General methods and properties to evaluate continuum limits of the 1D discrete time quantum walk

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Abstract

Models of quantum walks which admit continuous time and continuous spacetime limits have recently led to quantum simulation schemes for simulating fermions in relativistic and nonrelativistic regimes (Molfetta GD, Arrighi P. A quantum walk with both a continuous-time and a continuous-spacetime limit, 2019). This work continues the study of relationships between discrete time quantum walks (DTQW) and their ostensive continuum counterparts by developing a more general framework than was done in Molfetta and Arrighi (A quantum walk with both a continuous-time and a continuous-spacetime limit, 2019) to evaluate the continuous time limit of these discrete quantum systems. Under this framework, we prove two constructive theorems concerning which internal discrete transitions (“coins”) admit nontrivial continuum limits. We additionally prove that the continuous space limit of the continuous time limit of the DTQW can only yield massless states which obey the Dirac equation. Finally, we demonstrate that for general coins the continuous time limit of the DTQW can be identified with the canonical continuous time quantum walk when the coin is allowed to transition through the continuous limit process.

Keywords Discrete time quantum walk · Continuous time quantum walk · Lattice fermions · Quantum simulation

1 Introduction

The discrete time quantum walk (DTQW) has been the subject of much attention since it was introduced in Ref. [1] and independently in Ref. [2], and also its applications

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to quantum computing were discovered in the analysis of Hadamard Walks [3]. The DTQW has since been used in a variety of quantum computing algorithms, including the Oracular Search [4] and Element distinctness [5] algorithms (for a full list, see Ref. [6]).

As noted in Ref. [7], a now well-studied limit of the DTQW was introduced by Feynman and Hibbs [8] in constructing a path integral formulation for the propagator of the Dirac equation. According to Feynman, a particle zig-zags at the speed of light across a spacetime lattice, flipping its chirality from left to right with an infinitesimal probability at each time step [7]. The Dirac equation results when the continuous spacetime limit is taken, with the mass of the particle determined by the flipping rate. More recent works have produced notions of discrete spacetimes (see Refs. [9,10]) and consequent questions regarding how they produce our apparent continuum.

Since the writing of this paper it has been communicated to us that our work has intersected the results of Ref. [11]. By analyzing different scalings among Δx , Δt , and the speed of propagation c , the authors in Ref. [11] have developed a quantum simulation scheme known as a Plastic Quantum Walk which supports a continuous spacetime limit and a continuous time-discrete space limit. They also show that the procedure for obtaining such a walk yields a curved spacetime Hamiltonian for lattice-fermions with synchronous coordinates. In particular, the results in Sect. 4 of our work intersect those in Ref. [11], as we both find all parametrizations of unitary coins which permit continuous time-discrete space 1D continuum limits. However, our work deviates from theirs when we use these parametrizations to find solutions to the resultant continuum limit in Corollary 1, and in Sect. 7 we use the parametrization to show how the DTQW is related to the CTQW in general.

Other notable recent work includes Mlodinow and Brun in Ref. [12] demonstrating how to constrain a 3D DTQW to obtain a resulting fully Lorentz invariant continuum limit. They showed that their symmetry requirement necessitates the inclusion of antimatter, and, in Ref. [13], discuss experimental methods to distinguish between the DTQW and its continuum limiting Dirac equation as a description of fermion dynamics. These limits were also central to Refs. [14,15]. Their continuum limits for DTQWs transformed discrete time evolution equations to partial differential equations (PDEs), as the PDEs analyzed were much simpler than the discrete recursion relations of the DTQW.

Strauch [7] also used the continuum limit to connect the DTQW and CTQW, and Refs. [16,17], and more recently [18], demonstrate that the free particle Dirac evolution could be obtained by taking continuum limits of the DTQW. Strauch also demonstrated, in Ref. [16], the DTQW's connections with zitterbewegung, which is an interference effect among free relativistic Dirac particles between their positive and negative energy parts that produces a quivering motion [19]. Strauch shows that zitterbewegung in the DTQW can be tuned based on the value of its coin rotation parameter, and shows that the CTQW contains zitterbewegung-like oscillations (which Strauch denotes as anomalous zitterbewegung) even though there is only one energy for the CTQW [16].

At this time, several forms of continuum limits have already been rigorously developed, including general space and time limits with coin variations, in Refs. [16,20], and the continuous time limit for a very particular choice of coin in Ref. [7].

The purpose of this work is to formulate a general framework within which continuum limits of the DTQW can be taken, and to analyze the corresponding dynamics in the various limits. From our analysis, we determine all possible coins with which a continuous time and discrete space limit can be taken in 1D+1 (Sect. 4), and we show that the previous result in [11] is a special case of our general procedure. We also show that taking time and space limits simultaneously with a fixed coin is possible when steps in the walk are allowed and yields a massless dirac equation (Sect. 5). We then show that the ensuing time evolution derived from taking a continuous space limit of the continuous time limit of the DTQW is a massless dirac equation as well (Sect. 6). Lastly, we prove that the solutions of the continuous time limit of the DTQW can always be related to the solutions of the CTQW for any choice of coin allowed to undergo the continuous time limit of the DTQW (Sect. 7).

1.1 DTQW definition

The one-dimensional DTQW assumes a time dependent probability amplitude $\vec{\Psi}(x, t) = \begin{pmatrix} \psi_L(x, t) \\ \psi_R(x, t) \end{pmatrix}$ for a random walker's position and spin (assumed to point left or right). Compared with the classical probabilistic random walk, this (i) involves an internal (left/right) spin degree of freedom and (ii) involves quantum probability amplitudes instead of classical random walk probabilities. The time dynamics are given as

$$\vec{\Psi}(x, t + \Delta t) = SC\vec{\Psi}(x, t), \quad (1)$$

where the operations S and C (defined below) represent external and internal unitary operations, respectively, S being an external translation operation and C being an internal rebalancing of the two spin amplitudes ψ_R and ψ_L .

For example, if the coin operation C is implemented by the Hadamard matrix, then:

$$C\vec{\Psi}(x, t) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \vec{\Psi}(x, t). \quad (2)$$

With Δt and Δx the time and space intervals for the quantum walk, the full change SC acting in one time iteration Δt is then:

$$\begin{aligned} \vec{\Psi}(x, t + \Delta t) &= SC\vec{\Psi}(x, t) \\ &= \frac{S}{\sqrt{2}} \begin{pmatrix} \psi_L(x, t) - \psi_R(x, t) \\ \psi_L(x, t) + \psi_R(x, t) \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_L(x + \Delta x, t) - \psi_R(x + \Delta x, t) \\ \psi_L(x - \Delta x, t) + \psi_R(x - \Delta x, t) \end{pmatrix} \end{aligned} \quad (3)$$

The unitary time evolution is then:

$$\vec{\Psi}(x, t) = (SC)^m \vec{\Psi}(x, 0), \quad (4)$$

letting $m = \frac{t}{\Delta t}$. We also express this in discrete differential form for the purpose of forming subsequent continuum limits:

$$\Delta_t \vec{\Psi}(x, t) \equiv \frac{SC - \mathbb{I}}{\Delta t} \vec{\Psi}(x, t). \quad (5)$$

We will also often represent the walk in Fourier space and define our discrete Fourier transform convention here. Let $\vec{\tilde{\Psi}}(k, t)$ be the Fourier transform of $\vec{\Psi}(x, t)$ and $x = n\Delta x$ for $n \in \mathbb{Z}$. We use the following conventions for the forward and inverse Fourier transforms, for Fourier variable $k \in [-\frac{\pi}{\Delta x}, \frac{\pi}{\Delta x}]$:

$$\vec{\tilde{\Psi}}(k, t) = \sum_{n=-\infty}^{\infty} e^{-ikn\Delta x} \vec{\Psi}(n\Delta x, t) \equiv \mathcal{F}(\vec{\Psi}) \quad (6)$$

$$\vec{\Psi}(n\Delta x, t) = \frac{\Delta x}{2\pi} \int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}} dk e^{ikn\Delta x} \vec{\tilde{\Psi}}(k, t) \equiv \mathcal{F}^{-1}(\vec{\tilde{\Psi}}). \quad (7)$$

A standard procedure here will be to represent operators in Fourier space as follows: given an operator O on a function space Y , its Fourier conjugate operator $\tilde{O}$ is defined by $\tilde{O}\tilde{f}(k) = \mathcal{F}(O(f(x)))$, with $f(x) \in Y$, so that $\tilde{O}$ is the Fourier representation of O . The operator we will be most commonly representing in Fourier space is the shift operator S , defined by $\tilde{S}$:

$$\mathcal{F}(S\vec{\Psi}(x, t)) = \tilde{S}\vec{\tilde{\Psi}}(k, t) = e^{ik\Delta x\sigma_z} \vec{\tilde{\Psi}}(k, t), \quad (8)$$

where σ_z is a Pauli matrix.

2 Defining continuum limits

Skipping steps Before formulating a universal definition of continuum limits for the quantum walk, we want to establish the important notion of so-called alternating limits, in which only steps of a certain parity (e.g. even or odd) are considered observed. We first provide an informal example demonstrating that trivial divergences occur in the $\Delta t \rightarrow 0$ limit arising from multiple parity-dependent limits in the discrete walk. Such limits were considered in Ref. [7].

Consider the DTQW with coin $C = ie^{i\theta\sigma_x}$, with σ_x a standard Pauli matrix and $\theta \equiv \theta(\Delta t)$ a real number (modulo 2π) depending on the time discretization parameter Δt . For the example we construct an informal continuous time limit, to be formalized in Definition 1. Essentially we will take the $\Delta t \rightarrow 0$ limit in Eq. (5). The continuous time limit then amounts to identifying the limiting operator

$$\lim_{\Delta t \rightarrow 0} \frac{\tilde{S}(\Delta x)C(\Delta t) - \mathbb{I}}{\Delta t} = \lim_{\Delta t \rightarrow 0} \frac{ie^{ik\Delta x\sigma_z}e^{i\theta(\Delta t)\sigma_x} - \mathbb{I}}{\Delta t},$$

assuming a fixed space of functions $\mathbb{X}$ on which it acts; here $\mathbb{I}$ is the identity. This is defined more carefully later in this section within *Formal definitions*.

