Continuous Time Quantum Walks (CTQW)

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1 Introduction

Quantum computing became a prominent area of research with publications such as Feynman's 1986 paper suggesting a construction for a Hamiltonian that can implement any quantum circuit [1]. Some of the key results in quantum information science such as Shor's algorithm [2] and Grover's algorithm [3] which show speed up over classical algorithms for integer factorisation and database searching have motivated a wealth of research in the field. A particular field of interesting research among these are quantum random walks - the quantum counterpart to classical random walks, used in studies of the fundamentals and applications of diffusion [4–7], modelling of transport for solvents [8], electrons [9], mass, [10], heat [11], radiation, [12], photon motion in isotropic media [13], polymer dynamics [14, 15] among other applications not limited to modelling of stock exchanges in finance, peer to peer networks, astrophysics and the creation of new classical algorithms [16–22]. If the classical random walks are so widely used, then why would one wish to study their quantum counterpart? Grover's algorithm is an example that can be interpreted as a discrete time quantum walk which offers a polynomial speed up over a classical algorithm when searching an unstructured database for a given marked element. Ambainis discovered a quantum algorithm based off of a quantum random walk to solve the element distinctness problem quicker than a classical algorithm [23]. That is, given a set of elements $x_1, x_2 ... x_n \in [M]$ how many times do we have to query to determine if all elements are distinct? This problem is solved by a classical algorithm if we sort $\Omega(N)$ times. Shi et. al worked out that this problem requires at most $\Omega(N^{\frac{2}{3}})$ queries for a quantum algorithm [24]. By using quantum interference and superposition, Ambainis discovered the complexity of this operation is $\mathcal{O}(N^{\frac{2}{3}})$ queries. Other quantum algorithms based off of the quantum walk have been reported for other cases too, including the claw finding algorithm [25], related to cryptographic applications which goes as follows: given two functions $f : X \to Z$ and $g : Y \to Z$ promised as an oracle, determine if a pair $(x, y) \in X \times Y$ called a *claw* exists such that $f(x) = g(y)$. X and Y are domains of size N and M respectively where $N \leq M$. A lot of work has gone in to trying to prove quantum speed ups, but also research exists on optimising current quantum algorithms. The claw finding algorithm is an example of this. Tani showed the complexity of solving this problem was $\mathcal{O}(N^{\frac{1}{2}}M^{\frac{1}{4}})$ for $N \leq M < N^2$ and $\mathcal{O}(M^{\frac{1}{2}})$ for $M \geq N^2$. Zhang [26] improved the algorithm to $\mathcal{O}(N^{\frac{1}{3}}M^{\frac{1}{3}})$ for $N \leq M < N^2$ and $\mathcal{O}(M^{\frac{1}{2}})$ for $M \geq N^2$. The algorithmic speed up of the quantum walk has encouraged studies on various structures including 1D lines [27], hypercubes, [28] and periodic crystal lattices [29] which may in turn lead to the development of new quantum algorithms to implement on a quantum computer. Other applications extend to biology. Mohseni et. al showed how quantum walks can be used to study quantum interference effects occurring in energy transfer dynamics. This is relevant for delocalised excitonic transport in photosynthetic systems [30, 31].

This essay starts by a brief discussion of the first paper on quantum random walks, followed by outlining the formalism of the continuous time quantum walk, how it is different from a discrete-time quantum walk and how to define it based on the local properties of a graph. Hilbert spaces and limits are then discussed for simulating a continuous time quantum walk in discrete time and a discussion of its advantages and drawbacks. The final section then discusses how to achieve universal quantum computation using a continuous time quantum walk. This is by no means exhaustive of what has been studied with respect to continuous time quantum walks - there are a vast amount of publications in the literature and this essay will cover only a small amount in detail. References will be given for other details not talked about in this work.

