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Local Probability Conservation in Discrete Time Quantum Walks

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We show that probability is locally conserved in discrete time quantum walks, corresponding to a particle evolving in discrete space and time. In particular, for a spatial structure represented by an arbitrary directed graph, and any unitary evolution of a particle which respects that locality structure, we can define probability currents which also respect the locality structure and which yield the correct final probability distribution.

I. INTRODUCTION

For a particle evolving via the Schrodinger equation in continuous space and time, it is well known that any changes in its probability density can be explained by local probability currents. This result has recently been extended to discrete space and continuous time [1, 2]. In this paper we will demonstrate that this is also the case for discrete space and time, hence ensuring local conservation of probability for discrete time quantum walks [3–5]. Probability currents have previously been defined for particular cases of quantum walks in one and two spatial dimensions [6–8]. However, here we give a general approach that proves the existence of a probability current for walks on arbitrary directed graphs.

In continuous space and time the local conservation of probability for a single particle is expressed by the continuity equation

$$\frac{\partial \rho(\vec{x},t)}{\partial t} + \nabla \cdot J(\vec{x},t) = 0, \tag{1}$$

where $\rho(\vec{x},t) = |\psi(\vec{x},t)|^2$ is the probability density and $J(\vec{x},t)$ is a vector field describing the probability current. For a particle governed by the non-relativistic Schrödinger equation

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{x},t) + V\psi(\vec{x},t) \tag{2}$$

we find that

$$J(\vec{x},t) = -\frac{i\hbar}{2m}[\psi^*(\vec{x},t)\nabla\psi(\vec{x},t) - \psi(\vec{x},t)\nabla\psi^*(\vec{x},t)], \tag{3}$$

is real and satisfies equation (1). From this we can conclude that probability is conserved locally in this case. A similar probability current can be defined for relativistic systems governed by the Dirac equation [9].

The same is true if we make space discrete. In this picture we represent space as a graph. Then the continuity equation representing local conservation of probability becomes

$$\frac{dP_n(t)}{dt} + \sum_m J_{mn}(t) = 0, \tag{4}$$

where $P_n(t)$ represents the probability of being at vertex n at time t and $J_{mn}(t)$ is a matrix element representing the probability current between vertexes n and m (where $J_{mn}(t) > 0$ implies a net flow of probability from n to m). To ensure locality we require that $J_{mn}(t) = 0$ whenever n and m are not linked by an edge in the graph, and in order to obtain meaningful results, we also require that $J_{mn}(t)$ be real and anti-symmetric. It has been shown that for any system undergoing Schrödinger evolution with Hamiltonian $H(t)$, we can take $J_{mn}(t)$ to have the form [1]

$$J_{mn}(t) = \frac{1}{i\hbar}(H_{mn}(t)\rho_{nm}(t) - \rho_{mn}(t)H_{nm}(t)). \tag{5}$$

Here $\rho(t)$ represents the density operator of the particle at time t. Similar results have been obtained by considering probability currents in tight-binding models and other discrete solid state structures [2, 10–12]. Given that $H_{mn}(t)$ and $H_{nm}(t)$ are zero whenever n and m are not linked by an edge, $J(t)$ is a local probability current which satisfies (4) and is real and antisymmetric. Hence again in these systems probability is locally conserved.

We now take this further by also making time discrete. Instead of the Schrödinger equation, in each time step a unitary operator is applied to the state. Labelling the discrete times by integers, we have $|\psi(t+1)\rangle = U(t)\,|\psi(t)\rangle$. This corresponds to a discrete time quantum walk. For simplicity in what follows, we will focus on a single time-step and omit the explicit time parameter t, writing $|\psi'\rangle = U\,|\psi\rangle$. A quantum walk of many time-steps can be considered by treating each time-step individually.

As time derivatives are not applicable in this case, the continuity equation (4) must be modified to refer to the change in probability $\Delta P_n = P_n^{'} - P_n$ at vertex n in one time step, and the probability current J_{mn} flowing between n and m in that time step, giving

$$\Delta P_n + \sum_m J_{mn} = 0. \tag{6}$$

There are four main properties that the probability current J should satisfy. As in the previous case it should

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be real, anti-symmetric and non–zero only when n and m are connected by an edge in the graph. However, here an additional property to enforce locality is required - that the probability flux out of a given vertex in one time step is less than the initial probability of being at that vertex. This property can be written concisely as

$$\sum_{m^*} J_{m^*n} \leq P_n, \tag{7}$$

where $m^* = \{m : J_{mn} > 0\}$. We will use this notation for m^* throughout the paper.