For this analysis of a continuous time limit for the discrete space and time quantum walk, we will seek the most general scaling of walk parameters that admit nontrivial limits as $\Delta t \rightarrow 0$. In this case we will admit all scalings for the coin parameter of the form $\theta = \pi/2 + \gamma \Delta t$, with $\gamma > 0$, which were introduced by Strauch [7]. Thus from the operator standpoint we seek a limit of the form $\lim_{\Delta t \rightarrow 0} \frac{ie^{ik\Delta x\sigma_z} i\sigma_x e^{i\gamma\Delta t\sigma_x} - \mathbb{I}}{\Delta t}$, which in fact does not exist generically. We show here however, that if we consider only even parity steps (i.e. even numbers of steps, effectively considering only every other step), then non-trivial limits exist. Thus, we will be considering only iterations of the even parity operator $SCSC$ rather than the fundamental step SC , and we will identify a limit $\lim_{\Delta t \rightarrow 0} \frac{\tilde{S}(\Delta x)C(\Delta t)\tilde{S}(\Delta x)C(\Delta t) - \mathbb{I}}{\Delta t}$, which structurally is:

$$\begin{aligned} & \lim_{\Delta t \rightarrow 0} \frac{\tilde{S}(\Delta x)C(\Delta t)\tilde{S}(\Delta x)C(\Delta t) - \mathbb{I}}{\Delta t} \\ &= \lim_{\Delta t \rightarrow 0} \frac{-e^{ik\Delta x\sigma_z} i\sigma_x e^{i\gamma\Delta t\sigma_x} e^{ik\Delta x\sigma_z} i\sigma_x e^{i\gamma\Delta t\sigma_x} - \mathbb{I}}{\Delta t} \\ &= \lim_{\Delta t \rightarrow 0} \frac{(\mathbb{I} + i\gamma\Delta t(\sigma_x \cos 2k\Delta x + \sigma_y \sin 2k\Delta x) + O(\Delta t^2))(\mathbb{I} + i\gamma\Delta t\sigma_x + O(\Delta t^2) - \mathbb{I})}{\Delta t} \\ &= i\gamma(\sigma_x(\cos 2k\Delta x + 1) - \sigma_y \sin 2k\Delta x). \end{aligned}$$

As might be expected, it will be clear below that replacing the above even power $(SC)^n$ with $n = 2$ by $n = 3$, the above limiting process will no longer exist; existence of the limit will hold only for even powers n . In general, restricting to fixed even step sizes n will lead to continuous limiting processes as above (with scaling of the coin based on Δt), while non-even step sizes will never admit such limits (see Theorem 2, proved in Appendix A).

Formal definitions. Definitions of our operator limits require common spaces for their domains. We will redefine all operators on such a common space, given as

$$\mathbb{X} = \{ \vec{\Psi}(x, t) : \vec{\Psi}(\cdot, t) \in L^2(\mathbb{R}) \otimes L^2(\Sigma) \text{ for all } t \geq 0 \text{ and } \vec{\Psi}(x, \cdot) \in C^1(\mathbb{R} \rightarrow \mathbb{C}^2) \},$$

where Σ is the space spanned by $|L\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|R\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Note that the effective domain space of the above tensor product space is $\mathbb{R} \times \Sigma$, with $\Sigma = L, R$. Thus, $\vec{\Psi}(x, t)$ is assumed once continuously differentiable in t , with two components in L^2 (i.e. square integrable functions in $x \in \mathbb{R}$ for fixed t).

We will consider general quantum walks that have $\Delta t \rightarrow 0$ limits when step numbers $n = km$ are restricted to whole multiples of an integer n , i.e. generalizing the above parity restriction for step numbers ($n = 2$) to accommodate more general step number restrictions. Thus, let $\vec{\Psi}(x, t) \in \mathbb{X}$, n be the number of skipped steps, ∂_t be the time derivative operator, and define the discrete derivative as $\Delta_t \vec{\Psi}(x, t) = \frac{\vec{\Psi}(x, t+n\Delta t) - \vec{\Psi}(x, t)}{n\Delta t}$. If $\vec{\Psi}(x, t) \in \mathbb{X}$ is a wave function, then the DTQW time evolution

equation is

$$\vec{\Psi}(x, t + n\Delta t) = (S(\Delta x)C(\Delta t))^n \vec{\Psi}(x, t). \quad (9)$$

We denote the level of discretization of our space and time operations by $\eta = (\Delta x, \Delta t)$. We will consider a discrete space and time quantum walk governed by

$$i\Delta_t \vec{\Psi} = H_\eta \vec{\Psi} \equiv i \frac{(SC)^n - \mathbb{I}}{n\Delta t} \vec{\Psi}(x, t) \quad (10)$$

on $\mathbb{X}$, with H_η the above family of operators parametrized by $\eta = (\Delta x, \Delta t)$. The continuous time limit of the walk in Eq. (10) exists if the right hand side of the equation has a limit (for $\vec{\Psi} \in \mathbb{X}$) as $\eta \rightarrow (0, 0)$ along a given prescribed path, for which both the DTQW functions and continuum limit of the DTQW functions are in $\mathbb{X}$. Continuum space limits in the absence of any change in Δt will not be considered here because $S \rightarrow \mathbb{I}$ as $\Delta x \rightarrow 0$, so the walk reduces simply to a coin acting on the spin portion of the wave function at each time step. With no traversal of the lattice there results a trivial walk. Formally, we state the definition of continuous time limit and continuous limit as:

Definition 1 Let the operators $H_\eta \equiv H_{\Delta x, \Delta t}$ and $H_{\Delta t}$ act on functions $\vec{\Psi}(x, t) \in \mathbb{X}$. Then, we have the following definitions:

- The *continuous time limit of the DTQW governed by coin C skipping n steps* is the time evolution equation $i\partial_t \vec{\Psi}(x, t) = H_{\Delta t} \vec{\Psi}(x, t)$ where $H_{\Delta t}$ is defined (when the limit exists) by $H_{\Delta t} \vec{\Psi}(x, t) = \lim_{\eta \rightarrow (\Delta x, 0)} H_\eta \vec{\Psi}(x, t)$, with the limit taken in the space $\mathbb{X}$.
- The *continuous spacetime limit of the DTQW governed by coin C skipping n steps* is the time evolution equation $i\partial_t \vec{\Psi}(x, t) = H_{\Delta x, \Delta t} \vec{\Psi}(x, t)$, where $H_{\Delta x, \Delta t}$ is defined (when the limit exists) by $H_{\Delta x, \Delta t} \vec{\Psi}(x, t) = \lim_{\eta \rightarrow (0, 0)} H_\eta \vec{\Psi}(x, t)$, (where in the limit $\Delta x = v\Delta t$ for some $v > 0$).

We call the operators $H_{\Delta t}$ and $H_{\Delta x, \Delta t}$ the generators of time evolution, or Hamiltonians, in their respective continuum limits. Note that the second limit above may depend on the ratio $v = \frac{\Delta x}{\Delta t}$, and can also be generalized to allow any manner of approach of $\eta \rightarrow (0, 0)$.

Our goal is to explore the most general possibilities for these two cases. We remark that our inclusion of n expands the number of continuum limits that exist; in particular this possibility was not considered in Ref. [20]

Additionally, we need the following definition to allow parametrized coin variations:

Definition 2 Consider a continuous spacetime limit where Δx and Δt have the same scaling, so $\Delta x = v\Delta t = v\epsilon$ for some nonzero $v \in \mathbb{R}$. A coin *varies* in this continuum limit if the coin depends on $\epsilon = \Delta t$.

3 General conditions for continuum limits

The following discussion is based on terminology and results explored in Ref. [20]. We will study a critical aspect of coins that change under the continuous time and spacetime limits; this, in turn, will help to interpret the theorems in Sects. 4 and 5. To obtain these results, we will follow the DTQW wave function through n time steps of length Δt . All limits in this section will be in the topology of the space $\mathbb{X}$. We begin with the basic equation

$$\vec{\Psi}(x, t + n\Delta t) = (S(\Delta x)C(\Delta t))^n \vec{\Psi}(x, t), \quad (11)$$

with $S = S(\Delta x)$ and $C = C(\Delta t)$ both dependent on the increment $\eta = (\Delta x, \Delta t)$. If a continuous spacetime limit is taken with $(\Delta t, \Delta x) \rightarrow (0, 0)$, then due to $S \rightarrow \mathbb{I}$ when $\Delta x \rightarrow 0$, we must have

$$\lim_{\Delta t, \Delta x \rightarrow 0} (C(\Delta t))^n = \mathbb{I},$$

as the limit could otherwise not exist. In particular, unless $C(\Delta t)$ is constantly the identity, it must vary (as in Definition 2) in the continuous time limit.

If only a continuous time limit is taken (i.e. $\Delta t \rightarrow 0$), then (by continuity of the left side in t) for the left and right sides of Eq. (11) to be equal, we must have

$$\lim_{\Delta t \rightarrow 0} (S(\Delta x)C(\Delta t))^n = \mathbb{I}$$

where we include Δt dependence in C for generality. Note that the constraint in the continuous time limit involves both the coin and the shift operator, not just the coin as in the continuous spacetime limit. Now for the following definition:

Definition 3 Consider a matrix $A(t)$ which depends on some continuous parameter t . $A(t)$ homotopically approaches a root of unity if $A(t)$ depends continuously on t and there exists some nonzero integer m and some real number t' such that $\lim_{t \rightarrow t'} A(t)^m = \mathbb{I}$.

By the previous definition and the above analysis of Eq. (11), we have the following theorem:

Theorem 1 A coin for which a continuous space and time limit exists must homotopically approach a root of unity. The product of the shift and coin operator for which a continuous time limit exists must homotopically approach a root of unity as well.

Proof Recall from Definition 1 that we define the spacetime limit $H_{\Delta x, \Delta t}$ with $\Delta x = v\Delta t = v\epsilon$ as:

$$H_{\Delta x, \Delta t} \vec{\Psi}(x, t) \equiv i \lim_{\epsilon \rightarrow 0} \frac{(S(\epsilon)C)^n - \mathbb{I}}{n\epsilon} \vec{\Psi}(x, t) \quad (12)$$

for $\vec{\Psi}(x, t) \in \mathbb{X}$. Because $\lim_{\epsilon \rightarrow 0} S = \mathbb{I}$, we have the following:

$$i \lim_{\epsilon \rightarrow 0} \frac{C^n - \mathbb{I}}{n\epsilon} \vec{\Psi}(x, t) = H_{\Delta x, \Delta t} \vec{\Psi}(x, t) \quad (13)$$

Now we see that for the left hand side to equal the right hand side, C must be of the form $C^n = \mathbb{I} - in\epsilon H_{\Delta x, \Delta t} + O(\epsilon^2)$. Thus, by Definition 3, C must homotopically approach a root of unity in the continuous spacetime limit. The proof for the continuous time limit is similar, except now S does not converge to identity, so instead SC must be of the form $(SC)^n = \mathbb{I} - in\epsilon H + O(\Delta\epsilon^2)$, thereby satisfying definition once again. $\square$

From this analysis, we have obtained a general property of coins which undergo continuum limit transformations, and we will refer to this property in the future.

4 General continuous time limit

In this section, we will identify the set of DTQWs for which a continuous time limit exists, as according to Definition 1. We will then analyze the properties of the resulting time evolutions in the continuous time limit.

