transfer from one position to another can be realized within DTQWs. We concentrate on the acclaimed perfect-state transfer protocol introduced by Christandl *et al.* [11]. This protocol relies on properly engineered couplings, i.e., properly chosen terms of the Hamiltonian governing the corresponding CTQW. These couplings depend on position; therefore, by our analogy, the corresponding particle has position-dependent mass. On the other hand, mass is related to coin flip rate and so the corresponding DTQW should have a position-dependent coin. Below we examine how the choice of such coins affects the dynamics of DTQWs.

The chain coupling between nodes n and $n+1$ in the protocol is given by $J_n = \frac{\lambda}{2}\sqrt{n(N-n)}$, where $n = 1,2,\ldots,N-1$ and λ is a real parameter common for all couplings. As a result, the effective mass of the particle for the transfer between positions n and $n+1$ is

$$m_n = \frac{1}{2J_n} = \frac{1}{\lambda\sqrt{n(N-n)}}. \tag{17}$$

Next, consider a step operator of the form

$$U = U(n) = e^{ip\sigma_z}e^{i\sigma_y\theta_n}, \tag{18}$$

where θ_n depends on position. The matrix form of the coin operator is given by

$$C_n = \begin{pmatrix} \cos\theta_n & \sin\theta_n \\ -\sin\theta_n & \cos\theta_n \end{pmatrix}. \tag{19}$$

Recall that we consider a double-step operator U^2, since our walk on a chain of length $N/2$ is simulated by a walk on an even-N cycle for which even positions correspond to edges and we are interested in a walk on positions corresponding to vertices. Coins associated with edge positions correspond to mass, but there are also coins associated with vertices—odd positions of the cycle. Here, we set all of them to be identities ($\theta_{2k-1} = 0$), although we note that a different choice (equal for all vertices) leads to similar results. The edge coins

(even positions) are chosen according to the analogy between couplings and mass ($m = \tan\theta$),

$$\theta_{2k} = \arctan \frac{1}{2\lambda\sqrt{k\left(\frac{N}{2}-k\right)}}, \tag{20}$$

where $k = 1, 2, \ldots, N/2 - 1$.

Our studies show that the transfer strongly depends on the parameter λ. For small values of λ (large mass limit), the transfer is perfect. Around $\lambda = \frac{\pi}{N}$ it starts to drop down and it recovers back to a perfect transfer for λ of the order $O(1)$ and greater (small mass limit). We show that the nature of transport for the two limiting cases is drastically different. In the small-mass limit, perfect transfer occurs due to the dispersionless nature of the operator $e^{ip\sigma_z}$ whose spectrum is linear, whereas in the large-mass limit the generator of the operator U^2 is effectively given by a Hermitian operator whose action is the same as the action of the Hamiltonian introduced by Christandl *et al.* [11]. Interestingly, in both cases we found that the transfer fidelity does not depend on the initial coin state. Moreover, we checked numerically that a number of initial coin states, among which were eigenvectors of the three Pauli matrices, are always perfectly transferred. This fact allows us to conjecture that in the DTQW case not only the particle but also its intrinsic coin state is perfectly transferred: $\alpha|1, \rightarrow\rangle + \beta|1, \leftarrow\rangle \rightarrow \alpha|N-1, \rightarrow\rangle + \beta|N-1, \leftarrow\rangle$.

In Fig. 3 we present the transfer of a particle from position 1 to position $N-1$ for the corresponding DTQW with respect to evolution operator U^2. In this particular case $N = 30$ and $\lambda = 0.03$. As one can see the transfer is perfect, and moreover the dynamics is periodic because after twice the transfer time the system goes back to the initial state, as in the continuous-time case.

The main idea of the authors of the protocol [11] was to find a mirror-symmetric Hamiltonian with a harmonic spectrum, which would provide periodicity of evolution and a perfect transfer between mirror-symmetric positions for times equal to half of a period. Numerical simulations confirm that the spectrum of U^2 is also harmonic, yet it possesses an additional