1.1 Seminal paper on quantum walks (Aharonov et. al)

The notion of a quantum random walk was originally discovered by Aharonov et al in 1993 [32]. Contrary to the classical random walk where the walker has an equal probability of making a step of a given length in a given direction (for one dimension this is left and right, two dimensions would also includes upwards and downwards, etc), quantum walks are based upon probability amplitudes. An observable plays the role of a 'quantum coin' of which there are distinct measurement outcomes which influence the movement of the walker. Aharonov exemplified the concept by a spin-$\frac{1}{2}$ particle undergoing a one dimensional motion. In this case, measurement of the z component of the particles spin determines which path the walker will take. They suggest that the effective unitary operator governing the time translation is:

$$\hat{U} = exp(\frac{-i\hat{S}_z\hat{P}l}{h}) \tag{1}$$

Where $\hat{S}_z$ is an operator corresponding to the z component of the spin, $\hat{P}$ is the momentum operator and l is the length of a step. The eigenstates of $\hat{S}_z$ are given below in the operators spectral decomposition:

$$\hat{S}_z = \frac{\hbar}{2}\left|+\right\rangle\left\langle+\right| - \frac{\hbar}{2}\left|-\right\rangle\left\langle-\right| \tag{2}$$

Where $|\pm\rangle$ denotes spin up or spin down. Suppose we have the initial state of the particle given by:

$$\left|\psi\right\rangle = \left|\psi(x_0)\right\rangle\left(c_+\left|+\right\rangle + c_-\left|-\right\rangle\right) \tag{3}$$

Subject to the normalization condition $|c_+|^2 + |c_-|^2 = 1$ and $\psi(x_0)$ denotes the wavefunction centered around an initial point x_0. Thus after one step the state can be described as:

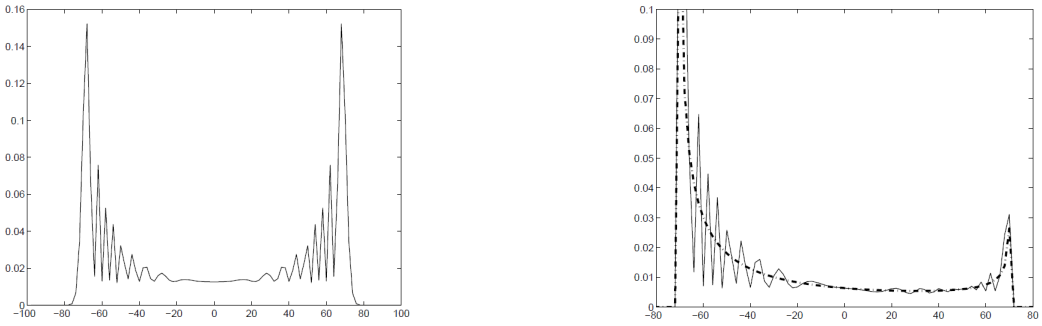
$$\left|\Psi\right\rangle = c_-\left|-\right\rangle\left|\psi(x_0 - l)\right\rangle + c_+\left|+\right\rangle\left|\psi(x_0 + l)\right\rangle \tag{4}$$

Thus, measuring $\hat{S}_z$ will collapse the wavefunction into either $|+\rangle$ or $|-\rangle$ which correspond to a translation of $x_0 + l$ and $x_0 - l$. If this is repeated N times then the average displacement is given by:

$$< x >= Nl(|c_+|^2 - |c_-|^2) \tag{5}$$

It is notable that this result is exactly the same as a random walk if we interpret $|c_+|^2$ and $|c_-|^2$ as the probabilities of being in the states $|+\rangle$ and $|-\rangle$ respectively. Thus, in the case of a balanced walk i.e. $|c_+|^2 = |c_-|^2 = \frac{1}{2}$ then $< x >= 0$, denoting that the average (most likely position of the walker is to stay at $x = 0$). If this is computed for all outcomes x then we find a Gaussian distribution centered around $x = 0$. This wavefunction collapse from quantum measurement recovers the dynamics of the classical random walk.