We consider a general unitary coin, which can be written via:

$$\begin{aligned} C &= e^{i\delta} R_z(\psi) R_y(\theta) R_z(\phi) = e^{i\delta} e^{-i\psi\sigma_z/2} e^{-i\theta\sigma_y/2} e^{-i\phi\sigma_z/2} \\ &= e^{i\delta} \begin{pmatrix} \cos \frac{\theta}{2} \exp -i \frac{\phi+\psi}{2} & -\sin \frac{\theta}{2} \exp i \frac{\phi-\psi}{2} \\ \sin \frac{\theta}{2} \exp i \frac{-\phi+\psi}{2} & \cos \frac{\theta}{2} \exp i \frac{\phi+\psi}{2} \end{pmatrix} \end{aligned} \quad (14)$$

We wish to know for which 2×2 matrices, as parametrized by Eq. (14), does the continuum limit exist, according to Definition 1. Before introducing the relevant theorem we make a few remarks. First, a constraint on δ is necessary to satisfy the finiteness condition for existence of the limit in Definition 1. The value of δ is arbitrary as it amounts to an overall energy shift in the Hamiltonian, which does not change measureables. This point is explained further in the proof of Lemma 4. Second, assuming that the elements of C cannot depend on the elements of S , observe that the limit in Definition 1 cannot be finite unless C depends on Δt . Thus, we will assume that the coin varies in the process of the continuum limit; here we have defined such variation in Definition 2. A proof of the following theorem is presented in Appendix A.

Theorem 2 *Let $C(\delta, \psi, \theta, \phi)$ be the 2×2 unitary matrix in Eq. (14), with the set of angles ψ, θ, ϕ parametrizing C depending on Δt as: $\phi = \phi_0 + \phi_1 \Delta t + O(\Delta t^2)$, $\psi = \psi_0 + \psi_1 \Delta t + O(\Delta t^2)$, and $\theta = \theta_0 + \theta_1 \Delta t + O(\Delta t^2)$, with $\phi_0, \psi_0, \theta_0, \phi_1, \psi_1, \theta_1 \in \mathbb{R}$ constants. The continuous time limit as defined in Definition 1 will exist for such a class of coins if and only if $\theta_0 = p\pi$, $\delta = -\frac{p\pi}{2}$ (for odd integer p), and n is even. The Hamiltonian obtained in such a limit is*

$$H = -\frac{\theta_1}{4} (R_z(-2\phi_0) + S^2 R_z(2\psi_0)) \sigma_y, \quad (15)$$

with S the shift operator defined in Eq. (8).

Thus, the class of coins that admit continuous time limits have the form

$$C = e^{-i\psi_0\sigma_z/2}\sigma_y e^{-i\theta_1\Delta t\sigma_y/2}e^{-i\phi_0\sigma_z/2} \quad (16)$$

(here parameters are ψ_0 , θ_1 , and ϕ_0). We observe that the Hamiltonian obtained from the continuous time limit does not depend on any parameters that are coefficients in terms $O(\Delta t)$ except θ_1 [so they do not need to be included in Eq. (16)]. θ_1 can be interpreted as a driving factor for the final Hamiltonian's time evolution. Its value completely determines how much of the mixing between the left and right states will be due to the evolution operator SC . Note that when $\theta_1 = 0$ all operators in the coin commute with the shift operator and no mixing occurs, which corresponds to the wave function recurring every other step in the DTQW.

Now we compare our Hamiltonian from Theorem 2 to the massless Hamiltonian obtained in Ref. [11]. We begin by writing the Hamiltonian obtained from the continuous time limit in Ref. [11] (Eq. (4) in [11]) in a way we can easily compare to the Hamiltonian in Theorem 2:

$$\begin{aligned} H_L &= c\sigma_x \sin(i\Delta_x\partial_x)e^{\Delta_x\sigma_z\partial_x} \\ &= c\sigma_x \left(\frac{e^{-\Delta_x\partial_x} - e^{\Delta_x\partial_x}}{2i} \right) e^{\Delta_x\sigma_z\partial_x} \\ &= \frac{c\sigma_x}{2i} \begin{pmatrix} 1 - e^{2\Delta_x\partial_x} & 0 \\ 0 & -(1 - e^{-2\Delta_x\partial_x}) \end{pmatrix} \\ &= \frac{c\sigma_x\sigma_z}{2i} \begin{pmatrix} 1 - e^{2\Delta_x\partial_x} & 0 \\ 0 & 1 - e^{-2\Delta_x\partial_x} \end{pmatrix} \\ &= -\frac{c\sigma_y}{2} (1 - e^{2\Delta_x\sigma_z\partial_x}) \\ &= -\frac{c}{2} (1 - e^{-2\Delta_x\sigma_z\partial_x})\sigma_y \\ &= -\frac{c}{2} (1 - S^2)\sigma_y. \end{aligned} \quad (17)$$

We see that $\frac{c}{2} = \frac{\theta_1}{4}$, and that H_L is a special case of Eq. (15) with $\phi_0 = 0$ and $\psi_0 = \pi$. It is the degrees of freedom possessed by the parameters ϕ_0 and ψ_0 which cause our procedure to be more general.

We now make an additional observation on the need for skipping steps (i.e. for an even n) for a sensible limit to occur. An explicit proof justifying this can be seen in Appendix A; for a more intuitive explanation, note that for existence of a continuous DTQW time limit, the Fourier Hamiltonian

$$\tilde{H}(k) = \lim_{\Delta t \rightarrow 0} \frac{(e^{ik\Delta x\sigma_z}C(\Delta t))^n - \mathbb{I}}{\Delta t} \quad (18)$$

must be finite. The operator $e^{ik\Delta x\sigma_z}C$ does not homotope to the identity as $\Delta t \rightarrow 0$ for any C , so no continuous time limit can exist for $n = 1$. However, for the coin in Eq. (16), the operator $e^{ik\Delta x\sigma_z}C e^{ik\Delta x\sigma_z}C$ does homotope to the identity since for coins in Eq. (16) $C e^{ik\Delta x\sigma_z}C = e^{-ik\Delta x\sigma_z} + O(\Delta t)$. That is, the coins in Theorem 2 invert the shift operator up to $O(\Delta t)$, making the $O(\Delta t^0)$ term in $SCSC$ the identity. After identities cancel in Eq. (18) only the $O(\Delta t)$ term remains, i.e., the Hamiltonian in the Theorem.

It should be noted that Ref. [7] derives a special version of the Hamiltonian in Theorem 2, using the coin $C = e^{-i\theta\sigma_x}$, and has $\theta = \frac{\pi}{2} - \gamma\Delta t$. The angle values parametrizing the general unitary coin in Theorem 2 for the particular choice in Ref. [7] including Δt dependence have the form:

$$\begin{aligned}\psi_0 &= -\frac{\pi}{2}, & \phi_0 &= \frac{\pi}{2}, & \theta_0 &= \pi \\ \psi_1 &= 0, & \phi_1 &= 0, & \theta_1 &= 4\gamma, \\ \delta &= 0\end{aligned}\quad (19)$$

with γ the jumping rate from vertex to vertex. If we do not have $\delta = p\pi$ for odd integer p , we obtain a final H with constant infinite energy contributions, which should then be ignored, as only energy differences lead to observable quantities.

Another important property of the coins derived in Theorem 2 is that they themselves homotopically approach a root of unity in that, as can be checked, $\lim_{\Delta t \rightarrow 0} C^n = \mathbb{I}$. This does not follow directly from our analysis in Sect. 3 of the continuous time limit, and a full characterization of all coins that admit continuous time limits was needed to obtain this property. Also, the limiting Hamiltonian in Theorem 2 will be used in Sect. 6 to determine how a continuous time limit followed by a continuous space limit compares to a simultaneous continuous spacetime limit.

We now analyze wave functions which that undergo the time evolution dictated by the Hamiltonian in Theorem 2. A proof of the following corollary is found in Appendix B.

Corollary 1 Let $\vec{\Psi}(x, t)$ be a solution to the time evolution equation with the Hamiltonian from Theorem 2, $i\partial_t \vec{\Psi}(x, t) = H\vec{\Psi}(x, t) = -\frac{\theta_1}{4}(R_z(-2\phi_0) + S^2 R_z(2\psi_0))\sigma_y \vec{\Psi}(x, t)$. Also, let $\vec{\Psi}(x, 0) = \begin{pmatrix} \Psi_L(x, 0) \\ \Psi_R(x, 0) \end{pmatrix}$ be the initial condition for $\vec{\Psi}(x, t)$. Then, the following is the analytical form of the time evolution for $\vec{\Psi}(x, t)$ for all t in terms of its initial state, where $x = m\Delta x$ for $m \in \mathbb{Z}$ and $J_m(t)$ is the m th order Bessel function of the first kind, $\alpha = \frac{\phi_0 + \psi_0}{2}$, and $\beta = \frac{\phi_0 - \psi_0}{2}$:

$$\begin{aligned}\vec{\Psi}(m\Delta x, t) &= \begin{pmatrix} \Psi_L(m\Delta x, t) \\ \Psi_R(m\Delta x, t) \end{pmatrix} \\ &= \frac{1}{2} \sum_{n=-\infty}^{\infty} i^{m-n} e^{i\alpha(m-n)} J_{m-n}\left(\frac{\theta_1 t}{2}\right) \\ &\quad \times \begin{pmatrix} (1 + (-1)^{m-n})\Psi_L(n\Delta x, 0) + i e^{i\beta}(1 - (-1)^{m-n})\Psi_R((n+1)\Delta x, 0) \\ -i e^{-i\beta}(1 - (-1)^{m-n})\Psi_L((n-1)\Delta x, 0) + (1 + (-1)^{m-n})\Psi_R(n\Delta x, 0) \end{pmatrix}\end{aligned}$$

This solution reduces to that found in Ref. [7] when the corresponding parameters in Eq. (19) are used, except for a sign difference stemming from the shift operator in Ref. [7] being defined as the inverse of S . The locations for which $\vec{\Psi}_L(x, 0)$ is nonzero will contribute to $\vec{\Psi}_L(m\Delta x, t)$ if they are an even number of steps away from m , and the nonzero locations of $\vec{\Psi}_R(x, 0)$ will contribute to $\vec{\Psi}_L(m\Delta x, t)$ if they are an odd number of steps away from m , and the opposite scenario is true for $\vec{\Psi}_R(m\Delta x, t)$. For a full description of the effects α and β have on the probability distribution, see Sect. 7.

5 Continuous spacetime limit with no coin variation

In this section we will demonstrate for which DTQWs the continuous spacetime limit exists and what the ensuing time evolution is if there is no coin variation involved, as defined in Definition 2. We present a theorem to illustrate that it is possible to obtain a continuous spacetime limit of a DTQW with non-varying coin, and to identify the necessary properties of coins which can undergo this type of limit. A proof of the following theorem is presented in Appendix C.

Theorem 3 *Let $\vec{\Psi}(x, t)$ be a two-component wave function undergoing the DTQW, as defined in Eq. (1). Also, let $|\hat{n}| = \sqrt{n_x^2 + n_y^2 + n_z^2} = 1$, $l = 0, 1, 2, \dots$, $m = 1, 2, \dots$, and $v\Delta t = \Delta x$, where Δt and Δx are the time step and lattice spacings of the DTQW for $\vec{\Psi}(x, t)$, respectively. The continuous spacetime limit will exist for $\vec{\Psi}(x, t)$ if and only if the DTQW skips every m steps and the coin operator dictating its DTQW is of the form*

$$C = \exp \frac{i\pi l}{m} \exp \frac{-i\pi l}{m} \hat{n} \cdot \vec{\sigma}. \quad (20)$$

The ensuing Hamiltonian for this walk will be the following massless Dirac Hamiltonian:

$$H = -vn_z \hat{n} \cdot \vec{\sigma} \frac{\partial}{\partial x}. \quad (21)$$

The massless Dirac Hamiltonian is the limiting Hamiltonian of this continuum limit. In the continuous spacetime limit, the mass term is generated by the coin's variation with time step, as can be seen in Appendix F. The ensuing continuous spacetime Hamiltonian will have no mass because the coin in Theorem 3 does not vary in the continuum limit.