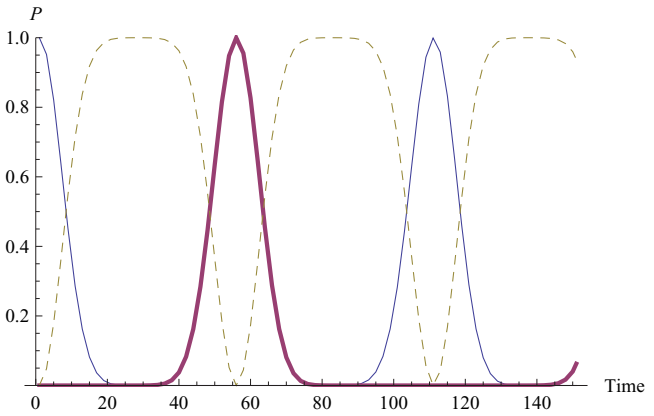

FIG. 3. (Color online) The evolution of perfect-state transfer from position 1 to position $N-1$ for DTQW with position-dependent coin ($N = 30$ and $\lambda = 0.03$). Thin (blue) line, probability of occupying position 1; thick (purple) line, probability of occupying position $N-1$; dashed line, probability of occupying remaining vertices of the chain.

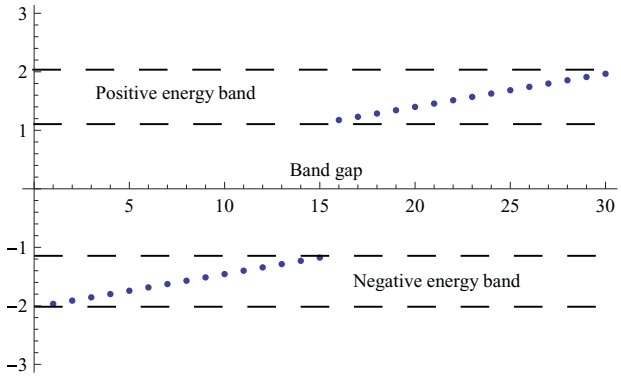

FIG. 4. (Color online) Arguments $\varphi \in [-\pi, \pi]$ of eigenvalues $e^{i\varphi}$ of a position-dependent coin DTQW double-step operator U^2 for $N = 30$ and $\lambda = 0.03$. Each dot corresponds to a doubly degenerated eigenvalue.

relativistic property (see Fig. 4). The arguments of eigenvalues of U^2 can be interpreted as quasienergies. They split into two bands, which can be related to positive and negative energy bands just like in the Dirac equation. Moreover, the two bands are separated by a band gap corresponding to the rest energy $2mc^2$. Due to the discrete nature of time for quasienergies the band gap occurs twice, the first occurrence centered around zero and the second centered around π. Numerical simulations show that the width of the band gap is related to the inverse of λ: in the limit $\lambda \to 0$ the band gap goes to π, and for $\lambda \to \infty$ the band gap goes to zero. This is as expected, since the corresponding mass scales as $\frac{1}{\lambda}$ [see Eq. (17)].

A. Large-mass limit

Recall the formulas for position-dependent coin (19) and coin flip rate (20) and recall that $\arctan\theta$ can be expressed as

$$\arctan\theta = \arcsin\left(\frac{\theta}{\sqrt{1+\theta^2}}\right) = \arccos\left(\frac{1}{\sqrt{1+\theta^2}}\right). \tag{21}$$

The entries of the coin matrix can be rewritten as

$$\cos\theta_{2k} = \frac{2\lambda\gamma_k}{\sqrt{1+4\lambda^2\gamma_k^2}}, \quad \sin\theta_{2k} = \frac{1}{\sqrt{1+4\lambda^2\gamma_k^2}}, \tag{22}$$

where $\gamma_k = \sqrt{k\left(\frac{N}{2}-k\right)}$. In the large-mass limit $\lambda \to 0$, which allows us to keep only the highest terms of the Taylor expansion,

$$\cos\theta_{2k} \approx 2\lambda\gamma_k, \quad \sin\theta_{2k} \approx 1. \tag{23}$$

The above limit resembles the one of Strauch [12], $\theta_{2k} \to \frac{\pi}{2}$. The action of the double-step operator U^2 on positions corresponding to vertices (odd positions) can be approximated by

$$U^2|2k-1, \rightarrow\rangle \approx 2\lambda\gamma_k|2k+1, \rightarrow\rangle + |2k-1, \leftarrow\rangle, \tag{24}$$

$$U^2|2k-1, \leftarrow\rangle \approx 2\lambda\gamma_{k-1}|2k-3, \leftarrow\rangle + |2k-1, \rightarrow\rangle. \tag{25}$$