Ideally, it would be possible to find an equation for J_{mn} in terms of U and $|\psi\rangle$ which satisfies all of the above requirements. A promising candidate is [13]

$$\begin{aligned} J_{mn} = \frac{1}{2}[(\rho U^\dagger)_{nm} U_{mn} + (U^\dagger)_{nm}(U\rho)_{mn} \\ - U_{nm}(\rho U^\dagger)_{mn} - (U\rho)_{nm}(U^\dagger)_{mn}]. \end{aligned} \tag{8}$$

where $\rho = |\psi\rangle\langle\psi|$. This is anti-symmetric, real-valued, and equal to zero whenever n and m are not connected by an edge in the graph (in which case $U_{mn}, (U^\dagger)_{nm}, U_{nm}$ and $(U^\dagger)_{mn}$ are all equal to zero). Furthermore we show in appendix A that this definition satisfies (6). However, we also show that this definition does not always satisfy (7), and therefore is not a suitable discrete-time probability current.

Whilst it is possible that an alternative general equation for J_{nm} could be found which satisfies all the requirements, we conjecture that one does not exist, due to the complex nature of the constraints encoded by (7), which only arise in discrete time. Instead we give in this paper a general non-constructive proof that a probability current satisfying all of the requirements exists. This resolves the key foundational issue, showing that probability is locally conserved in discrete space and time. We also give an efficient numerical method for computing the probability current, and extend the results to cases with internal degrees of freedom and directed graphs, for which we require that $J_{mn} > 0$ only if there is a directed edge from n to m.

II. SETUP

A suitable description of our discrete space is a graph, consisting of a set of vertices V and a set of edges E. For full generality, we consider directed graphs, for which an edge is associated with a particular direction of travel. Examples of these types of graphs are shown in figure 1. These graphs allow us to include novel space-time structures in which the particle is restricted to travel in certain directions. An edge is specified by an ordered pair of vertices $E \subseteq \{n \to m \,|\, n, m \in V\}$. For example, the edge $n \to m$ would allow the particle to move from n to m. We assume that the particle is always allowed to remain at its current location, so all self loops are included in E ($n \to n \in E$ for all n) [1]. To restrict to the simpler case of undirected graphs, we would require that $n \to m \in E \implies m \to n \in E$.

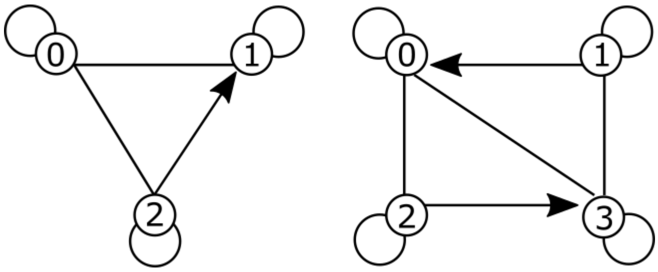

FIG. 1. Examples of directed graphs that allow discrete time Quantum walks. Edges without arrows are undirected and can be traversed in either direction.

The time evolution of a quantum particle in our discrete space-time model corresponds to a discrete time quantum walk on this graph. To define such a quantum walk, we associate an orthonormal quantum state $|n\rangle$ to each vertex (corresponding to the particle being at that point), and specify a unitary operator U describing the evolution, for which the matrix elements $U_{mn} = \langle m| U |n\rangle$ satisfy $n \to m \notin E \implies U_{mn} = 0$. Hence the unitary evolution cannot move the particle between vertices which are not connected by an edge. Given an initial pure state $|\psi\rangle$, we have $P_n = |\langle n|\psi\rangle|^2$ and $P'_n = |\langle n|U|\psi\rangle|^2$

Note that in the case of discrete space and continuous time, it is unnecessary to consider directed graphs. If there was a directed edge from m to n but no corresponding edge in the opposite direction (i.e. $m \to n \in E$ but $n \to m \notin E$) then we must have $H_{mn}(t) = 0$ for all time t. However, the Hermitian nature of the Hamiltonian would then imply that $H_{nm}(t) = 0$ as well. Such cases would be the same as if there was no edge at all between m and n, with no probability flowing in either direction ($J_{mn}(t) = 0$ for all t).

In the case of discrete space and discrete time, directed graphs can lead to interesting results, because there exist unitaries with $U_{mn} = 0$ but $U_{nm} \neq 0$. Hence we can find examples in which particles propagate along directed edges only in the allowed direction. Directed graphs have been previously studied in the context of discrete time quantum walks. In particular it has been shown that reversibility of the graph is a necessary and sufficient condition to define a coined Quantum walk [5]. An edge from $n \to m$ is reversible if there exists a path from m to n, and a graph is reversible if every edge in it is reversible. We give the extension of our results to coined quantum

[1] If we allow graphs for which some self loops are not included, then we can still prove local probability conservation using the probability flow approach given in the next section. However, the corresponding restrictions on the probability current are more complicated.

walks, and other cases in which the vertices have internal states in section III D.