The above theorem also states that a coin with no variation will have a continuum limit if it is a root of unity. This is expected in light of Theorem 1, as the continuous parameter in the coin is no longer present, so the coin itself must be a root of unity. This theorem may seem at odds with the discussion at the start of Ref. [20] (which we repeat in Sect. 3), but skipping steps in the walk was not considered when taking the

continuum limit, which is how a limit was obtained for this walk, even when the coin did not vary in the continuum limit.

6 Simultaneous continuous spacetime limit vs continuous time followed by continuous space limit

In this section we state a theorem on the existence of non-trivial continuous space limits of the continuous time limit of the DTQW. We begin with the theorem (proof in Appendix D):

Theorem 4 *Let ϕ_0 and ψ_0 be unable to vary in the continuous space limit (i.e. ϕ_0, ψ_0 cannot depend on Δx). Then, the only time evolution equation which is not infinite and contains spatial derivative(s) for the continuous space limit ($\Delta x \rightarrow 0$) of the continuous time limit of the DTQW is a massless dirac equation.*

The reason why ϕ_0 and ψ_0 cannot depend on Δx is given by the following conjecture:

Conjecture 1 There is no dependence ϕ_0 and/or ψ_0 can have on Δx that would allow for spatial derivative(s) in the continuum limit

If no spatial derivatives are present, no spatial translation will occur for the wave function in the continuous space limit, resulting in a trivial stationary walk. Another observation of Theorem 4 is that a different time evolution equation occurs when a *simultaneous* continuous spacetime limit is taken. As can be seen in Appendix F, when a simultaneous spacetime continuum limit is taken, a massive Dirac equation results.

7 General DTQW relationship to CTQW

In the following section, we will build on Strauch's result from Ref. [7], in which a connection was found between the DTQW and CTQW by taking a continuous time limit of the DTQW. Strauch used a specific coin $e^{-i\theta\sigma_x}$, and let $\theta = \frac{\pi}{2} - \gamma\Delta t$ when the continuous time limit was taken. Now that a general parametrization of all the possible coins which can undergo a continuous time quantum walk has been obtained from Theorem 2, we will investigate whether or not a relationship between the CTQW and DTQW exists for a general coin. We begin by reviewing Strauch's specific results in Ref. [7].

7.1 Review of Strauch

To begin, consider a DTQW with shift operator (in Fourier space) $\tilde{S} = e^{ik\Delta x\sigma_z}$ and coin operator $C = e^{-i\theta\sigma_x}$ such that the time evolution of a Fourier space wave function $\vec{\Psi}(k, t)$ is given by $\vec{\Psi}(k, t + \Delta t) = \tilde{S}C\vec{\Psi}(k, t)$. When a continuous time limit ($\Delta t \rightarrow 0$) is taken on $\vec{\Psi}(x, t)$, letting $\theta = \frac{\pi}{2} - \gamma\Delta t$ and skipping every other step,

the following time evolution is recovered for $\vec{\Psi}(x, t)$:

$$i\partial_t \vec{\Psi}(x, t) = -\gamma(\mathbb{I} + S^2)\sigma_x \vec{\Psi}(x, t) \quad (22)$$

Strauch observed that if we define two wave functions $\vec{\Psi}_+(x, t)$ and $\vec{\Psi}_-(x, t)$ such that $\vec{\Psi}_\pm(x, t) \equiv \frac{e^{\mp 2i\gamma t}}{2}(\mathbb{I} \pm S\sigma_x)\vec{\Psi}(x, t)$, then it can be shown that $\vec{\Psi}(x, t) = e^{2i\gamma t}\vec{\Psi}_+(x, t) + e^{-2i\gamma t}\vec{\Psi}_-(x, t)$ and $i\partial_t \vec{\Psi}_\pm(x, t) = \mp\gamma[\vec{\Psi}_\pm(x + \Delta x, t) + \vec{\Psi}_\pm(x - \Delta x, t) - 2\vec{\Psi}_\pm(x, t)]$ (which is the CTQW time evolution equation). In other words, Strauch found that the continuous time limit of the DTQW with $C = e^{-i\theta\sigma_x}$ can be written as a superposition of two copies of the CTQW. This relation helped clarify the then longstanding mystery about the exact relationship between the two ways of quantizing the quantum walk, the DTQW and CTQW. Next we show that this relationship holds for a general coin, and we will use the relation to see how the DTQW coin parameters effect the solutions of the time evolution equations in the discussion following the Theorem 5.

7.2 General coin CTQW-DTQW relation

We summarize our findings in the following theorem, the proof of which is in Appendix E:

Theorem 5 *Let $\vec{\Psi}(x, t)$ be the following two-component wave function resulting from the continuous time limit of the DTQW with a general coin as found in Theorem 2:*

$$i\partial_t \vec{\Psi}(x, t) = -\frac{\theta_1}{4}(R_z(-2\phi_0) + S^2 R_z(2\psi_0))\sigma_y \vec{\Psi}(x, t)$$

where θ_1 , ϕ_0 , and ψ_0 are real numbers which cannot depend on x or t . Additionally, let $\vec{\Psi}_\pm(x, t)$ be wave functions which satisfy the following CTQW time evolution equations:

$$i\partial_t \vec{\Psi}_\pm(x, t) = \mp \frac{\theta_1}{4}[\vec{\Psi}_\pm(x + \Delta x, t) + \vec{\Psi}_\pm(x - \Delta x, t) - 2\vec{\Psi}_\pm(x, t)].$$

Then, $\vec{\Psi}(x, t)$ can be written as a superposition of $\vec{\Psi}_+(x, t)$ and $\vec{\Psi}_-(x, t)$ in the following way (where $\alpha = \frac{\phi_0 + \psi_0}{2}$):

$$\vec{\Psi}(x, t) = e^{i\alpha \frac{x}{\Delta x}}(e^{-\frac{i\theta_1 t}{2}}\vec{\Psi}_+(x, t) + e^{\frac{i\theta_1 t}{2}}\vec{\Psi}_-(x, t)). \quad (23)$$

Now that a general relationship has been established between the continuous time limit of the DTQW and the CTQW, the effect of the coin parameters α and β on the solutions of the continuous time limit can be analyzed. To begin, $\vec{\Psi}_\pm(x, t)$ are fixed momentum traveling wave states with time evolution which does not depend on α or β because $\vec{\Psi}_\pm(x, t)$ satisfy the CTQW (which does not depend on α or β), so the time

evolution of these wave functions would be a spreading of their initial distribution across the sites. Equation (23) can be written more suggestively:

$$\vec{\Psi}(x, t) = e^{i(\alpha \frac{x}{\Delta x} - \frac{\theta_1 t}{2})} \vec{\Psi}_+(x, t) + e^{i(\alpha \frac{x}{\Delta x} + \frac{\theta_1 t}{2})} \vec{\Psi}_-(x, t). \quad (24)$$

$e^{i(\alpha \frac{x}{\Delta x} - \frac{\theta_1 t}{2})}$ has the effect of boosting $\vec{\Psi}_+(x, t)$ to a frame traveling right (if $\alpha > 0$) at speed $|\frac{\alpha \theta_1}{2}|$ or left (if $\alpha < 0$), and $e^{i(\alpha \frac{x}{\Delta x} + \frac{\theta_1 t}{2})}$ boosts $\vec{\Psi}_-(x, t)$ to a frame moving at speed $|\frac{\alpha \theta_1}{2}|$ in the opposite direction as $\vec{\Psi}_+(x, t)$. The last effect these parameters have is on the initial condition of $\vec{\Psi}_\pm(x, t)$. The operator which projects $\vec{\Psi}(x, 0)$ onto $\vec{\Psi}_\pm(x, 0)$ is $P_\pm = e^{-i\alpha \frac{x}{\Delta x}} (\frac{1}{2} \mp S e^{i\beta z} y)$, so $P_\pm \vec{\Psi}(x, 0) = \vec{\Psi}_\pm(x, 0)$. The only effect β has is on the initial conditions, while α affects both the initial condition and the frames to which $\vec{\Psi}_+(x, t)$ and $\vec{\Psi}_-(x, t)$ are boosted.

8 Conclusion and open questions

8.1 Conclusions

Provided our definitions of continuum limit from Sect. 2, we have concluded by Theorem 2 that keeping space discrete while continuizing time is only possible for particular coins, which must be of the form $C = e^{-i(\psi_0)\sigma_z/2} \sigma_y e^{-i\theta_1 \Delta t \sigma_y/2} e^{-i(\phi_0)\sigma_z/2}$, granted the limit is taken two steps at a time. We have also concluded, from Theorem 5 in Sect. 7.2, that the continuous time limit of the DTQW can always be related to the CTQW if the coin is of the form $\exp -\frac{i\theta}{2} (\sigma_y \cos \psi_0 - \sigma_x \sin \psi_0)$, where $\theta \rightarrow p\pi + \theta_1 \Delta t$ in the continuum limit for some odd integer p and $\theta_1 \in \mathbb{R}$. These two theorems imply that there exists unitary matrices used as coins in the DTQW that do not have continuous time limits, and thus cannot be related to the CTQW.

We additionally concluded from Theorem 3 that certain coins do not need to vary in the continuum limit, as long as they are roots of unity. Finally, we deduced from Theorem 4 that various types of Dirac equations can be obtained depending on how the continuum limit of the DTQW is taken. Space and time limits taken simultaneously yield different answers than when time is taken followed by space.

8.2 Open questions

There are many open questions pertaining to these ideas. Which types of coins have continuum limits in higher spatial dimensions? What do the connections between the DTQW and CTQW look like in higher spatial dimensions? What would the analogous theorems look like if we introduced multiple coins? Which symmetry group is responsible for constraining the coins which undergo the continuous time limit of the DTQW?

The connections between various continuum limits of the DTQW to the massless/massive Dirac equation shown in this work and in others suggest the possibility of a new universal quantum computational architecture involving the scattering of

particles obeying the Dirac or Schrodinger equations. Are these connections the most that can be made on the topic of computation, or is there something more? Stated another way, do quantum walks involved in quantum computational algorithms have continuum limits which can be related to the Dirac or Schrodinger equation? If they do, would it imply there is a way to utilize the Dirac or Schrodinger dynamics to obtain the results of quantum walk algorithms? The results and techniques shown in this work would certainly help obtain such an answer.