Let us also introduce the following *almost normalized* states:

$$|\psi_\pm(k)\rangle = \frac{1}{\sqrt{2}}\left(|2k-1,\rightarrow\rangle \pm i|2k-1,\leftarrow\rangle \pm i2\lambda\gamma_k|2k+1,\rightarrow\rangle - 2\lambda\gamma_{k-1}|2k-3,\leftarrow\rangle\right), \tag{26}$$

and normalized states

$$|\phi_\pm(k)\rangle = \frac{1}{\sqrt{2}}\left(|2k-1,\rightarrow\rangle \pm i|2k-1,\leftarrow\rangle\right). \tag{27}$$

Note that $|\phi_\pm(k)\rangle$ and $|\psi_\pm(k)\rangle$ are almost equal up to the factor of $O(\lambda)$. The action of the double-step operator on $|\psi_\pm(k)\rangle$ yields

$$U^2|\psi_\pm(k)\rangle = i\left[|\phi_\pm(k)\rangle - i2\lambda\gamma_k|\phi_\pm(k+1)\rangle - i2\lambda\gamma_{k-1}|\phi_\pm(k-1)\rangle\right] + O(\lambda^2). \tag{28}$$

Now, it is enough to recognize that $2\lambda\gamma_k = J_{k,k+1}$ from the protocol [11] and that for short times the action of the unitary operator can be approximated by $U \approx \mathbb{1} - iHt$, where H is the Hamiltonian; therefore,

$$U^2|\psi_\pm(k)\rangle \approx i(\mathbb{1} - iH)|\phi_\pm(k)\rangle. \tag{29}$$

The above Hamiltonian is exactly the Hamiltonian of Christandl *et al.*; therefore, the CQTW behavior is restored. Moreover, the action of H does not mix $\pm$ states, which is the reason why we observe not only the transfer of the walker but also the transfer of its intrinsic coin state.

B. Small-mass limit

Let us consider $\lambda \to \infty$. In this case a dispersionless movement dominates the evolution, since Eq. (22) is approximately

$$\cos\theta_{2k} \approx 1, \quad \sin\theta_{2k} \approx 0. \tag{30}$$

Therefore, the double-step operator simplifies to $U^2 = e^{-2ip\sigma_z}$, except at position N, where we apply the reversing coin which also causes a π phase shift of the particle coming from the left. The transfer occurs in $N/2$ double steps. The initial state $\alpha|1,\rightarrow\rangle + \beta|1,\leftarrow\rangle$ evolves in the following way. The first part of this state, which is the right-moving part, moves to the right, is reflected at position N, and goes back to position $N-1$ to finish in state $-\alpha|N-1,\leftarrow\rangle$. The second, left-moving part goes left to $0 \equiv N \bmod N$, gets reflected, and moves right to position $N-1$ to finish in state $\beta|N-1,\rightarrow\rangle$. This also works for any initial state localized at x, for which the destination point is $N-x$. In order to restore the final coin state to the initial state, one has to apply the σ_y operation.

C. Transition between the two types of transfer

The unitary evolution operator U is the product of two operators S and C. Transfer properties rely on the interplay between this pair. In the small-mass limit, C does not play any significant role, since it is close to identity. On the other hand, in the large-mass limit, C is crucial because it makes the evolution similar to that of the protocol [11]. As we pointed out in the beginning of this section, we observed that the transition between the two types of behavior occurs around $\lambda = \frac{\pi}{N}$. Here, we give the heuristic explanation for this value.

The time of transfer over a chain of length N for the protocol [11] is $T = \frac{\pi}{\lambda}$. In our case we consider chains which are effectively of length $N/2$; that is why we have to multiply λ by 2, which is evident in Eq. (20). As a result, the corresponding time of transfer should be given by $\mathcal{T} = \frac{\pi}{2\lambda}$ and indeed this is approximately what we observe. Next, let us recall that the DTQW is related to relativistic quantum mechanics via its similarity to the Dirac equation. In relativistic physics, a distance traveled by a particle in time t can be at most ct. Similarly, in a DTQW, in one step the particle can move only to neighboring positions; that is why in order to travel the distance from one end of the chain to another the particle needs to take at least $N/2$ steps. This gives the critical value of $\lambda_{cr} = \frac{\pi}{N}$, above which the particle would move with velocity greater than the *speed of light*. Since this is impossible, a relativistic behavior has to dominate the evolution and as a consequence the transition between the two types of behavior can be interpreted as a nonrelativistic-to-relativistic transition.

