A Quantum Mechanical Travelling Salesman

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Abstract
A quantum simulation of a travelling salesman is described. A vector space for a graph is defined
together with a sequence of operators which transform a special initial state into a superposition states
representing Hamiltonian tours. The quantum amplitude for any tour is a function of the classical cost
of travelling along the edges in that tour. Tours with the largest quantum amplitude may be different
than those with the smallest classically-computed cost.

1 Introduction
In the problem of the travelling salesman we are given a graph with a fixed number of vertices. Every vertex
is connected to every other vertex by one edge. A vertex is not connected to itself. Every edge has a cost
which is a positive real number. A Hamiltonian tour of such a graph is a path which begins at a special
vertex, chosen arbitrarily but then fixed. Starting from this vertex, a sequence of steps is taken in each of
which a previously unvisited vertex is visited by travelling along the edge connecting the two. The cost of
travelling along that edge is accumulated. The classical cost of a tour is the sum of the costs associated with
the edges traversed during the tour. The tour ends when all vertices have been visited exactly once at which
point one more step is taken to return to the starting vertex. For a graph with \(N\) vertices, there are \((N-1)!\)
tours that begin and end at the starting vertex. The problem is to find the tour with the minimum cost.
This is the simplest version of the travelling salesman problem [1].

In section 2 I will describe a quantum simulation of this problem. The simulation occurs in a vector space
for a graph. This vector space is sufficient to describe Hamiltonian tours which are special basis states. The
simulation begins by placing the graph in a basis state corresponding to a choice of the starting vertex. A
sequence of operators will transform this initial state to a final state which is a superposition of only the
Hamiltonian tours. In this final state all tours have the same quantum amplitude. There are three goals for
the description in section 2. The first is to describe the vector space for a graph. The second is to show how
this vector space is capable of describing a Hamiltonian tour. The last goal is to construct operators which
perform the transformations which may be interpreted as carrying out all Hamiltonian tours.

The simulation is improved in section 3 by taking into account the cost of travelling along the edges. The
operators described in section 2 are modified so that the quantum amplitude of a path is built up as the tour
proceeds. The amplitude is now not a constant, but a function of the cost along the edges. Hamiltonian
tours with smaller classical costs have larger quantum amplitudes.

The dynamical system described is not a quantum algorithm that can execute on a universal quantum
Turing machine described by Deutsch [2]; it is a simulation of a special system by a quantum mechanical one.
Such systems [3, 4, 5] have long been in existence. The simulation requires a quantum mechanical computer
capable of executing it. The model of a computer most suitable has been described by Feynman [4] based on
work of Benioff [3] and others [4].

Feynman describes a universal quantum computer which is a one dimensional lattice of spin-half systems
with nearest neighbour interactions coupled to a system of logic gates. The state of the complete system
consists of the state of the spin lattice and the state of the registers on which the gates act. The Hamiltonian
for the system defines the dynamics of the lattice of spins as well as that of the gates. Nothing in Feynman’s
description requires the system to be a set of logic gates; they can be more general [5]. In the simulation

1See references in [3, 4, 5].
of the travelling salesman presented here, the state space of the registers are replaced by the state space of a graph while the operators which act on the registers are replaced by the operators for carrying out a Hamiltonian tour. The system coupled to the lattice of spins is not a set of logic gates but one which operates on a graph.

2 Simulating Hamiltonian tours

Let $G$ be a fully connected, symmetric graph with $N$ vertices. These two properties mean that every vertex is connected to every other vertex by an edge and that the same edge is used when travelling from one vertex to another in either direction. A vertex is not connected to itself. The vertices are labelled $1, 2, \ldots, N$. $V_i$ is the name for the vertex labelled $i$. Nothing that follows depends on the choice of labelling.

Associated with $G$ is the quantum system $\mathcal{G}$ which is the system that will simulate the travelling salesman. In the following, unless explicitly noted, the graph in question will be the quantum system $\mathcal{G}$ and not $G$ because it is $\mathcal{G}$ that is subject to dynamical evolution.

I will define a vector space for $\mathcal{G}$ and assign meaning to these states. These states will be sufficient to define a visit of a vertex and a Hamiltonian tour. $\mathcal{G}$ is prepared to be in a special initial state corresponding to starting at the chosen initial vertex. A sequence of $N$ operators applied to this state will transform it to a final state which is a superposition of all Hamiltonian tours and only the Hamiltonian tours. Let the initial and final states be $|g(0)\rangle$ and $|g(N)\rangle$ respectively and let $\hat{S}(1), \hat{S}(2), \ldots, \hat{S}(N)$, be the operators. The goal is to show that

$$|g(N)\rangle = \hat{S}(N)\hat{S}(N-1)\cdots \hat{S}(1)|g(0)\rangle,$$

and that $|g(N)\rangle$ is a superposition of states which may be interpreted as Hamiltonian tours. Moreover $|g(N)\rangle$ contains only such states and no others.