III. RESULTS

A. Probability flow

In order to analyse the locality of probability flows, it is helpful to break the probability current J_{mn} (which represents the net flow of probability between vertices n and m) into the individual flows of probability along the directed edges $n \to m$ and $m \to n$. In particular, we define the flow of probability along the edge $n \to m$ as f_{mn}. Then

$$J_{mn} = f_{mn} - f_{nm}. \tag{9}$$

Note that the 'diagonal' flow matrix element f_{nn} corresponds to the amount of probability which remains at vertex n.

In order to give meaningful results and satisfy local probability conservation, the flow matrix elements f_{mn} must satisfy the following properties:

$$f_{mn} \geq 0, \tag{10}$$

$$f_{mn} = 0 \quad \text{if} \quad n \to m \notin E, \tag{11}$$

$$\sum_m f_{mn} = P_n, \tag{12}$$

$$\sum_n f_{mn} = P'_m. \tag{13}$$

The first condition specifies that the probability flowing along an edge in a particular direction must be positive, the second that it must respect the locality structure of the graph. The third condition specifies that all probability initially at vertex n must either flow to a neighbouring vertex or remain there during one time-step. The fourth condition requires that all probability at vertex n after one time step must either have flowed to it from a neighbouring vertex or have remained there.

Note that these conditions would refer to any local probabilistic evolution on a graph. The quantum nature of the evolution enters because we use $|\psi\rangle$ and U to calculate the initial and final probability distributions via $P_n = |\langle n|\psi\rangle|^2$ and $P'_m = |\langle m|U|\psi\rangle|^2$. These probability distributions then enter the flow conditions (12) and (13) which will be used in the next two sections to prove the existence of a valid set of probability flows and to construct explicit solutions numerically. Not all pairs of distributions P_n and P'_m can arise from a quantum evolution on a particular graph.

We now show that properties (10) - (13) for f_{mn} yield all the required properties of J_{mn}. The flow f_{mn} is a positive number hence J_{mn} as defined in (9) is real. We also see that J_{mn} is anti-symmetric, and non-zero only when an edge exists between m and n. Note that

$$\begin{aligned}\Delta P_n + \sum_m J_{mn} &= (P'_n - P_n) + \sum_m f_{mn} - \sum_m f_{nm} \\ &= (P'_n - P_n) + P_n - P'_n \\ &= 0,\end{aligned} \tag{14}$$

hence J_{mn} satisfies equation (6). Finally, as

$$\begin{aligned}\sum_{m^*} J_{m^*n} &= \sum_{m^*} f_{m^*n} - \sum_{m^*} f_{nm^*} \\ &\leq \sum_m f_{mn} - \sum_{m^*} f_{nm^*} \ \leq P_n\end{aligned} \tag{15}$$

J_{mn} also satisfies equation (7).

Below, we show that a valid f_{nm} satisfying properties (10)-(13) always exists, hence we can also define a valid J_{nm} satisfying local probability conservation.

The converse is also true. If we can define a J_{nm} which is real, antisymmetric, satisfies (6) and (7), and for which $J_{mn} > 0$ only if $m \to n \in E$ then we can always generate flows f_{mn} satisfying conditions (10)-(13). This is shown in appendix B, and illustrates that flow conditions (10)-(13) are equivalent to the conditions on the J_{mn} given in the introduction.

B. Existence of local probability flows

In this section we prove that there exist flow matrix elements f_{nm} satisfying the conditions (10) to (13) for any discrete time quantum walk, and thus that probability is locally conserved.

We can show the existence of such probability flows using a result of Aaronson [14], which was proven in a different context (without considering locality). He showed that for any unitary evolution of a quantum state, and any fixed basis, there exist probability flows f_{mn} between basis states that take the initial probability distribution over the basis to the final probability distribution over that basis, and which satisfy $f_{mn} \leq |U_{mn}|$. In our case, $n \to m \notin E \implies U_{mn} = 0 \implies f_{mn} = 0$, hence such flows would satisfy our requirements. However, Aaronson's condition is stronger than we need, because it also constrains probability flows along edges which do exist. Therefore, for completeness and clarity, we provide here a simpler proof of a similar result which is sufficient for our purposes.

The key insight is to consider probability as a 'fluid', flowing through a network of 'pipes' with different capacities from a source to a sink. This can be described by a directed graph with edges which have a maximum capacity specifying the amount of probability allowed to flow along them. Figure 2 illustrates the configuration we will consider.