D. Other techniques for perfect transfer

As mentioned earlier, nearly perfect transfer in spin networks can be obtained in many ways. In principle, all transfer techniques can be employed in DTQWs. For example, wave packet encoding (see Ref. [9] and references therein) is straightforward since one can prepare the same spatial wave packet in DTQWs as the one considered in CTQWs. However, the position-dependent coupling method is the one for which the correspondence between DTQWs and CTQWs is the most nontrivial. Below we would like to mention another example based on our coin-mass-coupling analogy. We present the DTQW version of a protocol in which two spins are weakly coupled to the ends of a spin chain with uniform couplings [17,18].

The CTQW Hamiltonian of a chain with weakly coupled ends is determined by coupling constants $J_{i,i+1} = J$ for $i = 2,\ldots,N-2$ and $J_{1,2} = J_{N-1,N} = aJ$, where $a \ll 1$. Due to weak coupling to the rest of the chain, an interaction of the first and the last spins with the middle part can be treated as a perturbation. Without interaction the two spins would be in a degenerate state. Weak coupling breaks the degeneracy and perturbation theory predicts that there are new eigenstates which are even superpositions of two states (a state in which the first spin is up and one in which the last spin is up) or three states (the first spin up, the last spin up, or the middle of the chain is in one of its unperturbed eigenstates). The second case happens when the degenerated eigenvalue of the two spins is the same as one of the eigenvalues of the chain. Nearly perfect transfer is possible because the initial and final states are almost completely supported on these two or three states only (for a detailed discussion see Refs. [17,18]).

In DTQWs the above protocol can be realized in the following way. As before, we can simulate an $N/2$ chain on an N cycle with one reversing edge. All coins are the same $\theta_k = \theta$, except $\theta_2 = \theta_{N-2} = \frac{\pi}{2} - \varepsilon$. We observe that the DTQW behaves exactly like the corresponding CTQW. Moreover, we also observe the transfer of the coin state. In Fig. 5 we show the eigenstate population for $N = 30$, $\theta = \frac{\pi}{4}$, and initial state $|1,\rightarrow\rangle$. In the case $\varepsilon \ll 1$, the initial state is almost entirely supported on four eigenstates (two positive-energy eigenstates

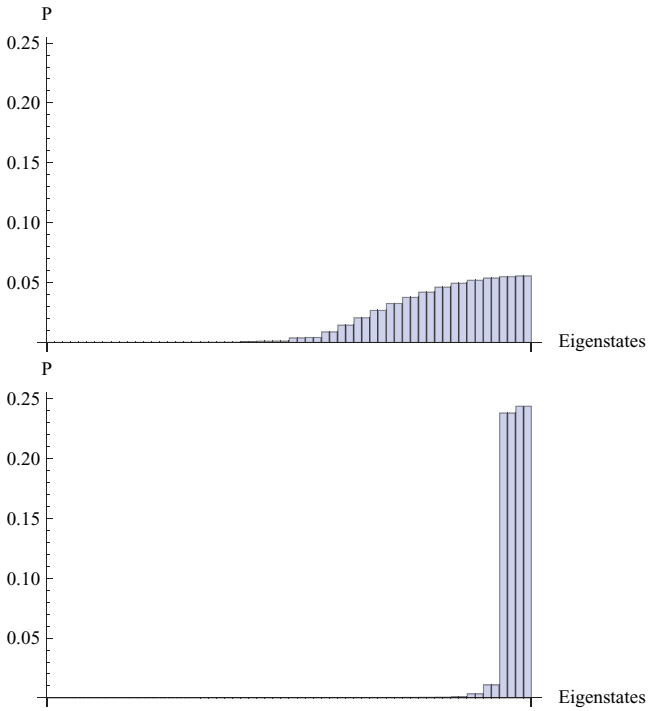

FIG. 5. (Color online) Eigenstate population for $N = 30$, $\theta = \pi/4$, and initial state $|1, \rightarrow\rangle$: (top) $\theta_1 = \theta_{N-1} = \theta = \pi/4$; (bottom) $\theta_2 = \theta_{N-2} = \pi/2 - \varepsilon$, where $\varepsilon = \frac{\pi}{2N}$. The initial state is almost entirely supported on four eigenstates only.

and two negative-energy eigenstates). In Fig. 6 we present the population of positions 1 and $N - 1$ in time. The time of transfer scales as $O(\frac{1}{\varepsilon^2})$.