The interesting aspect of the quantum random walk is that the coin operator which influences the translation of the walker can change. Superpositions of the coin operator can affect the distribution. This can lead to drastic differences between the quantum walk and the classical walk. Whereas the classical random walk is a Gaussian distribution, the quantum walk probability amplitudes can be greater at positions such as $x_0 + 3l$ and $x_0 - 2l$ when the spin has not been measured. This is also not necessarily symmetric. Figures 1a and 1b show the probability distributions for symmetric and asymmetric quantum walks respectively on one-dimensional lines [33, 34]. The quantum random walk spreads faster than a classical random walk. This aspect has encouraged studies of hitting times H_{ij}, which are defined as the number of steps required to visit a vertex j given an initial starting vertex i. The vertex definition is generally for higher dimensionality graph structures however they can equally represent points on a line. Whilst hitting times are intimately linked to algorithmic quantum speedup, they are not specifically of interest in this essay. For details on hitting times and other properties such as limiting distributions see the comprehensive review by Venegas-Andraca [35].



(a) Symmetric quantum walk

(b) Asymmetric quantum walk

Figure 1: Examples of discrete time quantum walk simulations. The y axes represent the probability of being in a location on the walk (x axes). (a) is a symmetric quantum walk from using a balanced Hadamard coin, whereas in (b) the walk is severely biased to one side due to the initial starting state. Both cases show a substantial deviation from a classical random walk due to quantum interference effects and that the probabilities are proportional to the modulus of the state amplitudes squared.

2 Continuous Time Quantum Walks

The continuous time quantum walk has some notable contrasts with the discrete random walk which will be described in this section, namely:

- CTQW are generally described by Markov processes;
- A CTQW evolves under a Hamiltonian which is defined with respect to a graph;
- No coin operator is required in a CTQW. The implications of this are discussed in section 2.2.

2.1 Formalism

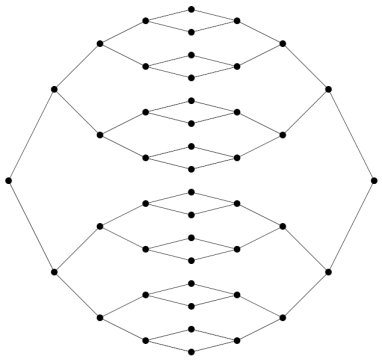


Figure 2: An example of a graph which a quantum walk is performed on. From [36].

The formalism for the continuous time quantum walk leads on fairly straightforwardly from its classical counterpart, the continuous time classical walk. This is a Markov process. A Markov process is best illustrated with a graph as in figure 2. Suppose the graph G has a set of vertices N indexed by integers $a = 1, 2...N$. The vertices may be connected to other vertices by an edge. If we let γ denote the jumping rate per unit time between vertices and impose the condition that the walk may only travel between nodes connected to an edge, the random walk can be described by a stochastic generator matrix M. Its matrix elements are defined by:

$$M_{ab} = \begin{cases} -\gamma & \text{for } a \neq b, \text{ a and b connected by an edge} \\ 0 & \text{for } a \neq b, \text{ a and b not connected} \\ k\gamma & \text{for } a = b, \ k \text{ is the valence of vertex a.} \end{cases}$$

So it is clear from the definition of M_{ab} above that the diagonal elements are the valences (the number of connections from a vertex to its other vertices) and only matrix elements concerning nearest neighbours will have non-zero entries. In a small time frame ϵ such that $\gamma\epsilon \approx 1$ is the probability of jumping from one vertex to another, the probability of being in vertex a at a given time t is [36]:

$$\frac{dp_a(t)}{dt} = -\sum_b M_{ab} p_b(t) \tag{6}$$

Where the probabilities are subject to the usual classical normalization condition i.e.

$$\sum_a p_a(t) = 1 \tag{7}$$

To go from the continuous time classical walk to its quantum counterpart, we construct an N-dimensional Hilbert space consisting of the vectors $|a\rangle$ where $a = 1, 2..N$ denote the graphs vertices as before. The Schrdinger equation in this case is:

$$i\frac{d\,\langle a|\psi(t)\rangle}{dt} = \sum_b \langle a|\, H\, |b\rangle\, \langle b|\psi(t)\rangle \tag{8}$$