This network consists of 3 different groups of edges. The first and final sets of edges have capacity corresponding to initial and final probabilities respectively. The intermediate edges represent the evolution of the state and

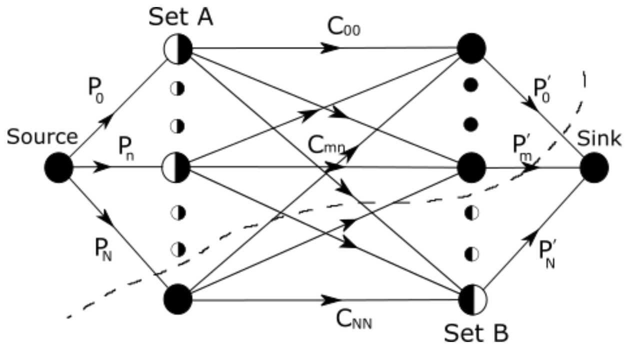

FIG. 2. A diagram showing the movement of probability in the network flow picture. The line on the graph is an example of a cut. Vertices corresponding to $n \in A$ and $m \in B$ are shown half-filled.

have capacity defined in the following way [2]

$$C_{mn} = \begin{cases} 0 & \text{if } n \to m \notin E \\ 1 & \text{otherwise} \end{cases} \tag{16}$$

If the total capacity of this network from source to sink is one, then for any flow configuration achieving this capacity the flow of probability along the edges in the middle section will give a valid f_{mn}. In particular, we set f_{mn} equal to the flow of probability along the intermediate edge with capacity C_{mn}.

Following a similar approach to [14], we will show that the maximum flow allowed by the network is one unit of probability by making use of the max-flow, min-cut theorem [15]. This states that the value of the minimum cut in the network is equal to the maximum flow of the network. A cut is a set of edges which if removed from the network disconnects the source from the sink, and its value is the total capacity of those edges.

Let us first write down the value K of a general cut. Let A be the set of n such that the edge $Source \to n$ is not in the cut and let B be the set of m such that the edge $m \to Sink$ is not in the cut. Then to disconnect the source from the sink the cut must contain all the edges $n \to m$ such that $n \in A$ and $m \in B$. Therefore the value of the cut can be written as

$$\begin{aligned} K &= \sum_{n \notin A} P_n + \sum_{m \notin B} P'_m + \sum_{n \in A, m \in B} C_{mn} \\ &= (1 - \sum_{n \in A} P_n) + (1 - \sum_{m \in B} P'_m) + \sum_{n \in A, m \in B} C_{mn} \\ &= 2 - \left(\sum_{n \in A} P_n + \sum_{m \in B} P'_m \right) + \sum_{n \in A, m \in B} C_{mn} \end{aligned} \tag{17}$$

In order for probability one to be able to flow through the network, we require that $K \geq 1$ for all cuts. We prove this by considering separately the two cases in which the sum over C_{mn} in (17) is either non-zero or zero.

Firstly, consider the case in which at least one of the C_{mn} elements in the cut is equal to one. In this case $\sum_{n \in A, m \in B} C_{mn} \geq 1$ and thus

$$K \geq 3 - \left(\sum_{n \in A} P_n + \sum_{m \in B} P'_m \right) \geq 1, \tag{18}$$

where we have used the fact that any partial sum over elements of a probability distribution is at most one.

Secondly, consider the case in which all of the C_{mn} elements in the cut are zero, such that $\sum_{n \in A, m \in B} C_{mn} = 0$. In this case, it is helpful to express the sum over probabilities in (17) in terms of projection operators as

$$\begin{aligned} \sum_{n \in A} P_n + \sum_{m \in B} P'_m &= \sum_{n \in A} |\langle n|\psi\rangle|^2 + \sum_{m \in B} |\langle m| U |\psi\rangle|^2 \\ &= \langle\psi| \Big(\sum_{n \in A} |n\rangle \langle n| + \sum_{m \in B} U^\dagger |m\rangle \langle m| U \Big) |\psi\rangle \\ &= \langle\psi| \Pi_A + \Pi_B |\psi\rangle \end{aligned} \tag{19}$$

where $|\psi\rangle$ is the initial state,

$$\Pi_A = \sum_{n \in A} |n\rangle \langle n| \quad \text{and} \quad \Pi_B = \sum_{m \in B} U^\dagger |m\rangle \langle m| U. \tag{20}$$

Π_A and Π_B are projectors onto the spaces spanned by $|n\rangle$ such that $n \in A$ and $U^\dagger |m\rangle$ such that $m \in B$ respectively. In this case, we can show that Π_A and Π_B are projectors onto orthogonal spaces, and thus that $\Pi_A + \Pi_B$ is itself a projection operator. In particular,

$$\Pi_B \Pi_A = \sum_{n \in A, m \in B} U^\dagger |m\rangle \langle m| U |n\rangle \langle n| = 0 \tag{21}$$

because by assumption $C_{mn} = 0$ for all terms in the sum, which means that $n \to m \notin E$ and thus $U_{mn} = \langle m| U |n\rangle = 0$. As $\Pi_A + \Pi_B$ is a projection operator, $\langle\psi| \Pi_A + \Pi_B |\psi\rangle \leq 1$ and thus

$$K = 2 - \langle\psi| \Pi_A + \Pi_B |\psi\rangle \geq 1. \tag{22}$$

Note that this second part of the proof, expressed in (19) - (22), depends critically on the quantum nature of the evolution.