$\mathcal{G}$ is driven from $|g(0)\rangle$ to $|g(N)\rangle$ by being coupled to an external system. In other words, the step operators $\hat{S}(1), \hat{S}(2), \ldots, \hat{S}(N)$ are components in a larger Hamiltonian for the dynamical system consisting of a one-dimensional lattice of spins and $\mathcal{G}$ $[4]$.

The vector space for $\mathcal{G}$ is defined to be the direct product of the space of each of its vertices. The space at each vertex is the direct product of $(N+1)$ qubit spaces. At each $V_i$, the basis vectors are

$$|v_i; a_{i1}, a_{i2}, \ldots, a_{iN}\rangle. \quad (1)$$

The values of $v_i$, and $a_{ij}$ can be 0 or 1. The basis vectors span a space of dimension $2^{N(N+1)}$ giving $\mathcal{G}$ a dimension of $2^{N(N+1)}$. These states can be transformed by the usual raising and lowering operators. So

$$\hat{v}_i |0\rangle = 0, \quad \hat{v}_i |1\rangle = |0\rangle, \quad \hat{v}_i^* |0\rangle = |1\rangle, \quad \hat{v}_i^* |1\rangle = 0, \quad i = 1, 2, \ldots, N.$$ 

Similarly for the states labelled by $a_{ij}$.

$$\hat{a}_{ij} |0\rangle = 0, \quad \hat{a}_{ij} |1\rangle = |0\rangle, \quad \hat{a}_{ij}^* |0\rangle = |1\rangle, \quad \hat{a}_{ij}^* |1\rangle = 0, \quad i, j = 1, 2, \ldots, N.$$ 

These operators obey the well known commutation rules.

$$\hat{v}_i \hat{v}_i^* + \hat{v}_i^* \hat{v}_i = 1, \quad \hat{v}_i \hat{v}_j^* + \hat{v}_j^* \hat{v}_i = 0, \quad (i \neq j)$$

$$\hat{a}_{ij} \hat{a}_{ij}^* + \hat{a}_{ij}^* \hat{a}_{ij} = 1, \quad \hat{a}_{ij} \hat{a}_{kl}^* + \hat{a}_{kl}^* \hat{a}_{ij} = 0, \quad (i, j) \neq (k, l).$$

Where $i, j, k, l = 1, 2, \ldots, N$. The $\hat{v}$ and $\hat{v}^*$ operators commute with the $\hat{a}$ and $\hat{a}^*$. The basis vectors of $\mathcal{G}$ are

$$\prod_{i=1}^{N} |v_i; a_{i1}, a_{i2}, \ldots, a_{iN}\rangle. \quad (2)$$
The meaning of \( v_i \), and \( a_{ij} \) is as follows. \( v_i = 1 \) means \( V_i \) is being visited while \( v_i = 0 \) means \( V_i \) is not being visited. \( a_{ij} = 1 \) means there is a directed edge from \( V_i \) to \( V_j \) while \( a_{ij} = 0 \) means there is no such edge. A state with \( a_{ii} = 1 \) means there is a self-edge from \( V_i \) to itself. For any \( i \) the set of values \( a_{ij} \) represents the edge-state of \( V_i \).

Let us first see how these states can describe a Hamiltonian tour. Consider a graph \( G^{(3)} \), with three vertices \( V_1, V_2 \) and \( V_3 \). The basis vectors of its quantum equivalent \( G^{(3)} \) are

\[
|v_1; a_{11}, a_{12}, a_{13}⟩ |v_2; a_{21}, a_{22}, a_{23}⟩ |v_3; a_{31}, a_{32}, a_{33}⟩
\]

for all values of the \( v_i \) and \( a_{ij} \). Begin by placing its \( G^{(3)} \) in a state in which one vertex \( V_1 \), is visited and all three vertices have only self-edges. According to the convention, in this state

\[
v_1 = 1, v_2 = v_3 = 0,
\]

\[
a_{ij} = \begin{cases} 1 & \text{if } i = j; \\ 0 & \text{if } i \neq j, \end{cases}
\]

where \( i, j = 1, 2, 3 \). This is the state

\[
|g^{(3)}(0)⟩ = |1; 1, 0, 0⟩ |0; 0, 1, 0⟩ |0; 0, 0, 1⟩.
\]

A shorthand for this state is

\[
|g^{(3)}(0)⟩ = |1; a_{11} = 1⟩ |0; a_{22} = 1⟩ |0; a_{33} = 1⟩.
\]

The underline indicates that all \( a_{ij} \) not appearing in the ket have a value of 0. In this state, only \( v_1 = 1 \) so \( V_1 \) is the vertex being visited. All \( a_{ij} = 0, (i \neq j) \) and \( a_{ii} = 1 \) so all vertices have only self-edges. The graph representing this state is shown in Figure 1.