We also observe another interesting phenomenon. If one changes the coin operator at position 2 from $e^{i\sigma_y \frac{\theta_2}{2}}$ to $e^{i\sigma_x \frac{\theta_2}{2}}$, the transfer is suppressed and the state is essentially localized at position 1 for all time. The reason for this behavior is that the initial energy at position 1 differs from the energy the particle would have at position $N - 1$; therefore, the transport is forbidden due to energy conservation. In the next section we explain this in further detail.

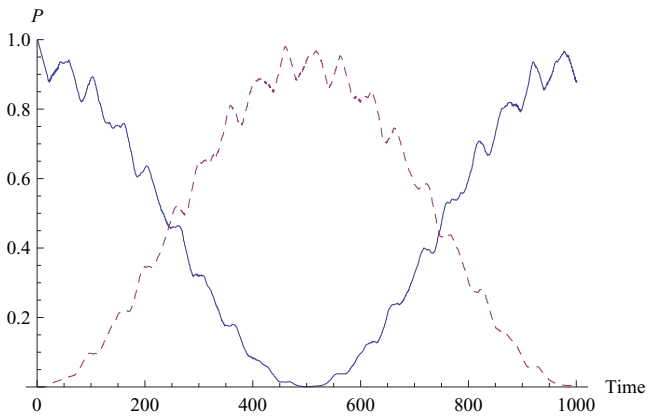

FIG. 6. (Color online) Probability of population of positions 1 (solid line) and $N - 1$ (dashed line) in subsequent time steps: $N = 30$, $\theta = \frac{\pi}{4}$, and $\varepsilon = \frac{\pi}{2N}$.

V. HOW DO WE CONVERT BETWEEN CTQW AND DTQW?

The conversion of CTQWs into DTQWs was considered by Childs [13]; however, his approach was purely mathematical and did not take into account the physical properties of the underlying quantum walks. On the other hand, our approach is based on physical aspects of quantum walks, and hence by studying the DTQW version of a continuous process one can learn many facts about the physics governing the corresponding system. In this section we show how, in general, to convert an arbitrary CTQW on a chain into a DTQW. Once again, we are going to implement a walk on an $N/2$ chain using an N cycle with vertex and edge positions.

Recall that in general CTQWs on a chain the only nonzero elements of the Hamiltonian are $H_{j,j+1}$, $H_{j,j-1}$, and H_{jj}. Diagonal terms, which are necessarily real, correspond to the potential energy

$$u(j) = H_{jj}. \tag{31}$$

Potential energy has been already considered in DTQWs, mostly in the context of localization (see, for example, Ref. [19]). The kinetic energy for the transition between positions j and $j + 1$, which is proportional to the second power of momentum divided by the mass, corresponds to the real part of the off-diagonal terms $H_{j,j+1}$ and $H_{j+1,j}$. In this case $\mathrm{Re}[H_{j,j+1}] = \frac{1}{2m_{j,j+1}}$. It was studied in the previous sections. The mass can be expressed as

$$m_{j,j+1} = \frac{1}{2\mathrm{Re}[H_{j,j+1}]}. \tag{32}$$

Finally, let us consider the imaginary part of $H_{j,j+1}$. First of all, note that the operator proportional to $-i|j\rangle\langle j+1| + i|j+1\rangle\langle j|$, which gives rise to the nonzero imaginary part of $H_{j,j+1}$, can be approximated as a first power of momentum operator for positions j and $j + 1$ (see Ref. [20]). Indeed,

$$\left(\sum_j -i|j\rangle\langle j+1| + i|j+1\rangle\langle j|\right)^2 = \sum_j 2|j\rangle\langle j| - |j+2\rangle\langle j| - |j\rangle\langle j+2|. \tag{33}$$