Where the completeness relation has been inserted for $|b\rangle$. Thus in the quantum case, the probabilities are conserved in the following way:

$$\sum_a |\langle a|\psi(t)\rangle|^2 = 1 \tag{9}$$

So compared to the classical walk, the sum of the overlap integrals squared over all vertices have to equal 1 in the quantum case. It is this normalization condition and the factor i that appears in (8) that gives rise to different dynamics over the classical continuous time walk. If we compare (8) to (6) we find a natural form for the matrix elements of $\hat{H}$:

$$M_{ab} = \langle a|\, H\, |b\rangle \tag{10}$$

Whilst (10) suggests that the Hamiltonian for a CTQW is based off of the graph's adjacency matrix, care should be taken as the adjacency matrix as defined in (6) may not be Hermitian and thus the evolution may not be unitary (reversible) [37]. Mathematically these conditions are expressed as:

$$\hat{U} = \hat{U}^\dagger \quad \text{Hermicity}; \quad \hat{U}\hat{U}^\dagger = \mathbb{1} \quad \text{Unitarity} \tag{11}$$

Where the unitarity condition shown above is follows from noting that the operator adjoint is equal to the inverse matrix of the operator i.e. $\hat{U}^\dagger = \hat{U}^{-1}$. Thus, the unitary evolution of a state is generated by a Hamiltonian i.e.:

$$\hat{U} = e^{-i\hat{H}t} \tag{12}$$

This leads on nicely to the broad definition of a CTQW as given in [38]:

Definition 1: *A continuous time quantum walk over a graph G is defined by the unitary transformation $\hat{U} = e^{-i\hat{H}t}$ such that the state vector in the Hilbert space at a time t is given by the evolution $|\Psi(t)\rangle = \hat{U}\,|\psi(0)\rangle$.*

2.2 Hilbert spaces and limits between CTQW and DTQW

Here we discuss the implications of the CTQW lifting the requirement of a coin operator and obtaining a CTQW from a DTQW. Unlike the classical walk counterpart where the continuous time case can be found by taking the limit in infinitesimally small time steps, the quantum case does not have such a trivial transition. This is because the coin space is an essential component in a DTQW to maintain unitary and non trivial dynamics. Thus, the Hilbert space of a DTQW is $\mathcal{H}_c \otimes \mathcal{H}_p$ where $\otimes$ denotes the tensor product and subscripts c and p denote the coin and position spaces respectively. Compare this with the CTQW, of which the Hilbert space is $\mathcal{H}_p$. The position space is based off of the graph as in the previous section where its general construction is an orthonormal basis of the vertices. One can immediately see from the Hilbert spaces of the DTQW and CTQW that an injective (one to one mapping) for every element may be lost from taking the continuous time limit of a DTQW which was not the case classically. Childs shows one way of simulating a CTQW with a DTQW which will form the main discussion in this section [39]. The DTQW corresponds to an $N \times N$ Hermitian matrix H. Considering an orthonormal basis $|j\rangle$ from $j = 1, 2.., N$ and the absolute value of the matrix elements H:

$$abs(H) = \sum_{j,k=1}^{N} |H_{jk}| \, |j\rangle \langle k| \tag{13}$$

There will exist principal eigenvectors of $abs(H)$ that take the form:

$$|d\rangle = \sum_{j=1}^{N} d_j \, |j\rangle \tag{14}$$

Which is the general form of a vector expressed as a linear combination of the basis vectors with coefficients given by $d_j = \langle j|d\rangle$. Then the Perron-Frobenius theorem is used [40], which states that the largest eigenvalue has an eigenvector with strictly positive coefficients d. This theorem is valid for a positive matrix i.e. one where all the entries are greater than zero and conditional on the irreducibility of $abs(H)$:

$$P^T abs(H) P \neq \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix} \tag{15}$$