We have shown that $K \geq 1$ for all cuts in the network shown in figure 2. Hence the minimum cut in the network has value greater than or equal to one. In fact, the minimum cut must have value exactly one, because a possible cut would be to separate the source from all nodes it is connected to, which has value $K = \sum_n P_n = 1$. Then by applying the Max-flow, Min-cut theorem we can conclude that the maximum flow allowed in the network is also one.

In appendix C, we show how this general proof applies to a specific example of a quantum walk on a three vertex graph, to further illustrate the method.

[2] Note that the similar result in [14] takes $C_{mn} = |U_{mn}|$. This leads to a valid flow satisfying $f_{mn} \leq |U_{mn}|$.

As we have shown that one unit of probability can flow through the network, there exists a valid local probability flow which changes P_n to P'_n. As this applies to each time step of a discrete time quantum walk, it proves that probability is locally conserved in such evolutions. In other words, probability is locally conserved for all quantum evolutions in discrete space time.

C. Constructing solutions

Although the above proof ensures the existence of a valid probability flow satisfying local probability conservation, it does not give a method of constructing such a flow. However, this can be achieved efficiently for cases with a finite number of vertices via linear programming.

If N is the number of vertices in V, we can think of the flow matrix elements f_{nm} as forming an N^2 dimensional real vector $\mathbf{f}$. The constraints (10)-(13) then correspond to a positivity constraint on each component of $\mathbf{f}$, and a number of linear equalities satisfied by the components. These can be expressed in the form

$$\mathbf{f} \geq 0, \tag{23}$$

$$\mathbf{A}.\mathbf{f} = \mathbf{b}, \tag{24}$$

where $\mathbf{A}$ and $\mathbf{b}$ are a matrix and vector expressing the linear equalities (11) - (13). Given such constraints, a linear program can find a vector $\mathbf{f}^*$ which satisfies the constraints and maximizes the value of some linear objective function $c = \mathbf{v}.\mathbf{f}$. In this case, as we are only interested in finding a feasible assignment $\mathbf{f}$, it does not really matter what we choose as our objective function, but one natural choice would be to maximize the amount of probability which remains stationary (i.e. taking $c = \sum_n f_{nn}$). This would prevent probability from flowing in both directions between two vertices. Note that this is not the only source of non-uniqueness of $\mathbf{f}$. Given any cycle on the graph around which probability of at least δ flows, there is another valid solution in which that probability remains stationary instead.

Various techniques exist to solve linear programming problems, including the simplex method [16], or Karmarkar's algorithm [17]. The latter approach is efficient in the computational complexity sense, requiring a time which is polynomial in N.

In appendix C, we show how to use this method to generate probability flows for a specific example of a quantum walk on a three vertex graph.

D. Systems with Internal Degrees of Freedom

Quantum systems with internal degrees of freedom are commonly used in the context of coined quantum walks. In particular, we could consider a particle which carries an internal degree of freedom, such as a spin, in addition to its location. Alternatively we could consider cases in which each spatial location has its own distinct set of internal states.

In both of these cases we can denote an orthonormal basis of quantum states by $|n, k\rangle$ where $n \in V$ gives the spatial location and $k \in \mathcal{S}_n$ gives the internal degree of freedom. In such cases, we can apply the results obtained earlier, and thus prove local probability conservation, by mapping the system to one with no internal degrees of freedom. In this mapping, a vertex with M internal degrees of freedom can be replaced with a set of M vertices that are all connected to each other. Note that this is similar to the staggered fermion approach used in discrete models of quantum field theory [18–20] where some issues arise. However, as we are using this as a mathematical tool to prove probability conservation on the original graph these issues do not affect the result.

In particular, suppose that initially the different spatial locations form a directed graph with edge set $E \subseteq \{n \to m \,|\, n, m \in V\}$, then we can construct a new graph to represent the situation including the internal degrees of freedom, with vertices $V' = \{(n,k) \,|\, n \in V, k \in \mathcal{S}_n\}$ and edge set $E' = \{(n,k) \to (m,l) \,|\, n \to m \in E, k \in S_n, l \in S_m\}$. For example any coined Quantum walk of a particle on a line with a two-dimensional degree of freedom is identical to a walk of a particle with no internal degrees on the graph shown in figure 3.