The above operator resembles the Laplacian, which is the kinetic energy operator proportional to the square of momentum. The first power of momentum can appear in the Hamiltonian if there is a vector potential $\vec{A}$ acting on the particle. In this case we have to substitute $(\vec{p})^2 \rightarrow (\vec{p} - \frac{e}{c}\vec{A})^2$, where e is the charge of the particle. As before, in the following, we assume $c = 1$ and we also set $e = 1$. Using this analogy one arrives at

$$\mathrm{Im}[H_{j,j+1}] = \frac{A_{j,j+1}}{m_{j,j+1}}, \tag{34}$$

where in general both the vector potential and the mass are position dependent. The vector potential alone can be estimated as follows:

$$A_{j,j+1} = \frac{1}{2}\frac{\mathrm{Im}[H_{j,j+1}]}{\mathrm{Re}[H_{j,j+1}]}. \tag{35}$$

Our approach is based on the analogy between DTQWs and the Dirac equation, whose general time-independent one-dimensional form is

$$\left(-i\frac{\partial}{\partial x}-A(x)\right)\sigma_z\psi+m(x)\sigma_y\psi=\left(i\frac{\partial}{\partial t}-u(x)\right)\psi. \tag{36}$$

At this point we can go to a DTQW via application of the Trotter formula. One step of the corresponding DTQW is given by

$$U=SCV=e^{ip\sigma_z}e^{i\left(m(j)\sigma_y-A(j)\sigma_z\right)}e^{iu(j)}, \tag{37}$$

where j denotes position. To include the account of the scalar potential, we introduced a new operator $V=e^{iu(j)}$. Moreover, the new coin operator C contains the vector potential term. It is worth noting that vector potentials allow us to implement Hadamard coins using a relativistic analogy. The relativistic limit of a Hadamard DTQW was considered in Ref. [16], where the mass term in the corresponding Dirac equation violated Lorentz covariance. Before we plug Eqs. (31), (32), and (35) into Eq. (37), let us emphasize that in some cases it might be convenient to consider the inverse tangent of both potentials, like we did previously with the mass, because of the periodicity of the arguments in the exponents. Moreover, since we consider the division of positions into edges and vertices, scalar potential terms should act on vertices, whereas mass and vector potential terms should act on edges. As a result the double-step operator can be taken as

$$U^2=SCSV=e^{ip\sigma_z}e^{i\left(\tilde{m}_{j,j\pm1}\sigma_y-\tilde{A}_{j,j\pm1}\sigma_z\right)}e^{ip\sigma_z}e^{i\tilde{u}_j}, \tag{38}$$

where $\tilde{A}_{j,j+1}=\arctan(\frac{1}{2}\frac{\mathrm{Im}[H_{j,j+1}]}{\mathrm{Re}[H_{j,j+1}]})$, $\tilde{m}_{j,j+1}=\arctan(\frac{1}{2\mathrm{Re}[H_{j,j+1}]})$, and $\tilde{u}_j=\arctan(H_{jj})$.

A similar conversion can be done for higher-dimensional quantum walks. Moreover, it is clear that, using the above analogy, one can convert the corresponding DTQW back into a CTQW. However, there are certain kinds of DTQWs which cannot be easily converted into CTQWs; therefore, let us now concentrate on the reverse problem of conversion of DTQWs into CTQWs. An example of a case in which the conversion is problematic is a DTQW with a position-dependent coin, where not only does the coin flip ratio θ_j depend on position, but also the generating operator σ_j changes from position to position. In the previous section we considered a DTQW version of a weakly coupled spin protocol and observed that the transfer can be suppressed due to a change of the first and the last coin flip generators from σ_y to σ_x. The coin degree of freedom is a qubit; therefore, the coin generator is a linear combination of σ_x, σ_y, and σ_z. In the Bloch sphere picture, coin operation is a rotation of a qubit about an axis $\vec{n}$, where the generator of rotation is $\vec{n}\cdot\vec{\sigma}$. In general, $\vec{n}$ can point in any direction on a surface of a three-dimensional sphere; however, in the case of the Dirac equation (36) it is bounded to the yz plane. Due to this fact, simple conversion from DTQWs into CTQWs is not possible. As a result, a DTQW offers a greater possibility of control over the transport than is allowed in the CTQW case.