Where P is a permutation matrix and X, Y and Z are square matrices. The action of P^T and P is conjugating the matrix i.e. swapping the rows and columns of $abs(H)$. So the statement above says that no permutation operation on $abs(H)$ can produce a block triangular matrix. An orthonormal set of quantum states $|\psi_1\rangle, ..., |\psi_N\rangle$. are defined on the tensor product space $\mathbb{C}^N \otimes \mathbb{C}^N$ as follows:

$$|\psi_j\rangle = \frac{1}{\sqrt{\|Abs(H)\|}} \sum_{k=1}^{N} \sqrt{H^*_{jk} \frac{d_k}{d_j}} \, |j, k\rangle \tag{16}$$

Where $\langle j, k|\psi_j\rangle \neq 0$ i.e. the coefficient of the vector $|\psi_j\rangle$ is finite-valued if and only if j is adjacent to k in the graph of non-zero entries of H. Under this construction, the DTQW over the matrix H is defined as the unitary operation reflecting in $span \in |\psi_j\rangle$ followed by the swap operation $\hat{S}$ i.e. $\hat{S} \, |j, k\rangle = |k, j\rangle$. The product of these reflections is related to the matrix of inner products as shown by Szegedy in another paper [41].

$$\langle \psi_j | \, \hat{S} \, |\psi_j\rangle = \frac{H_{jk}}{\|Abs(H)\|} \tag{17}$$

An isometry is defined which is the mapping for vectors in $\mathbb{C}^N \to \mathbb{C}^N \otimes \mathbb{C}^N$. This is significant as it allows the CTQW Hilbert space to be mapped to its DTQW counterpart. The operation is:

$$\hat{T} = \sum_{j=1}^{N} |\psi_j\rangle \langle j| \tag{18}$$

Whilst $\hat{T}$ is not self-adjoint (Hermitian), it can be observed that the product $\hat{T}\hat{T}^\dagger$ is the sum over projectors $|\psi_j\rangle \langle \psi_j|$. Thus, the overall walk operator $\hat{U}$ is:

$$\hat{U} = i\hat{S}(2\hat{T}\hat{T^{\dagger}} - 1) \tag{19}$$

Note the similarity of this expression to the unitary operation used in Grover's algorithm [3]. This leads on to the first theorem:

Theorem 1: if $\frac{H}{\|Abs(H)\|}\left|\lambda\right\rangle = \lambda\left|\lambda\right\rangle$ then the unitary $\hat{U} = i\hat{S}(2\hat{T}\hat{T^{\dagger}} - 1)$ has the eigenvectors:

$$\left|\mu_{\pm}\right\rangle = \frac{1 - e^{\pm iarcos\lambda}\hat{S}\hat{T}}{\sqrt{2(1-\lambda)^2}}\left|\lambda\right\rangle \tag{20}$$

With the eigenvalues:

$$\mu_{\pm} = \pm e^{\pm iarcsin\lambda} \tag{21}$$

The proof of this result is given in [42]. Let Π denote the projector onto $span \in \left\{\hat{T}\left|j\right\rangle, \hat{ST}\left|j\right\rangle\right\}$. This construction assumes that the eigenvalues from Theorem 1 are small i.e. $arcsin\lambda \approx \lambda$. Under this construction we may expand the exponential appearing in the eigenvector $\left|\mu\pm\right\rangle$ as follows:

$$\left|\mu_{\pm}\right\rangle \approx \frac{(\mathbb{1} \mp i\hat{S} + \lambda\hat{S})\hat{T}}{\sqrt{2}} \tag{22}$$

The action of the unitary $\hat{U}$ considering the projector Π is :

$$i\Pi\hat{U}\Pi \approx \sum_{\lambda,\pm} \mp e^{\pm i\lambda}\frac{(\mathbb{1} \mp i\hat{S} + \lambda\hat{S})\hat{T}}{\sqrt{2}}\left|\lambda\right\rangle\left\langle\lambda\right|\hat{T^{\dagger}}\frac{(\mathbb{1} \pm i\hat{S} + \lambda\hat{S})}{\sqrt{2}} \tag{23}$$