Local probability conservation on the expanded graph then implies local probability conservation for the original graph, with the probabilities and currents on the original graph being $P_n = \sum_k P_{(n,k)}$ and $J_{mn} = \sum_{k,l} J_{(m,l),(n,k)}$

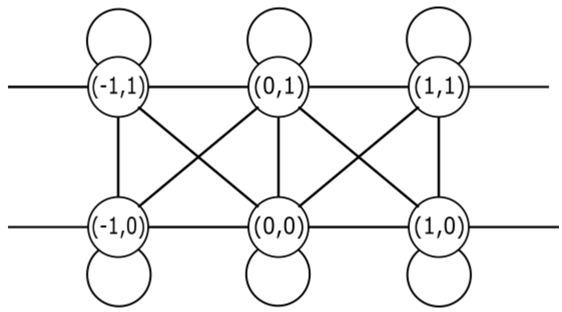

FIG. 3. Any quantum walk of a particle on a line with a two dimensional internal degree of freedom can be represented by a quantum walk on this expanded graph. For generality, all links are shown undirected, allowing travel in both directions.

E. Mixed states and general quantum processes

So far we have considered pure quantum states evolving unitarily. However, it is also possible to extend these results to mixed states and general quantum processes (represented by completely positive trace preserving maps), which may be useful when considering open quantum systems or situations involving uncertainty. In this case the state is represented by a density operator ρ, and the transformation during a single timestep is given by $\rho' = \sum_i K_i \rho K_i^\dagger$, where K_i are Kraus operators [21]. In order to respect the locality structure of the graph, such a transformation must satisfy $n \to m \notin E \implies \langle m| K_i |n\rangle = 0 \, \forall \, i$. Mixed states and general quantum dynamics can always be represented by pure states and unitary evolutions on a larger hilbert space composed of the original system and an ancilla [21]. By treating the ancilla as an internal degree of freedom as in the previous subection, it follows that local probability conservation also applies in these cases.

IV. DISCUSSION

For quantum evolutions in discrete space and time, in which the locality structure of space is described by an arbitrary directed graph and the evolution is unitary, we have shown that probability is locally conserved. Essentially, we can always explain the change in spatial probability distributions in terms of probability flows which respect the locality of space.

The constraint of local probability conservation can be expressed in terms of the probability current J_{nm} between vertices or probability flows f_{nm} along edges. Unlike in the continuous time examples which have been considered, the existence of a valid probability flow is established non-constructively, although valid solutions can be obtained efficiently via numerical methods.

A third approach to the probability flow is to consider a stochastic matrix[3] $P_{m|n}$ which evolves the initial probability distribution into the final distribution via

$$P'_m = \sum_n P_{m|n} P_n, \tag{25}$$

with $n \to m \notin E \implies P_{m|n} = 0$. This is equivalent to the formulation in terms of probability flows. To go from f_{mn} to $P_{m|n}$ we take

$$P_{m|n} = \frac{f_{mn}}{P_n}, \tag{26}$$

whenever $P_n \neq 0$. If $P_n = 0$, (26) is not well defined. However, in such cases the distribution $P_{m|n}$ is irrelevant as there is no probability initially at n to flow, and we can simply take $P_{m|n} = \delta_{m,n}$ to avoid violating the locality structure. Similarly we can transform from $P_{m|n}$ to f_{mn} by taking $f_{mn} = P_{m|n} P_n$. As in the discussion of probability flows, note that the aim here is not to derive P'_n by computing $P_{m|n}$ and then evolving the initial state, as we need to calculate P'_n in order to find $P_{m|n}$. Rather, it is to show that there exists a $P_{m|n}$ which is consistent with the initial and final probability distributions and locality.

This result could be helpful in understanding quantum walk evolutions, and is also interesting from a foundational perspective, as it demonstrates that an intuitive property of quantum theory in continuous space and time and discrete space continuous time also holds in the discrete space and time formalism. This could be helpful for any approaches to particle physics in which discretization of time and space is pursued, such as [22–25].

ACKNOWLEDGMENTS

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[3] i.e. satisfying $P_{m|n} \geq 0$, and $\sum_m P_{m|n} = 1$ for all n

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Appendix A: A proposed general current

In this appendix we consider a proposed general form of the probability current [13], for arbitrary discrete time quantum walks on undirected graphs, given by

$$\begin{aligned} J_{mn} = \frac{1}{2}[&(\rho U^\dagger)_{nm}U_{mn} + (U^\dagger)_{nm}(U\rho)_{mn} \\ &- U_{nm}(\rho U^\dagger)_{mn} - (U\rho)_{nm}(U^\dagger)_{mn}]. \end{aligned} \tag{A1}$$