![Figure 1: A graph representing the state \( |g^{(3)}(0)⟩ \). The • marks the vertex being visited, here \( V_1 \). Every vertex is connected only to itself with a self edge.](image)

Let us take the first step by acting on \( |g^{(3)}(0)⟩ \) with the operator \( \hat{v}_1 \hat{a}_{11} \hat{a}_{12}^* \hat{a}_{13}^* \).

\[
\hat{v}_1 \hat{a}_{11} \hat{a}_{12}^* \hat{a}_{13}^* |1; a_{11} = 1⟩ |0; a_{22} = 1⟩ |0; a_{33} = 1⟩ = |0; a_{12} = 1⟩ |1; a_{22} = 1⟩ |0; a_{33} = 1⟩.
\]

In this new state, \( v_1 \leftarrow 0 \) and \( v_2 \leftarrow 1 \) so by convention this means \( V_2 \) is being visited. The other change is

\[
\hat{v}_1 \hat{a}_{11} \hat{a}_{12}^* \hat{a}_{13}^* \text{ is to make } V_2 \text{ the vertex being visited and replace the self edge at } V_1 \text{ with a directed edge from } V_1 \text{ to } V_2.
\]

The state of \( V_3 \) is unchanged. The meaning of this transformation is that we have carried out the first step of one tour from \( V_1 \) to \( V_2 \). Figure 2 shows the graph representing this state.

In the second step, visit \( V_3 \) from \( V_2 \) with the operator \( \hat{v}_2 \hat{a}_{22} \hat{a}_{23}^* \). \n
\[
(\hat{v}_2 \hat{a}_{22} \hat{a}_{23}^*)(\hat{v}_1 \hat{a}_{11} \hat{a}_{12}^* \hat{a}_{13}^*) |g^{(3)}(0)⟩ = |0; a_{12} = 1⟩ |0; a_{23} = 1⟩ |1; a_{33} = 0⟩.
\]

After this second step (Figure 3), \( V_3 \) is visited and we have recorded that the visit of \( V_2 \) took place along the (2, 3) edge of \( V_2 \) (\( a_{23} = 1 \)). No unvisited vertices remain, so we must return to the starting vertex with the operator \( \hat{v}_3 \hat{a}_{32}^* \hat{a}_{31}^* \). This produces the state
Figure 2: A graph representing the $|0; a_{12} = 1 \rangle |1; a_{22} = 1 \rangle |0; a_{31} = 1 \rangle$ produced as a result of the first step from $V_1$ to $V_2$. $V_1$ has no self-edge. $V_2$ is is being visited.

Figure 3: A graph representing the state $|0; a_{12} = 1 \rangle |0; a_{23} = 1 \rangle |1; a_{33} = 0 \rangle$. $V_3$ is is being visited.

$$(\hat{v}_3 \hat{a}_{33} \hat{a}_{31}^* \hat{v}_1^*)(\hat{v}_2 \hat{a}_{22} \hat{a}_{23}^* \hat{v}_3^*)(\hat{v}_1 \hat{a}_{11} \hat{a}_{12}^* \hat{v}_2^*) |g^{(3)}(0)\rangle = |1; a_{12} = 1 \rangle |0; a_{23} = 1 \rangle |0; a_{31} = 1 \rangle$$

which is a basis state corresponding to the Hamiltonian tour $V_1 \rightarrow V_2 \rightarrow V_3 \rightarrow V_1$. It is carried out with the three operators $\hat{v}_1 \hat{a}_{11} \hat{a}_{12}^* \hat{v}_2^*$, $\hat{v}_2 \hat{a}_{22} \hat{a}_{23}^* \hat{v}_3^*$ and $\hat{v}_3 \hat{a}_{33} \hat{a}_{31}^* \hat{v}_1^*$.