If we consider the general spectral decomposition of a function of an operator [43] i.e.:

$$f(\frac{H}{\|Abs(H)\|}) = \sum_{\lambda} f(\lambda)\left|\lambda\right\rangle\left\langle\lambda\right| \tag{24}$$

Comparing (24) with the right hand side of (23) we see that the expression is very similar to the evolution of $e^{(\frac{H}{\|Abs(H)\|})}$ for unit time with the exception of three caveats. These are as follows:

- The presence of the isometry mapping operator $\hat{T}$ and its adjoint $\hat{T^{\dagger}}$.
- Positive and negative phases for each eigenvalue λ, hence the sum over $\pm$ appearing in (23).
- Rotations by the factor $\frac{\mathbb{1}\pm i\hat{S}}{\sqrt{2}}$.

To obtain a good approximation of the CTQW dynamics, the basis is rotated by $(\frac{\mathbb{1}+i\hat{S}}{\sqrt{2}})$, and to make the fraction $h = \frac{\|H\|}{\|Abs(H)\|}$ arbitrarily small. This is achieved by constructing a lazy quantum walk which is analogous to a classical random walk that steps with probability $\epsilon \leq 1$. In order to do this the states in (16) are modified in the following way:

$$\left|\psi_j^{\epsilon}\right\rangle = \sqrt{\epsilon}\left|\psi_j\right\rangle + \sqrt{1-\epsilon}\left|\perp_j\right\rangle \tag{25}$$

So it is clear that this modification retains normalization. The states $\left|\perp_j\right\rangle$ form an orthonormal set as before. The isometry operator $\hat{T}$ is redefined for the modified state in (25):

$$\hat{T_{\epsilon}} = \sum_{j}\left|\psi_j^{\epsilon}\right\rangle\left\langle j\right| \tag{26}$$

Theorem 1 still holds under this transformation. The CTQW simulation is done in steps τ in the following algorithm:

Child's CTQW simulation algorithm:

1. Given an initial state $|\phi_o\rangle \in span\{|j\rangle : j = 1, ...N\}$, Apply T_ϵ followed by $\frac{\mathbb{1}+i\hat{S}}{\sqrt{2}}$.

2. Apply the unitary $\hat{U} = iS(2T_\epsilon T_\epsilon^\dagger - \mathbb{1})$ τ times.

3. Project onto the basis of states defined by $(\frac{\mathbb{1}+i\hat{S}}{\sqrt{2}})\hat{T}_\epsilon |j\rangle$

As the walk evolves, the probability of being in a state $|j\rangle$ is:

$$Pr(j) = |\langle j| e^{\frac{-i\tau\epsilon\hat{H}}{\|Abs(H)\|}} |\phi_o\rangle|^2 \tag{27}$$

Where (27) is only valid provided higher order terms including $\epsilon^2 h^2$ and $\epsilon^3 h^3 \tau$ are small. If we choose $\epsilon = \frac{\|Abs(H)\|t}{\tau}$ then we can obtain the evolution of the walk. This shows that if we increase the number of steps τ then we increase the accuracy of the walk. In order to satisfy an accuracy bound δ, i.e.

$$\|e^{-i\hat{H}t} |\psi_o\rangle - |\psi_t\rangle\| \leq \delta \tag{28}$$

It takes

$$\tau \geq \mathcal{O}\{\frac{(\|H\|t)^{\frac{3}{2}}}{\sqrt{\delta}}\|Abs(H)\|t\} \tag{29}$$

Steps. A natural and viable question to ask from this analysis is what benefit one might get from simulating a continuous time quantum walk with a discrete time one. It was found on particular types of graphs like shown in figure 2 that a continuous time quantum walk admits an exponential speed up over classical random walk when considering the time taken to traverse from one side to the other. In fact, with a modification to the graph as shown in figure 3 [44], the CTQW can beat *any* classical algorithm (random walk or not) exponentially. The reason for modifying the graph is because the original graph in figure 2 could be done in polynomial time classically as checking the degree of the central vertices allows one to confirm where they are in their random walk.