This is an appealing definition as it can be easily verified that J_{mn} is anti-symmetric, real-valued, and equal to zero whenever n and m are not connected by an edge in the graph (in which case $U_{mn}, (U^\dagger)_{nm}, U_{nm}$ and $(U^\dagger)_{mn}$ are all equal to zero). Furthermore, note that

$$\begin{aligned} \sum_m J_{mn} &= \frac{1}{2}[(\rho U^\dagger U)_{nn} + (U^\dagger U\rho)_{nn} - 2(U\rho U^\dagger)_{nn}] \\ &= \rho_{nn} - (U\rho U^\dagger)_{nn} \\ &= -\Delta P_n \end{aligned} \tag{A2}$$

and hence

$$\Delta P_n + \sum_m J_{mn} = 0. \tag{A3}$$

However, this definition does not always satisfy the requirement that

$$\sum_{m^*} J_{m^*n} \leq P_n, \tag{A4}$$

where $m^* = \{m : J_{mn} > 0\}$. In particular, it is possible to find cases in which the probability flow away from a vertex is greater than the initial probability located at that vertex. A simple example is provided by considering a quantum walk on three connected vertices with

$$U = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \tag{A5}$$

and an initial pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle)$, corresponding to

$$\rho = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{A6}$$

As U and ρ are both Hermitian and real in this case, (A1) simplifies to

$$J_{mn} = U_{mn}[(U\rho)_{mn} - (U\rho)_{nm}]. \tag{A7}$$

From this, one finds that

$$J_{21} = \frac{1}{2}\left[0 - \left(\frac{1}{4} - \frac{1}{2\sqrt{2}}\right)\right] = \frac{1}{8}(\sqrt{2} - 1) > 0. \tag{A8}$$

This implies that there is a positive flow of probability from vertex 1 to vertex 2. However, there is initially no probability of the particle being at vertex 1 ($P_1 = 0$). Hence we obtain a violation of (A4).

Appendix B: Equivalence of flow and current conditions

In this appendix, we show that if we can define a J_{nm} which is real, antisymmetric, satisfies (6) and (7), and for which $J_{mn} > 0$ only if $m \to n \in E$ then we can always generate flows f_{mn} satisfying conditions (10)-(13). As we showed in the main paper that these flow conditions always allow one to construct a probability current J_{mn} with the specified properties this shows that these two sets of properties are equivalent.

To achieve this, we set

$$f_{mn} = \begin{cases} J_{mn} & \text{if } J_{mn} > 0 \text{ and } m \neq n \\ P_n - \sum_{m^*} J_{m^* n} & m = n \\ 0 & \text{otherwise.} \end{cases} \tag{B1}$$

Property (10) is ensured by (7), property (11) follows because $n \to m \notin E \implies m \neq n$ and $J_{mn} \leq 0 \implies f_{mn} = 0$. The remaining two properties are given by

$$\begin{aligned} \sum_m f_{mn} &= \sum_{m \neq n} f_{mn} + f_{nn} \\ &= \sum_{m^*} J_{m^* n} + \left(P_n - \sum_{m^*} J_{m^* n} \right) \\ &= P_n \end{aligned} \tag{B2}$$

$$\begin{aligned} \sum_n f_{mn} &= \sum_{n \neq m} f_{mn} + f_{mm} \\ &= \sum_{n : J_{mn} > 0} J_{mn} + \left(P_m - \sum_{k : J_{km} > 0} J_{km} \right) \\ &= - \sum_{k : J_{km} < 0} J_{km} + P_m - \sum_{k : J_{km} > 0} J_{km} \\ &= - \sum_k J_{km} + P_m \\ &= \Delta P_m + P_m \\ &= P'_m \end{aligned} \tag{B3}$$

Appendix C: Example of Constructing Probability Flows

In this appendix we illustrate the existence proof for local flows given in section III B, and the method for constructing probability flows in section III C for a specific example.

We will consider a walk on the three vertex graph shown in figure 4, according to the unitary

$$U = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}. \tag{C1}$$

for the initial state

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}. \tag{C2}$$

Note that $U_{32} = 0$ as required by the fact that there is no edge from vertex 2 to vertex 3 in the graph. To proceed,

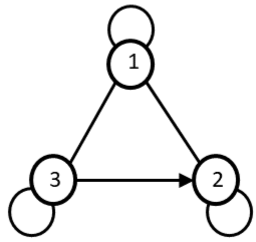

FIG. 4. A three vertex graph on which we consider an example quantum walk in appendix C.

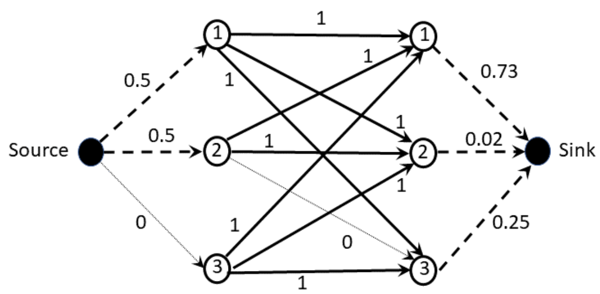

FIG. 5. A flow network with each edge labelled by its capacity

we first calculate the final state

$$|\psi'\rangle = U |\psi\rangle = \begin{pmatrix} \frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right) \\ \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right) \\ \frac{1}{2} \end{pmatrix}. \tag{C3}$$

We can then calculate the initial and final probability distributions from $|\psi\rangle$ and $|\psi'\rangle$. For all numerical calculations these are stored and manipulated using machine precision, but for simplicity we present them below to 2 d.p.

$$P_n = |\langle n|\psi\rangle|^2 = \begin{pmatrix} 0.50 \\ 0.50 \\ 0 \end{pmatrix} \quad P'_m = |\langle m|\psi'\rangle|^2 = \begin{pmatrix} 0.73 \\ 0.02 \\ 0.25 \end{pmatrix}. \tag{C4}$$

Our aim is to find a local probability flow that explains the transition from P_n to P'_n.