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A Proof of general continuous time limit of the DTQW (Theorem 2)

Before we begin, let's reiterate the theorem we wish to prove:

Theorem 2 *Let $C(\delta, \psi, \theta, \phi)$ be the 2×2 unitary matrix in Eq. (14), with the set of angles ψ, θ, ϕ parametrizing C depending on Δt as: $\phi = \phi_0 + \phi_1 \Delta t + O(\Delta t^2)$, $\psi = \psi_0 + \psi_1 \Delta t + O(\Delta t^2)$, and $\theta = \theta_0 + \theta_1 \Delta t + O(\Delta t^2)$, with $\phi_0, \psi_0, \theta_0, \phi_1, \psi_1, \theta_1 \in \mathbb{R}$ constants. The continuous time limit as defined in Definition 1 will exist for such a class of coins if and only if $\theta_0 = p\pi$, $\delta = -\frac{p\pi}{2}$ (for odd integer p), and n is even. The Hamiltonian obtained in such a limit is*

$$H = -\frac{\theta_1}{4}(R_z(-2\phi_0) + S^2 R_z(2\psi_0))\sigma_y, \quad (25)$$

with S the shift operator defined in Eq. (8).

We begin by stating the continuous time limit of the DTQW for coin C and skipping n steps, from Definition 1:

$$i\partial_t \vec{\psi}(x, t) = i \lim_{\Delta t \rightarrow 0} \frac{(SC)^n - \mathbb{I}}{n\Delta t} \vec{\psi}(x, t) \quad (26)$$

Now we construct lemmas to prove Theorem 2. Our first lemma will be an algebraic expansion of $(\tilde{S}C)^n$ that will help make manifest later lemmas, where $\tilde{S}$ is the Fourier transform of S , which is defined by $\tilde{S} = e^{ik\Delta x\sigma_z}$.

Lemma 1 *Let $\psi'_0 = \psi_0 - 2k\Delta x$, $A = R_z(\psi'_0)R_y(\theta_0)R_z(\phi_0)$, $B = \psi_1\sigma_z A + \theta_1\sigma_y R_z(-2\psi'_0)A + \phi_1 A\sigma_z$, and $\tilde{S}$ be the Fourier transform of S . Then, the following*

is true up to $O(\Delta t)$:

$$(\tilde{S}C)^n = (e^{i\delta}A)^n \left(1 - \frac{i\Delta t}{2}A^{-1} \sum_{j=0}^{n-1} A^{-j}BA^j \right) \quad (27)$$

Proof After substituting ψ , ϕ , and θ in terms of ϕ_0 , ψ_0 , θ_0 , ϕ_1 , ψ_1 , and θ_1 , the rotation matrices in Eq. (14) become $R_z(\psi) = R_z(\psi_0) \left(1 - \frac{i\psi_1\Delta t}{2}\sigma_z + O(\Delta t^2) \right)$ and so on for $R_z(\phi)$ and $R_y(\theta)$. After doing this substitution and going to Fourier space (so $S \rightarrow \tilde{S} = R_z(-2k\Delta x)$), we get the following for $(\tilde{S}C)^n$:

$$\begin{aligned} (\tilde{S}C)^n = & e^{i\delta n} \left(R_z(-2k\Delta x)R_z(\psi_0) \left(1 - \frac{i\psi_1\Delta t}{2}\sigma_z + O(\Delta t^2) \right) \right. \\ & \left. \times R_y(\theta_0) \left(1 - \frac{i\theta_1\Delta t}{2}\sigma_y + O(\Delta t^2) \right) R_z(\phi_0) \left(1 - \frac{i\phi_1\Delta t}{2}\sigma_z + O(\Delta t^2) \right) \right)^n \end{aligned} \quad (28)$$

We now make the substitution $\psi'_0 = \psi_0 - 2k$ and expand Eq. (28) further:

$$\begin{aligned} (\tilde{S}C)^n = & e^{i\delta n} [R_z(\psi'_0)R_y(\theta_0)R_z(\phi_0) - \frac{i\Delta t}{2}(\psi_1\sigma_z R_z(\psi'_0)R_y(\theta_0)R_z(\phi_0) \\ & + \theta_1\sigma_y R_z(-2\psi'_0)R_z(\psi'_0)R_y(\theta_0)R_z(\phi_0) + \phi_1 R_z(\psi'_0)R_y(\theta_0)R_z(\phi_0)\sigma_z) + O(\Delta t^2)]^n \\ = & e^{i\delta n} \left(A - \frac{i\Delta t}{2}B + O(\Delta t^2) \right)^n \\ = & e^{i\delta n} \left(A^n - \frac{i\Delta t}{2}(A^{n-1}B + A^{n-2}BA + \dots + ABA^{n-2} + BA^{n-1}) + O(\Delta t^2) \right) \\ = & e^{i\delta n} \left(A^n - \frac{i\Delta t}{2} \sum_{j=0}^{n-1} A^{n-1-j}BA^j + O(\Delta t^2) \right) \\ = & (e^{i\delta}A)^n \left(1 - \frac{i\Delta t}{2}A^{-1} \sum_{j=0}^{n-1} A^{-j}BA^j + O(\Delta t^2) \right) \end{aligned} \quad (29)$$

□

Now we make a statement concerning the $O(\Delta t^2)$ terms:

Lemma 2 *The continuous time limit as defined in Eq. (26) will be independent of any $O(\Delta t^2)$ terms in the parameters ψ , θ , and ϕ .*

Proof Examining the last line of Eq. (29), we see that the only contribution of the $O(\Delta t^2)$ terms in the parameters ψ , θ , and ϕ will be in the $O(\Delta t^2)$ term. The $O(\Delta t^2)$ term in the last line of Eq. (29) does not contribute to the continuous time limit defined in Eq. (26) because it goes to zero as the limit is taken. Thus, the $O(\Delta t^2)$ terms in the parameters ψ , θ , and ϕ do not contribute to the continuous time limit. □

The next lemma uses Lemma 1 to constrain the values n can take for a finite limit in Eq. (26) to exist.

Lemma 3 *There is no continuous time limit as defined in Eq. (26) for $n = 1$.*

Proof For the Hamiltonian in Eq. (26) to be finite, $(SC)^n$ must equal $\mathbb{I} + O(\Delta t)$, and thus $\tilde{SC}$ must equal $\mathbb{I} + O(\Delta t)$ as well. Therefore, from Eq. (27), $(e^{i\delta}A)^n$ must equal identity if $\tilde{SC} = \mathbb{I} + O(\Delta t)$. The only unitary operator $e^{i\delta}A$ that could possibly satisfy $(e^{i\delta}A)^n = \mathbb{I}$ for $n = 1$ is the identity operator itself, but $e^{i\delta}A$ cannot even equal identity, as A has k dependence from containing $\tilde{S}$, and the angles are not permitted to depend on k , so there is no possible way to cancel out the k dependence. Thus, there is no continuous time limit defined in Eq. (26) for $n = 1$. $\square$

Next we use the reasoning from Lemma 3 to further constrain the values θ_0 and δ can take.

Lemma 4 *For the limit defined in Eq. (26) to be finite, θ_0 and δ must be constrained such that $\theta_0 = p\pi$ and $\delta = \frac{2\pi l}{n} - \frac{p\pi}{2}$ for odd integer p and any integer l .*

Proof Following up on the constraint that $(e^{i\delta}A)^n = \mathbb{I}$ from Lemma 3, let U be the diagonalization matrix of A , and let D be the matrix of eigenvalues of A . Then, we have the following:

$$(e^{i\delta}A)^n = e^{in\delta}(U^{-1}DUU^{-1}DUU^{-1}DU \dots) = e^{in\delta}U^{-1}D^nU = \mathbb{I} \quad (30)$$

$$\rightarrow e^{in\delta}D^n = UU^{-1} = \mathbb{I} \rightarrow e^{in\delta}D^n = \mathbb{I} \quad (31)$$

so if we set the eigenvalues of $e^{i\delta}A$ equal to an n th root of unity $e^{2\pi l/n}$ where $l = 0, 1, 2, \dots$ (which is equivalent to the constraint $(e^{i\delta}A)^n = \mathbb{I}$), we recover the following constraint for θ_0 :

$$\cos \theta_0/2 = \frac{\cos\left(\frac{2\pi l}{n} - \delta\right)}{\cos\left(\frac{\psi'_0 + \phi_0}{2}\right)} \quad (32)$$

Because none of the angles have k dependence, the only way this condition can hold true is if $\cos \theta_0/2 = 0$ or $\theta_0 = p\pi$ where $p = 1, 3, 5, \dots$. This also gives a constraint on δ , being $\delta = \frac{2\pi l}{n} - \frac{p\pi}{2}$. As a remark, the reason why the choice of overall phase is important here is that it shifts the zero point energy of the Hamiltonian in question and will make the dependence on other variables more manifest in the continuum limit (physical quantities are the differences in energies/eigenvalues of a Hamiltonian, not the eigenvalues themselves). $\square$

The next lemma uses the constraints on θ_0 and δ from Lemma 4 to impose a constraint on n .

Lemma 5 *For the limit defined in Eq. (26) to be finite, n must be even.*

Proof Substituting our constraint for θ_0 from Lemma 4 into A , we get the following:

$$A = -i \sin \frac{p\pi}{2} R_z(\psi'_0 - \phi_0) \sigma_y \quad (33)$$

Now consider n even. Substituting this form of A and our constraint on δ from Lemma 4 into $(e^{i\delta}A)^n$ in the last line of Eq. (29), where $n = 2w$ for some integer w , we find that $(e^{i\delta}A)^{2w} = (-e^{2i\delta}\mathbb{I})^w = \mathbb{I}$, as $A^2 = -\mathbb{I}$ and $(-e^{2i\delta})^w = \mathbb{I}$ for all w . This implies that even powers of n will satisfy $(e^{i\delta}A)^n = \mathbb{I}$. As for odd n , we can write $n = 2m + 1$ for some integer m to obtain the following:

$$(e^{i\delta}A)^n = (e^{i\delta}A)^{2m+1} = e^{i\delta}A \quad (34)$$

This cannot equate to identity, as we showed in Lemma 3 that for $n = 1$ no parametrization of A can make $e^{i\delta}A = \mathbb{I}$. Thus, n must be even to have a finite continuum limit as defined in Eq. (26). $\square$

Because the constraints on n and θ_0 hold true for all l from the last two lemmas, we will choose $l = 0$ for the remainder of the proof without loss of generality.

Now we plug in the constraints from Lemmas 4 and 5 to obtain the final forms of C , $\tilde{S}C$, $(\tilde{S}C)^n$, and most importantly H .