Up to now we have considered only one-dimensional graphs, like chains. In two and higher dimensions, one encounters even more complicated obstacles. First, the typical formulation of a DTQW on a d-dimensional grid uses a $2d$-dimensional coin. Each coin dimension corresponds to a different direction for the walker to take in the next step. This is in contrast to the Dirac formulation of relativistic motion, where, for example, in the three-dimensional case the *coin* space is only four-dimensional. The conditional shift operator of the corresponding DTQW is of the form

$$\exp\left(i\sum_j p_j\otimes\gamma_j\right), \tag{39}$$

where $j=1,2,\ldots,d$ enumerates different orthogonal directions, $\gamma_j=|2j\rangle\langle 2j|-|2j-1\rangle\langle 2j-1|$ acts on the coin space, and p_j is the corresponding momentum operator for direction j. Note that $[\gamma_j,\gamma_k]=0$ for all values of j and k, whereas the corresponding Dirac matrices anticommute: $\{\tilde{\gamma}_j,\tilde{\gamma}_k\}=2\delta_{jk}$. Moreover, $\tilde{\gamma}_j^2=\mathbb{1}$ for all j, whereas for DTQWs $\sum_j\gamma_j^2=\mathbb{1}$. Due to this reason, one is unable to recover the relativistic energy relation $E^2=|\vec{p}|^2+m^2$ but rather obtains $E^2=\sum_j|\alpha_j|^2p_j^2+\beta^2$, where $\sum_j|\alpha_j|^2=1$ and β^2 is a parameter related to properties of the relevant coin operator, which can be interpreted as the mass. Since our method of conversion is closely related to the similarity of quantum walks to the Schrödinger and the Dirac equations, it is somehow expected that problems with conversion of DTQWs into CTQWs appear when the description of the DTQW departs from the Dirac one.

It is important to mention here the research on quantum-walk search protocols on d-dimensional grids. The efficiencies of the two protocols, the DTQW [21,22] and the CTQW [23], are quite similar. Only in dimensions $d=2,3$ is the DTQW protocol faster than the corresponding CTQW protocol. In Ref. [20], the authors of the CTQW protocol improved the efficiency of their model; however, this was done at the cost of an additional *coin* degree of freedom, which had to be included—departure from the standard CTQW structure was inevitable. The heart of the DTQW protocol [21] is the so-called Grover coin, which for $d=2$ is of the following form:

$$C_G=\frac{1}{2}\begin{pmatrix}-1&1&1&1\\1&-1&1&1\\1&1&-1&1\\1&1&1&-1\end{pmatrix}. \tag{40}$$

For the two-dimensional Grover walk the probability distribution remains localized at the initial position for all time. This effect was explained by Inui *et al.* [24], who noticed that eigenvalues of the Grover walk are highly degenerated. More than half of the eigenvalues are ±1. There is no CTQW analogy of the Grover walk. Since the Grover walk obeys translational symmetry, the corresponding CTQW version should also possess this property. However, for a translational symmetric CTQW on an $N\times N$ grid with periodic boundary conditions, coupling constant $J=|J|e^{i\varphi}$, and diagonal term A, the set of eigenvalues is given by $A+2|J|[\cos(\varphi-2\pi k_x/N)+\cos(\varphi-2\pi k_y/N)]$, where $k_x,k_y=0,1,\ldots,N-1$, and it is clear that there is no possibility of such a high degeneracy.

VI. CONCLUSIONS

In this work we studied the DTQW version of the quantum-state transfer, which is originally described as a continuous-time process. While in the continuous-time scenario the transfer properties depend on couplings between neighboring positions, in the discrete-time case it is the coin operator which is responsible for the perfect transmission from one position to another. We applied the analogy between the DTQW and the Dirac equation and between the CTQW and the Schrödinger equation to show that both coins and couplings can be interpreted as the mass of a particle, which allowed us to transform the CTQW into the DTQW. We examined the DTQW versions of perfect-state transfer protocols studied in Refs. [11,17,18]. We found that in DTQW versions not only the particle but also its intrinsic coin state is perfectly transferred. The general method of the CTQW transformation into the DTQW has been also discussed. Finally, we argued that some DTQWs do not have the corresponding CTQW versions due to the fact that in some cases the dynamics of a DTQW is much richer than that of the CTQW.

One of the biggest advantages of a CTQW is that it can be easily defined on any graph, whereas a DTQW is natural on regular graphs only, where the same coin degree of freedom can be used for all vertices. However, many problems in physics, as well as in computer science, are defined on regular graphs. The above discussion shows that in many cases the DTQW is more general than the CTQW, since it allows us to observe some effects which cannot be observed in a CTQW. It would be interesting to find phenomena which can be observed in CTQWs only.

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