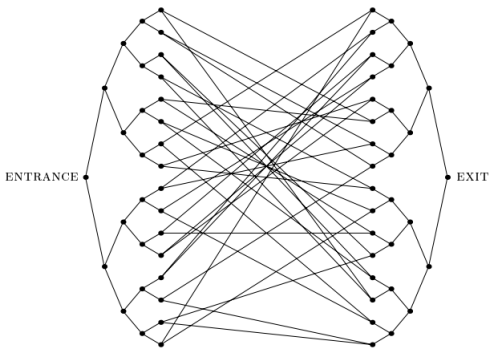


Figure 3: An example of a modified graph which a continuous time quantum walk grants an exponential speed up over any classical algorithm. From [44].

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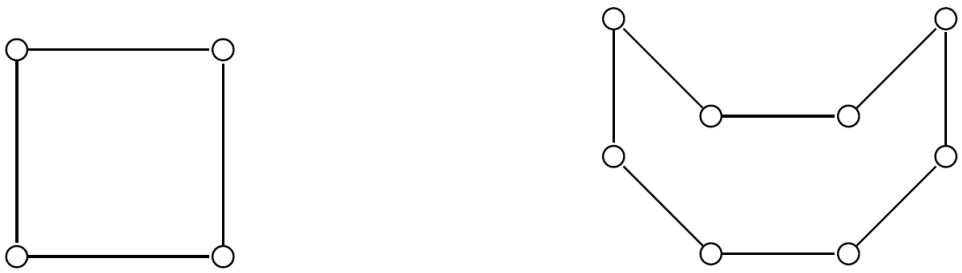
The CTQW simulation shown can also be used in Hamiltonian simulation - this can be used to find the dynamics or energies of a system with a given Hamiltonian. Hamiltonian simulation is efficient for sparse matrices (those with many zeros in their entries) and local - a sum of terms acting on a constant number of qubits. An ordinary discrete time process takes $t^{\frac{3}{2}}$ steps to obtain evolution for a time t. But with the continuous time quantum walk here, a linear time scaling can be obtained and is optimal without the requirement of a sparse Hamiltonian. There are two caveats with the simulation. Firstly, the exponential speedup (and in fact, no polynomial speedup so there is no benefit) does not carry at all in some non linear hidden structures because $\|abs(H)\| >> \|H\|$ - requiring an exponential number of steps [45]. The second

caveat comes from the construction - requiring a low energy subspace as ϵ is chosen such that the eigenvalues are small. This may be limiting for attempting to perform adiabatic quantum computation by a quantum walk. Other simulations of continuous time quantum walks exist. For example, a continuous limit has been found for 1D from the Dirac equation based off of a variational principle [46]. However, no complexity is given, and it does not make sense to compare because the cases are different. Other approaches also involve modifications of the graph. This is shown in figure 4.



(a) Arbitary graph G. **(b)** Modified graph G'.

Figure 4: Graphs G and G'. The Graph G allows for a coin of dimension 2, thus it may be represented by a 2 x 2 matrix that is unitary and Hermitian. The continuous time quantum walk is defined on the graph G' such that the number of vertices is the same as the state space dimension of G and each vertex subspace of the original walk is mapped on a collection of vertices in G. Figures from [38].

3 Universal quantum computation

In 2009 Childs showed a way in which a continuous time quantum walk allows for universal quantum computing [47]. The quantum walk takes place on an N-vertex graph. The walk begins at a vertex and ends at a vertex which is measured at $t = poly(logN)$. The computational basis states are represented by virtual quantum wires i.e. for an n-qubit circuit there are 2^n wires. Quantum gates are implemented by scattering off widgets that connect and attach to the quantum wires. These are shown in figure 5.

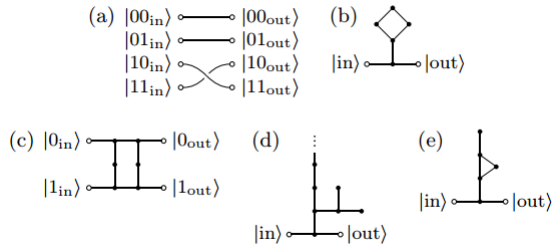


Figure 5: Widgets used for quantum computation via CTQW. a) CNOT gate. b) Phase shift gate. c) Basis-changing gate. d) Momentum filter. e) Momentum seperator. Figure from [47].