Lemma 6 Equation (26) will have a finite limit if C , $\tilde{S}C$, $(\tilde{S}C)^n$, and H are the following, where S is the shift operator defined in Eq. (8):

$$\begin{aligned} C &= (-1)^{p\pi} (R_z(\psi_0 - \phi_0)\sigma_y - \frac{i\Delta t}{2} [i(\phi_1 - \psi_1)R_z(\psi_0 - \phi_0)\sigma_x + \theta_1 R_z(\psi_0 - \phi_0)]) \\ \tilde{S}C &= (-1)^{p\pi} (R_z(\psi'_0 - \phi_0)\sigma_y - \frac{i\Delta t}{2} [i(\phi_1 - \psi_1)R_z(\psi'_0 - \phi_0)\sigma_x + \theta_1 R_z(\psi'_0 - \phi_0)]) \\ (\tilde{S}C)^n &= 1 - \frac{in\theta_1\Delta t}{4} (R_z(-2\phi_0) + R_z(2\psi'_0))\sigma_y \\ H &= -\frac{\theta_1}{4} (R_z(-2\phi_0) + S^2 R_z(2\psi_0))\sigma_y. \end{aligned} \quad (35)$$

Proof To find $\tilde{S}C$, we take the n_{th} root of both sides of the third line of Eq. (29). This will yield the following:

$$\tilde{S}C = e^{i\delta} \left(A - \frac{i\Delta t}{2} B \right). \quad (36)$$

Plugging in for the constrained versions of A and B and reducing, we obtain the following:

$$\tilde{S}C = (-1)^{p\pi} \left(R_z(\psi'_0 - \phi_0)\sigma_y - \frac{i\Delta t}{2} [i(\phi_1 - \psi_1)R_z(\psi'_0 - \phi_0)\sigma_x + \theta_1 R_z(\psi'_0 - \phi_0)] \right) \quad (37)$$

To find C , we simply multiply Eq. (37) by $\tilde{S}^{-1} = R_z(2k)$, obtaining the following:

$$C = (-1)^{p\pi} \left(R_z(\psi_0 - \phi_0)\sigma_y - \frac{i\Delta t}{2} [i(\phi_1 - \psi_1)R_z(\psi_0 - \phi_0)\sigma_x + \theta_1 R_z(\psi_0 - \phi_0)] \right) \quad (38)$$

Next we will find $(\widetilde{SC})^n$ by evaluating the sum in the last line of Eq. (29) using the constrained form of A in Eq. (33). One can show that $A^2 = -1$ and $A^{-1} = -A$, so the sum in Eq. (29) becomes the following:

$$A^{-1} \sum_{j=0}^{n-1} A^{-j} B A^j = -A \sum_{j=0}^{n-1} (-1)^j A^j B A^j \quad (39)$$

Now we split up the sum into even and odd terms:

$$\begin{aligned} -A \sum_{j=0}^{n-1} (-1)^j A^j B A^j &= -A \left(\sum_{j=\text{odds}}^{n-1} (-1)^j A^j B A^j + \sum_{j=\text{evens}}^{n-2} (-1)^j A^j B A^j \right) \\ &= -A \frac{n}{2} (-ABA + B) = -\frac{n}{2} \{A, B\} \\ &= \frac{n\theta_1}{2} (R_z(-2\phi_0) + R_z(2\psi'_0))\sigma_y \end{aligned} \quad (40)$$

We used Eq. (33) in the last line, so Eq. (29) becomes the following:

$$(SC)^n = 1 - \frac{in\theta_1 \Delta t}{4} (R_z(-2\phi_0) + R_z(2\psi'_0))\sigma_y \quad (41)$$

Now we can find $\widetilde{H}$ by evaluating the limit in Eq. (26) using Eq. (41) to obtain the following Hamiltonian in Fourier space:

$$\widetilde{H} = -\frac{\theta_1}{4} (R_z(-2\phi_0) + R_z(2\psi'_0))\sigma_y \quad (42)$$

Fourier transforming back and resubstituting for ψ'_0 , we obtain the following H :

$$H = \frac{\theta_1}{4} (R_z(-2\phi_0) + S^2 R_z(2\psi_0))\sigma_y \quad (43)$$

where S is the shift operator defined in Eq. (8). □

Combining Lemmas 4–6, we prove Theorem 2.

B Proof of time evolution from continuous time limit of DTQW Hamiltonian (Corollary 1)

We start by reiterating the corollary:

Corollary 1 Let $\vec{\Psi}(x, t)$ be a solution to the time evolution equation with the Hamiltonian from Theorem 2, $i\partial_t \vec{\Psi}(x, t) = H \vec{\Psi}(x, t) = -\frac{\theta_1}{4} (R_z(-2\phi_0) +$

$S^2 R_z(2\psi_0))\sigma_y \vec{\Psi}(x, t)$. Also, let $\vec{\Psi}(x, 0) = \begin{pmatrix} \Psi_L(x, 0) \\ \Psi_R(x, 0) \end{pmatrix}$ be the initial condition for $\vec{\Psi}(x, t)$. Then, the following is the analytical form of the time evolution for $\vec{\Psi}(x, t)$ for all t in terms of its initial state, where $x = m\Delta x$ for $m \in \mathbb{Z}$ and $J_m(t)$ is the m th order Bessel function of the first kind, $\alpha = \frac{\phi_0 + \psi_0}{2}$, and $\beta = \frac{\phi_0 - \psi_0}{2}$:

$$\begin{aligned} \vec{\Psi}(m\Delta x, t) &= \begin{pmatrix} \Psi_L(m\Delta x, t) \\ \Psi_R(m\Delta x, t) \end{pmatrix} \\ &= \frac{1}{2} \sum_{n=-\infty}^{\infty} i^{m-n} e^{i\alpha(m-n)} J_{m-n}\left(\frac{\theta_1 t}{2}\right) \\ &\quad \times \begin{pmatrix} (1 + (-1)^{m-n})\Psi_L(n\Delta x, 0) + ie^{i\beta}(1 - (-1)^{m-n})\Psi_R((n+1)\Delta x, 0) \\ -ie^{-i\beta}(1 - (-1)^{m-n})\Psi_L((n-1)\Delta x, 0) + (1 + (-1)^{m-n})\Psi_R(n\Delta x, 0) \end{pmatrix} \end{aligned}$$

We begin the theorem by finding the eigenvalues and eigenvectors of the Hamiltonian in Fourier space:

Lemma 7 *The eigenvalues of the Hamiltonian in Fourier space are $\pm\lambda(k) = \pm \cos(k - \frac{\phi_0 + \psi_0}{2})$ with corresponding eigenvectors $\vec{\pm\lambda} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm ie^{i(k + \frac{\phi_0 + \psi_0}{2})} \\ 1 \end{pmatrix}$.*

Proof The Hamiltonian written in Fourier space is the following:

$$\tilde{H}(k) = -\frac{\theta_1}{4} (R_z(-2\phi_0) + e^{2ik\Delta x} R_z(2\psi_0))\sigma_y \quad (44)$$

It follows from straightforward eigenvalue decomposition that the eigenvalues and eigenvectors are those in Lemma 7 $\square$

Our next lemma relates the Fourier transform of $\vec{\Psi}(x, t)$, denoted $\vec{\widetilde{\Psi}}(k, t)$, to the Fourier transform of the initial conditions of $\vec{\Psi}(x, t)$, denoted $\vec{\widetilde{\Psi}}(k, 0)$.

Lemma 8 *Let U be the unitary diagonalization matrix of eigenvectors of $\tilde{H}(k)$, so $U = \frac{1}{\sqrt{2}} \begin{pmatrix} ie^{i(k + \frac{\phi_0 - \psi_0}{2})} & -ie^{i(k + \frac{\phi_0 - \psi_0}{2})} \\ 1 & 1 \end{pmatrix}$. Then $\vec{\widetilde{\Psi}}(k, t) = Ue^{-i\lambda(k)\sigma_z t} U^\dagger \vec{\widetilde{\Psi}}(k, 0)$*

Proof If U is the diagonalization matrix of eigenvectors of $\tilde{H}(k)$, we can write $U^\dagger \tilde{H}(k) U = \lambda\sigma_z$. Therefore, because $UU^\dagger = \mathbb{I}$ by unitarity, we have the following:

$$\vec{\widetilde{\Psi}}(k, t) = e^{-i\tilde{H}(k)t} \vec{\widetilde{\Psi}}(k, 0) = UU^\dagger e^{-i\tilde{H}(k)t} UU^\dagger \vec{\widetilde{\Psi}}(k, 0) \quad (45)$$

$$= Ue^{iU^\dagger \tilde{H}(k) U t} U^\dagger \vec{\widetilde{\Psi}}(k, 0) = Ue^{-i\lambda(k)\sigma_z t} U^\dagger \vec{\widetilde{\Psi}}(k, 0) \quad (46)$$

$\square$

Our next lemma recovers the explicit expression for $Ue^{-i\lambda(k)\sigma_z t} U^\dagger \vec{\widetilde{\Psi}}(k, 0)$:

Lemma 9 Let U and $\lambda(k)$ be defined as in Lemma 7. Then, we have the following expression for $Ue^{-i\lambda(k)\sigma_z t}U^\dagger \widetilde{\Psi}(k, 0)$, where $\alpha = \frac{\phi_0 + \psi_0}{2}$ and $\beta = \frac{\phi_0 - \psi_0}{2}$:

$$Ue^{-i\lambda(k)\sigma_z t}U^\dagger \widetilde{\Psi}(k, 0) \quad (47)$$

$$= \frac{1}{2} \begin{pmatrix} (e^{\frac{i\theta_1 t}{2} \cos(k-\alpha)} + e^{-\frac{i\theta_1 t}{2} \cos(k-\alpha)})\widetilde{\Psi}_L(k, 0) + i(e^{\frac{i\theta_1 t}{2} \cos(k-\alpha)} - e^{-\frac{i\theta_1 t}{2} \cos(k-\alpha)})e^{i(k+\beta)}\widetilde{\Psi}_R(k, 0) \\ -i(e^{\frac{i\theta_1 t}{2} \cos(k-\alpha)} - e^{-\frac{i\theta_1 t}{2} \cos(k-\alpha)})e^{-i(k+\beta)}\widetilde{\Psi}_L(k, 0) + (e^{\frac{i\theta_1 t}{2} \cos(k-\alpha)} + e^{-\frac{i\theta_1 t}{2} \cos(k-\alpha)})\widetilde{\Psi}_R(k, 0) \end{pmatrix} \quad (48)$$

We obtain Lemma 9 through straightforward matrix multiplication. Our next lemmas will introduce some integrals and convolutions that we will need when computing the inverse Fourier transform of the equation in Lemma 9.