Let us first consider the proof that there exists such a flow, as given in section III B. To do this, we construct a flow network as shown in figure 5

If we can find a flow of one unit of probability through this network then the flows on the central edges will correspond to local flows f_{mn} on our original graph as desired. To prove that such flows exist we use the max-flow, min cut theorem. The maximal flow through the network is equal to the minimal total capacity of edges that we need to remove to disconnect the source from the sink.

One way to disconnect the source from the sink is to cut all three edges coming from the source. This cut has a value equal to the sum of the capacities of those edges, given by $K = 0.5 + 0.5 + 0 = 1$. Similarly, disconnecting all of the edges leading into the sink has $K = 0.73 + 0.02 + 0.25 = 1$. Any cut that includes one of the central solid edges with capacity 1 must yield a value of $K \geq 1$, so these offer no improvement to the minimal cut value and can be discounted. The only remaining interesting option is to cut the set of edges $\{Source \to 1, Source \to 3, 2 \to 3, 1 \to Sink, 2 \to Sink\}$. This does disconnect the source from the sink. However, this cut has value $K = 0.5 + 0 + 0 + 0.73 + 0.02 = 1.25$. Hence the minimal cut value is one, and thus a maximal flow of one through the network is possible.

In terms of the proof in section III B, the cut with $K = 1.25$ considered above corresponds to $A = \{2\}$ and $B = \{3\}$, leading to orthogonal projectors

$$\Pi_A = |2\rangle\langle 2|, \tag{C5}$$

$$\Pi_B = U^\dagger |3\rangle\langle 3| U = \frac{1}{2}(|1\rangle - |3\rangle)(\langle 1| - \langle 3|). \tag{C6}$$

This gives $\langle\psi|\Pi_A + \Pi_B|\psi\rangle = 0.75$, and thus $K = 2 - \langle\psi|\Pi_A + \Pi_B|\psi\rangle = 1.25$.

The above proves that a suitable probability flow exists, but does not give an explicit solution. To find one, we employ the method in section III C. In particular, we use the P_n and P'_n we calculated in (C4) to write down the constraint conditions (11) - (13) on f_{mn} in the form of equation (24)

$$\begin{pmatrix} 1&0&0&1&0&0&1&0&0 \\ 0&1&0&0&1&0&0&1&0 \\ 0&0&1&0&0&1&0&0&1 \\ 1&1&1&0&0&0&0&0&0 \\ 0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&0&1&1&1 \\ 0&0&0&0&0&0&0&1&0 \end{pmatrix} \begin{pmatrix} f_{11} \\ f_{12} \\ f_{13} \\ f_{21} \\ f_{22} \\ f_{23} \\ f_{31} \\ f_{32} \\ f_{33} \end{pmatrix} = \begin{pmatrix} 0.50 \\ 0.50 \\ 0 \\ 0.73 \\ 0.02 \\ 0.25 \\ 0 \end{pmatrix}, \tag{C7}$$

As discussed in the main body, we now consider a linear program which maximizes the objective function $c = f_{11} + f_{22} + f_{33}$ subject to the linear equations (C7) and the positivity constraints $f_{mn} \geq 0$ for all n and m (23). Such a linear program can be solved computationally using several algorithms. In this example the simplex method was used and the following values for the probability flows were determined

$$f = \begin{pmatrix} 0.25 & 0.48 & 0 \\ 0 & 0.02 & 0 \\ 0.25 & 0 & 0 \end{pmatrix}. \tag{C8}$$

These are illustrated in figure 6, where it can be verified that they correctly account for the change in probability distribution from P_n to P'_m, and satisfy all constraints given by (10)-(13) as we would expect.

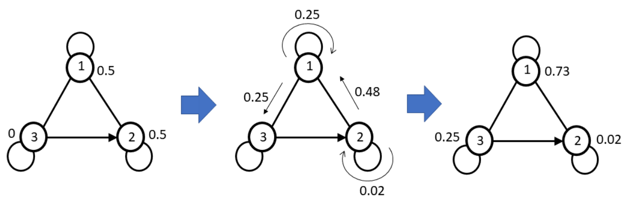

FIG. 6. For the example considered, the graphs on the left and right show the initial and final probability distributions P_n and P'_m respectively,and the central graph shows the probability flows f_{mn}.