Childs utilises scattering theory of graphs in order to show universal quantum computation. An infinite line of vertices are represented by computational basis states $|x\rangle$ for $x \in \mathbb{Z}$. Each vertex is connected by nearest neighbours $x \pm 1$. The eigenstates are momentum states $|\tilde{k}\rangle$ with:

$$\langle x|\tilde{k}\rangle = e^{ikx} \tag{30}$$

For $k \in \big[-\pi, \pi)$ and $\langle \tilde{k}|\tilde{k'}\rangle = 2\pi\delta(k-k')$. The eigenvalues are $2cos(k)$. G is then a finite graph and an infinite graph with adjacency matrix H is produced by attaching semi infinite lines to M vertices. For each $j \in (1, ..., M)$ and $k \in \big[-\pi, 0\big]$ there is an incoming scattering state $|\tilde{k}, sc\rangle$ of the form:

$$\langle x, j|\tilde{k}, sc\rangle = e^{-ikx} + R_j(k)e^{ikx} \tag{31}$$

$$\langle x, j'|\tilde{k}, sc\rangle = T_{j,j'}(k)e^{ikx} \tag{32}$$

for $j \neq j'$ and where the reflection and transmission coefficients $R_j(k)$ and $T_{j,j'}(k)$ as well as the amplitude on the vertices of a graph G are determined by the eigenvalue condition:

$$\hat{H}\,|\tilde{k}, sc\rangle = 2cos(k)\,|\tilde{k}, sc\rangle \tag{33}$$

For a further and more advanced discussion of this topic, see the reference. Using the widgets and scattering theory introduced here, the phase gate U_b can be achieved:

$$U_b = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix} \tag{34}$$

By altering the transmission coefficient, the unitary matrix U_c is achieved:

$$U_c = \frac{1}{\sqrt{2}} \begin{bmatrix} i & 1 \\ 1 & i \end{bmatrix} \tag{35}$$

By noting that the matrix product $iU_b^2U_cU_b^2$ is the Hadamard gate, these two matrices can generate SU(2) algebra. Figure 6 shows an example of an entangling circuit generated from these widgets. Using widgets a), b) and c) from figure 5 it is possible to achieve universal quantum computation.

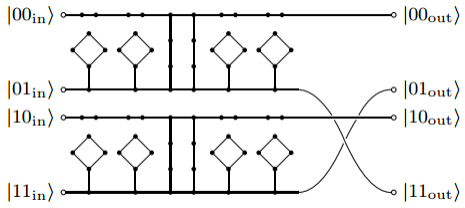


Figure 6: Quantum circuit for implementing an entangling gate using the scattering theory on graphs. This circuit implements a Hadamard on the second qubit followed by a CNOT gate with the second qubit acting as a control.

This construction shows that any quantum circuit may be simulated by a continuous time quantum walk on a sparse graph. This might find applications in quantum algorithms and binary game trees [48].

4 Summary

Quantum walks are going to play an important role in the future of quantum computation. Whether it is in the development of new quantum algorithms that offer a polynomial or exponential speed up over classical counterparts or if it is integral to the computation itself - in Hamiltonian simulation, or as a vehicle for universal quantum computation as discussed in this essay it is clear that their study will be important. They come in two varieties, discrete time and continuous time. Both have their advantages and disadvantages. In this essay the issue with taking the continuous time limit was addressed and motivations for simulating a continuous time quantum walk were discussed. It is thought that future studies on quantum walks will involve decoherences and adopt a Lindblad formalism as this may be useful in many applications such as non sparse density matrices of tensor product spaces. However, further studies on various types of graphs will persist - as solving a problem will involve requirement of knowledge of a graphs symmetry. This was the basis for the search algorithms using vertices for marked elements.

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