Lemma 10 Let $\mathcal{F}^{-1}$ denote the inverse Fourier transform, and $*$ denote the convolution. Then, we have the following inverse Fourier transforms, where $J_n(t)$ is the n th order Bessel function of the first kind:

$$\begin{aligned} \mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \cos(k-\alpha)}\widetilde{\Psi}_{L,R}(k, 0)) \\ = \mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \cos \alpha \cos k} e^{\pm \frac{i\theta_1 t}{2} \sin \alpha \sin k} \widetilde{\Psi}_{L,R}(k, 0)) \end{aligned} \quad (49)$$

$$= \mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \cos \alpha \cos k}) * \mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \sin \alpha \sin k}) * \mathcal{F}^{-1}(\widetilde{\Psi}_{L,R}(k, 0)) \quad (50)$$

$$= \sum_{n=-\infty}^{\infty} (\pm i)^{m-n} J_{m-n} \left(\frac{\theta_1 t}{2} \right) e^{i\alpha(m-n)} \Psi_{L,R}(n\Delta x, 0) \quad (51)$$

Proof The first equality of the equation in Lemma 10 is true by elementary trigonometric identities, and the second line is true by the convolution theorem. For the third line, we need the following inverse Fourier transforms

$$\mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \cos \alpha \cos k}) = \frac{\Delta x}{2\pi} \int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}} dk e^{ikn\Delta x} e^{\pm \frac{i\theta_1 t}{2} \cos \alpha \cos k} = (\pm i)^n J_n \left(\frac{\theta_1 t}{2} \cos \alpha \right) \quad (52)$$

$$\mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \sin \alpha \sin k}) = \frac{\Delta x}{2\pi} \int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}} dk e^{ikn\Delta x} e^{\pm \frac{i\theta_1 t}{2} \sin \alpha \sin k} = (\mp 1)^n J_n \left(\frac{\theta_1 t}{2} \sin \alpha \right) \quad (53)$$

$$\mathcal{F}^{-1}(\widetilde{\Psi}_{L,R}(k, 0)) = \Psi_{L,R}(m\Delta x, 0) \quad (54)$$

Now we find $\mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \cos \alpha \cos k}) * \mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \sin \alpha \sin k})$:

$$\mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \cos \alpha \cos k}) * \mathcal{F}^{-1}(e^{\pm \frac{i\theta_1 t}{2} \sin \alpha \sin k}) \quad (55)$$

$$= (\mp 1)^n \sum_{j=-\infty}^{\infty} (-i)^j J_j \left(\frac{\theta_1 t}{2} \cos \alpha \right) J_{n-j} \left(\frac{\theta_1 t}{2} \sin \alpha \right) \quad (56)$$

$$= (\pm i)^n J_n \left(\frac{\theta_1 t}{2} \right) e^{i\alpha n}, \quad (57)$$

where in the last line we used one of Graf's and Gegenbauer's addition theorems (Ref. [21], Eq. 10.23.7). Now we convolve this with $\Psi_{L,R}(m\Delta x, 0)$:

$$(\pm i)^n J_n \left(\frac{\theta_1 t}{2} \right) e^{i\alpha n} * \Psi_{L,R}(m\Delta x, 0) \quad (58)$$

$$= \sum_{n=-\infty}^{\infty} (\pm i)^{m-n} J_{m-n} \left(\frac{\theta_1 t}{2} \right) e^{i\alpha(m-n)} \Psi_{L,R}(n\Delta x, 0) \quad (59)$$

□

Next we have our last lemma:

Lemma 11 *Given the expression for $Ue^{-i\lambda(k)\sigma_z t} U^\dagger \widetilde{\Psi}(k, 0)$ in Lemma 9, we have the following:*

$$\begin{aligned} \mathcal{F}^{-1}(Ue^{-i\lambda(k)\sigma_z t} U^\dagger \widetilde{\Psi}(k, 0)) &= \vec{\Psi}(m\Delta x, t) \\ &= \frac{1}{2} \sum_{n=-\infty}^{\infty} i^{m-n} e^{i\alpha(m-n)} J_{m-n} \left(\frac{\theta_1 t}{2} \right) \\ &\quad \begin{pmatrix} (1 + (-1)^{m-n})\Psi_L(n\Delta x, 0) + ie^{i\beta}(1 - (-1)^{m-n})\Psi_R((n+1)\Delta x, 0) \\ -ie^{-i\beta}(1 - (-1)^{m-n})\Psi_L((n-1)\Delta x, 0) + (1 + (-1)^{m-n})\Psi_R(n\Delta x, 0) \end{pmatrix} \end{aligned} \quad (60)$$

Proof Observing the expression for $Ue^{-i\lambda(k)\sigma_z t} U^\dagger \widetilde{\Psi}(k, 0)$ in Lemma 9, we use Lemma 10 to go through each term and calculate the convolution. □

Thus, Lemma 11 recovers the time evolution equation in position space for the Hamiltonian from Theorem 2.

C Proof of continuous spacetime limit with no coin variation (Theorem 3)

We begin by restating the theorem:

Theorem 3 *Let $\vec{\Psi}(x, t)$ be a two-component wave function undergoing the DTQW, as defined in Eq. (1). Also, let $|\hat{n}| = \sqrt{n_x^2 + n_y^2 + n_z^2} = 1$, $l = 0, 1, 2, \dots$, $m = 1, 2, \dots$, and $v\Delta t = \Delta x$, where Δt and Δx are the time step and lattice spacings of the DTQW for $\vec{\Psi}(x, t)$, respectively. The continuous spacetime limit will exist for $\vec{\Psi}(x, t)$ if and only if the DTQW skips every m steps and the coin operator dictating its DTQW is of the form*

$$C = \exp \frac{i\pi l}{m} \exp \frac{-i\pi l}{m} \hat{n} \cdot \vec{\sigma}. \quad (62)$$

The ensuing Hamiltonian for this walk will be the following massless Dirac Hamiltonian:

$$H = -vn_z \hat{n} \cdot \vec{\sigma} \frac{\partial}{\partial x}. \quad (63)$$

To prove Theorem 3 we will construct lemmas as was done in Sect. 4. We will use Theorem 1 from Sect. 3 to prove Theorem 3. First we prove that the coin must be of the form of Eq. (20) by considering the following general unitary coin, where again $|\hat{n}| = \sqrt{n_x^2 + n_y^2 + n_z^2} = 1$:

$$C = e^{i\delta} R_n(\theta) = e^{i\delta} \exp -i\theta \hat{n} \cdot \vec{\sigma} / 2 \quad (64)$$

Lemma 12 *Let C be a general unitary operator as defined in Eq. (64). For the continuous spacetime limit to exist for this coin, it must be of the form in Eq. (20).*

Proof The only coins that will have a continuous spacetime limit will be those that possess the property such that for some integer m , $C^m = 1$, as stated in Theorem 1. Constraining this property onto the coins in Eq. (64), we get the following:

$$\begin{aligned} C^m &= e^{im\delta} \exp -im\theta \hat{n} \cdot \vec{\sigma} / 2 \\ &= e^{im\delta} (\cos m\theta / 2 - i \hat{n} \cdot \vec{\sigma} \sin m\theta / 2) = 1 \end{aligned} \quad (65)$$

The $\hat{n} \cdot \vec{\sigma}$ must go away, which constrains θ to satisfy $\theta = \frac{2\pi l}{m}$, where $l = 0, 1, 2, \dots$. Applying this constraint yields $C^m = e^{im\delta} (-1)^l$, so we must have that $\delta = \frac{\pi l}{m}$. Thus our original coin has become the following:

$$C = \exp \frac{i\pi l}{m} \exp \frac{-i\pi l}{m} \hat{n} \cdot \vec{\sigma} \quad (66)$$

□

Now we will be taking a continuous spacetime limit of the DTQW with this coin, and we will see what resultant PDE we obtain.

Lemma 13 *The Hamiltonian for the continuous spacetime limit of the DTQW with coin of the form in Eq. (20) will be the following:*

$$H = -vn_z \hat{n} \cdot \vec{\sigma} \frac{\partial}{\partial x}. \quad (67)$$

Proof We have the following continuous spacetime limit time evolution equation, where H is the resulting Hamiltonian or generator of time evolution for Ψ :

$$H = i \lim_{\Delta t, \Delta x \rightarrow 0} \frac{(S(\Delta x)C)^m - \mathbb{I}}{m \Delta t} \quad (68)$$

Let $\Delta x = v\Delta t$, so both space and time go to the continuum at the same scale. We focus our attention on the Fourier transformation of the operator in the middle of Eq. (68). We have the following:

$$\begin{aligned}\widetilde{S}(\Delta x)C^n - \mathbb{I} &= (e^{ikv\Delta t\sigma_z}C)^m - \mathbb{I} \\ &= ((1 + ikv\sigma_z\Delta t + O(\Delta t^2))C)^m - \mathbb{I}\end{aligned}\quad (69)$$

Next, we can ignore the $O(\Delta t^2)$ terms, as they will be zero in the end. So we obtain the following:

$$\begin{aligned}(\widetilde{S}(\Delta x)C)^n - \mathbb{I} &= (C + ikv\sigma_zC\Delta t)^m - \mathbb{I} \\ &= C^m + ikv\Delta t(C^{m-1}\sigma_zC + C^{m-2}\sigma_zC^2 + \dots \\ &\quad + C\sigma_zC^{m-1} + \sigma_zC^m + O(\Delta t^2)) - \mathbb{I} \\ &= ikv\Delta t \sum_{j=0}^{m-1} C^{m-j}\sigma_zC^j = ikv\Delta t \sum_{j=0}^{m-1} C^{-j}\sigma_zC^j\end{aligned}\quad (70)$$

Again, we can ignore the $O(\Delta t^2)$ terms, and we used the fact that $C^m = 1$. We can reduce the series in the last expression of (70) in the following way, setting $\alpha = \frac{\pi j}{m}$:

$$\begin{aligned}C^{-j}\sigma_zC^j &= \exp(i\alpha\hat{n} \cdot \vec{\sigma})\sigma_z\exp(-i\alpha\hat{n} \cdot \vec{\sigma}) \\ &= (\cos\alpha + i\hat{n} \cdot \vec{\sigma}\sin\alpha)\sigma_z(\cos\alpha - i\hat{n} \cdot \vec{\sigma}\sin\alpha) \\ &= 2\sin\alpha(-n_y\cos\alpha + n_xn_z\sin\alpha)\sigma_x + (2n_yn_z\sin^2\alpha + n_x\sin 2\alpha)\sigma_y \\ &\quad + (\cos 2\alpha + 2n_z^2\sin^2\alpha)\sigma_z\end{aligned}\quad (71)$$

The only terms to survive the sum will be those proportional to $\sin^2\alpha$ and $\cos^2\alpha$. Thus, we recover the sum:

$$\sum_{j=0}^{m-1} C^{-j}\sigma_zC^j = mn_z\hat{n} \cdot \vec{\sigma}\quad (72)$$

And thus our Hamiltonian is the following:

$$\widetilde{H} = ikvn_z\hat{n} \cdot \vec{\sigma}\quad (73)$$

Inverse Fourier transforming, we recover the Hamiltonian:

$$H = -vn_z\hat{n} \cdot \vec{\sigma}\frac{\partial}{\partial x}\quad (74)$$

□

Combining Lemmas 13 and 12 we obtain Theorem 3.

D Proof of continuous time and then space limit of DTQW (Theorem 4)

What follows is a short proof of Theorem 4. Here is the theorem for reference:

Theorem 4 *Let ϕ_0 and ψ_0 be unable to vary in the continuous space limit (i.e. ϕ_0, ψ_0 cannot depend on Δx). Then, the only time evolution equation which is not infinite and contains spatial derivative(s) for the continuous space limit ($\Delta x \rightarrow 0$) of the continuous time limit of the DTQW is a massless dirac equation.*

We begin with writing the Fourier space Hamiltonian of the continuous time limit of the DTQW, parametrized by ϕ_0, ψ_0 , and θ_1 (from Theorem 2):

$$H_C = -\frac{\theta_1}{4}(e^{i\phi_0\sigma_z} + e^{2ik\Delta x\sigma_z}e^{-i\psi_0\sigma_z})\sigma_y \quad (75)$$

The parameters ϕ_0, ψ_0 , and θ_1 are real numbers which cannot depend on k . If none of these parameters depend on Δx , we see that $\lim_{\Delta x \rightarrow 0} H_C = -\frac{\theta_1}{4}(e^{i\phi_0\sigma_z} + e^{-i\psi_0\sigma_z})\sigma_y$, which contains no spatial derivatives, thereby making it trivial. Therefore the parameters must depend on Δx . By Conjecture 1, the only parameter that can depend on Δx is θ_1 . Now for the following lemma:

Lemma 14 $\theta_1 = \frac{\alpha}{\Delta x}$ for some $\alpha \in \mathbb{R}$ in order for $\lim_{\Delta x \rightarrow 0} H_C$ to contain a spatial derivative.

Proof Spatial derivatives in Fourier space look the following way, where $\mathcal{F}(g(x))$ is the Fourier transform of $g(x)$:

$$\lim_{\Delta x \rightarrow 0} \frac{e^{ik\Delta x} - 1}{\Delta x} = ik = \mathcal{F}(\partial_x) \quad (76)$$

Now we expand H_C for small Δx :

$$H_C = -\frac{\theta_1}{4}(e^{i\phi_0\sigma_z} + e^{-i\psi_0\sigma_z} + 2ik\Delta x\sigma_z e^{-i\psi_0\sigma_z} + O(\Delta x^2))\sigma_y \quad (77)$$

Given that the only parameter that can depend on Δx is θ_1 , and that the only term which can contain a spatial derivative is the 3rd term, but only if it is divided by Δx , it must be the case that θ_1 is proportional to $\frac{1}{\Delta x}$. $\square$

Henceforth, we will set $\theta_1 = \frac{\alpha}{\Delta x}$ for some $\alpha \in \mathbb{R}$. Now for the next lemma:

Lemma 15 *The only parametrizations that will allow H_C to be finite in the limit $\Delta x \rightarrow 0$ are those consistent with the constraint $\phi_0 + \psi_0 = \pi$.*

Proof We rewrite H_C as above, but now we factor out $e^{-i\psi_0\sigma_z}$:

$$H_C = -\frac{\alpha}{4\Delta x} e^{-i\psi_0\sigma_z} (e^{2ik\Delta x\sigma_z} + e^{i(\phi_0+\psi_0)\sigma_z}) \sigma_y \quad (78)$$

In order for the term $e^{2ik\Delta x\sigma_z} + e^{i(\phi_0+\psi_0)\sigma_z}$ to look like a spatial derivative, $e^{i(\phi_0+\psi_0)\sigma_z}$ must be proportional to $-\text{identity}$, which equates to $\phi_0 + \psi_0 = \pi$. $\square$

For the sake of completeness, these conditions on the parameters of the coin correspond to the following pre-continuous time limit coin:

$$-\exp(i\phi_0\sigma_z/2)\sigma_x \exp\left(-i\frac{\alpha\Delta t}{2\Delta x}\sigma_y\right)\exp(-i\phi_0\sigma_z/2) \quad (79)$$

[from Eq. (16)]. Putting these two lemmas together, we get that the only finite continuous space limit H_C can have which contains spatial derivatives is the following:

$$\lim_{\Delta x \rightarrow 0} H_C = -\frac{\alpha}{2} e^{-i\psi_0\sigma_z} k \sigma_x \quad (80)$$

This equates to the following time evolution equation in position space for wave function $\vec{\psi}(x, t)$

$$i\partial_t \vec{\psi}(x, t) = i\frac{\alpha}{2} e^{-i\psi_0\sigma_z} \sigma_x \partial_x \vec{\psi}(x, t) \quad (81)$$

which is in the form of a dirac Hamiltonian for a massless particle in the σ_x basis (and reduces to the familiar form when $\psi_0 = 0$).

E Proof of general coin CTQW-DTQW relation (Theorem 5)

We begin by restating the theorem:

Theorem 5 Let $\vec{\Psi}(x, t)$ be the following two-component wave function resulting from the continuous time limit of the DTQW with a general coin as found in Theorem 2:

$$i\partial_t \vec{\Psi}(x, t) = -\frac{\theta_1}{4} (R_z(-2\phi_0) + S^2 R_z(2\psi_0)) \sigma_y \vec{\Psi}(x, t)$$

where θ_1 , ϕ_0 , and ψ_0 are real numbers which cannot depend on x or t . Additionally, let $\vec{\Psi}_{\pm}(x, t)$ be wave functions which satisfy the following CTQW time evolution equations:

$$i\partial_t \vec{\Psi}_{\pm}(x, t) = \mp \frac{\theta_1}{4} [\vec{\Psi}_{\pm}(x + \Delta x, t) + \vec{\Psi}_{\pm}(x - \Delta x, t) - 2\vec{\Psi}_{\pm}(x, t)].$$

Then, $\vec{\Psi}(x, t)$ can be written as a superposition of $\vec{\Psi}_+(x, t)$ and $\vec{\Psi}_-(x, t)$ in the following way (where $\alpha = \frac{\phi_0 + \psi_0}{2}$):

$$\vec{\Psi}(x, t) = e^{i\alpha \frac{x}{\Delta x}} (e^{-\frac{i\theta_1 t}{2}} \vec{\Psi}_+(x, t) + e^{\frac{i\theta_1 t}{2}} \vec{\Psi}_-(x, t)). \quad (82)$$

To begin, we introduce the following lemma:

Lemma 16 Let $\tilde{H} = -\frac{\theta_1}{4}(R_z(-2\phi_0) + \tilde{S}^2 R_z(2\psi_0))\sigma_y$. Then, the eigenvalues of $\tilde{H}$ are $\pm \frac{\theta_1}{2} \cos(k\Delta x - \frac{\phi_0 + \psi_0}{2})$.

This lemma is obtained from straightforward eigenvalue decomposition of $\tilde{H}$. Now for our next lemma:

Lemma 17 Let $\vec{\Psi}_\pm(x, t)$ be the inverse Fourier transform of the eigenvectors of $\tilde{H}$. The inverse Fourier transform of the time evolution equation of the eigenvectors of $\tilde{H}$ is $i\partial_t \vec{\Psi}_\pm(x, t) = \pm \frac{\theta_1}{4} (e^{-i\alpha} \vec{\Psi}_\pm(x + \Delta x, t) + e^{i\alpha} \vec{\Psi}_\pm(x - \Delta x, t))$

Proof From Lemma 16 we have the following, where $\vec{\Psi}_\pm(k, t)$ are eigenvectors of $\tilde{H}$ and $\alpha = \frac{\phi_0 + \psi_0}{2}$:

$$i\partial_t \vec{\Psi}_\pm(k, t) = \pm \frac{\theta_1}{2} \cos(k\Delta x - \alpha) \vec{\Psi}_\pm(k, t) \quad (83)$$

$$= \pm \frac{\theta_1}{4} (e^{ik\Delta x} e^{-i\alpha} + e^{-ik\Delta x} e^{i\alpha}) \vec{\Psi}_\pm(k, t). \quad (84)$$

Inverse Fourier transforming this, we get $i\partial_t \vec{\Psi}_\pm(x, t) = \pm \frac{\theta_1}{4} (e^{-i\alpha} \vec{\Psi}_\pm(x + \Delta x, t) + e^{i\alpha} \vec{\Psi}_\pm(x - \Delta x, t))$. $\square$

Now for our next lemma:

Lemma 18 The wave functions $\vec{\Psi}'_\pm(x, t) = e^{i(\pm \frac{\theta_1 t}{2} - \alpha \frac{x}{\Delta x})} \vec{\Psi}_\pm(x, t)$ will satisfy the CTQW time evolution equation $i\partial_t \vec{\Psi}'_\pm(x, t) = \pm \frac{\theta_1}{4} [\vec{\Psi}'_\pm(x + \Delta x, t) + \vec{\Psi}'_\pm(x - \Delta x, t) - 2\vec{\Psi}'_\pm(x, t)]$.

Proof It can easily be seen that plugging in $\vec{\Psi}_\pm(x, t) = e^{i(\mp \frac{\theta_1 t}{2} + \alpha \frac{x}{\Delta x})} \vec{\Psi}'_\pm(x, t)$ to $i\partial_t \vec{\Psi}_\pm(x, t) = \pm \frac{\theta_1}{4} (e^{-i\alpha} \vec{\Psi}_\pm(x + \Delta x, t) + e^{i\alpha} \vec{\Psi}_\pm(x - \Delta x, t))$ will yield the CTQW time evolution equation for $\vec{\Psi}'_\pm(x, t)$. $\square$

Now for our last lemma:

Lemma 19 $\vec{\Psi}(x, t)$ can be written as a superposition of $\vec{\Psi}'_+(x, t)$ and $\vec{\Psi}'_-(x, t)$, which satisfy the CTQW time evolution equation, in the following way:

$$\vec{\Psi}(x, t) = e^{i\alpha \frac{x}{\Delta x}} (e^{-\frac{i\theta_1 t}{2}} \vec{\Psi}'_+(x, t) + e^{\frac{i\theta_1 t}{2}} \vec{\Psi}'_-(x, t)) \quad (85)$$

Proof Let P_+ and P_- be projectors onto the $+$ and $-$ eigenvectors of $H = -\frac{\theta_1}{4}(R_z(-2\phi_0) + S^2 R_z(2\psi_0))\sigma_y$. Then, we can write the following:

$$\vec{\Psi}(x, t) = (P_+ + P_-)\vec{\Psi}(x, t) \quad (86)$$

$$= P_+\vec{\Psi}(x, t) + P_-\vec{\Psi}(x, t) \quad (87)$$

$$= \vec{\Psi}_+(x, t) + \vec{\Psi}_-(x, t). \quad (88)$$

From Lemma 18, we plug in $\vec{\Psi}_{\pm}(x, t) = e^{i(\mp\frac{\theta_1}{2} + \alpha\frac{x}{\Delta x})}\vec{\Psi}'_{\pm}(x, t)$ and obtain the expression in Lemma 19. $\square$

F Continuous spacetime limit with coin variation for $n = 1$

The following will be a reiteration of some of the results from Ref. [20], but there will be an emphasis on relating the continuous spacetime limit to the Dirac equation, or “Dirac-Type” equations as we will denote them. Let $\vec{\Psi}(x, t) \in L^2(\mathbb{R}) \times L^2(\Sigma)$, where Σ is the space spanned by $|L\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|R\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, and let $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Then, the following is the Dirac equation in 1 space and 1 time dimension $(1 + 1)$:

$$i\partial_t \vec{\Psi}(x, t) = (i\sigma_z \partial_x + \sigma_x m)\vec{\Psi}(x, t). \quad (89)$$

A “Dirac-Type” equation is the following, where $\hat{A}$ and $\hat{B}$ are any 2×2 anti-hermitian and hermitian matrices, respectively:

$$i\partial_t \vec{\Psi}(x, t) = (i\hat{A}\partial_x + \hat{B})\vec{\Psi}(x, t). \quad (90)$$

Equation (89) can easily be obtained by taking the continuous spacetime limit of the DTQW with the coin $C = e^{im\Delta t\sigma_x}$ and the usual shift operator (in Fourier space) $\tilde{S} = e^{ik\Delta x\sigma_z}$. In the same fashion, Eq. (90) can easily be obtained by taking the continuous spacetime limit of the DTQW with the coin $C = e^{i\Delta t\hat{B}}$, but now with a different shift operator $\tilde{S} = e^{ik\Delta x\hat{A}}$.

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