This three-vertex graph has only one other Hamiltonian tour — $V_1 \rightarrow V_3 \rightarrow V_2 \rightarrow V_1$ — which can be navigated with the operators $\hat{v}_1 \hat{a}_{11} \hat{a}_{13}^* \hat{v}_3^*$, $\hat{v}_3 \hat{a}_{33} \hat{a}_{32}^* \hat{v}_2^*$ and $\hat{v}_2 \hat{a}_{22} \hat{a}_{21}^* \hat{v}_1^*$. If we can perform both transformations simultaneously the final state of the graph, ignoring normalisation, would be

$$|1; a_{12} = 1 \rangle |0; a_{23} = 1 \rangle |0; a_{31} = 1 \rangle + |1; a_{13} = 1 \rangle |0; a_{32} = 1 \rangle |0; a_{21} = 1 \rangle$$

In both terms $V_1$ is the vertex being visited and, since no vertex has a self edge, all vertices have been visited. This state is shown in Figure 4 This example has shown that the basis states in (2) are capable of encoding a Hamiltonian tour.

A Hamiltonian tour starting at $V_1$ is a basis state with the following properties ($i, j = 1, 2, \ldots, N$).

1. $v_1 = 1$, $v_i = 0$ ($i \neq 1$),
2. $a_{ii} = 0$,
3. for each $i$, one $a_{ij} = 1$; all other $a_{ij} = 0$ ($i \neq j$) and
4. the directed graph represented by the basis state is connected.
In the general case $G$ is prepared in an initial state in which $V_1$ is visited and all vertices are in a state corresponding to having only self edges.

$$|g(0)\rangle = |1; a_{11} = 1\rangle \prod_{j=2}^{N} |0; a_{jj} = 1\rangle.$$  \hspace{1cm} (3)

To take the first step, define the step operator $\hat{S}(1)$.

$$\hat{S}(1) = \frac{1}{\sqrt{N}} \sum_{i,j=1}^{N} A_{ij} \hat{a}_i \hat{a}_j \hat{a}^*_j \hat{v}_i \hat{a}^*_i \hat{v}_j.$$  \hspace{1cm} (4)

where $A_{ij}$ is the adjacency matrix of $G$.

$$A_{ij} = \begin{cases} 0 & \text{if } i = j; \\ 1 & \text{if } i \neq j. \end{cases}$$

Let $|g(1)\rangle$ be the state produced by acting on $|g(0)\rangle$ with $\hat{S}(1)$.

$$|g(1)\rangle = \hat{S}(1)|g(0)\rangle = \frac{1}{\sqrt{N}} \sum_{i,j=1}^{N} A_{ij} \hat{a}_i \hat{a}_j \hat{a}^*_j \hat{v}_i \hat{a}^*_i \hat{v}_j |1; a_{11} = 1\rangle \prod_{k=2}^{N} |0; a_{kk} = 1\rangle.$$  \hspace{1cm} (5)

In the sum over $i$ the only term that survives is the one with $i = 1$ because $v_1 = 1$ and $v_i = 0$, $(i \neq 1)$. So we have

$$|g(1)\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} A_{1j} \hat{a}_i \hat{a}_j \hat{a}^*_j \hat{v}_i \hat{a}^*_i \hat{v}_j |1; a_{11} = 1\rangle \prod_{k=2}^{N} |0; a_{kk} = 1\rangle.$$  \hspace{1cm} (5)

Of the remaining $N$ terms consider the first with $j = 1$ which is $A_{11} \hat{v}_1 \hat{a}_1 \hat{a}^*_1 \hat{v}_1^*$. This does not contribute because $A_{11} = 0$. Therefore $|g(1)\rangle$ is a superposition of $(N - 1)$ basis states and does not contain a state resulting from visit of $V_1$ to itself. After the first step we have

$$|g(1)\rangle = \hat{S}(1)|g(0)\rangle = \frac{1}{\sqrt{N-1}} \sum_{i=2}^{N} |1 \rightarrow i \bullet\rangle.$$  \hspace{1cm} (5)

This is a convenient new notation to represent incomplete tours. Suppose we want to represent the state for the path $V_1 \rightarrow V_2 \rightarrow V_3$. Here, $V_3$ is being visited from $V_1$ via $V_2$. None of the other vertices have been visited and the tour is currently stopped at $V_3$. That is, no steps whatsoever have been taken from $V_3$. We will write this as

$$|1 \rightarrow 2 \rightarrow 3 \bullet\rangle.$$  \hspace{1cm} (5)

The number appearing last in the sequence identifies the vertex being visited, in this example $V_3$. All vertices whose labels appear in the sequence are in a state that is consistent with this path. The bullet after the last number signifies that the remaining vertices, whose labels do not appear in the sequence, have not taken part in the tour. The tour is stopped at the vertex whose number appears last in the sequence. Written out fully,

$$|1 \rightarrow 2 \rightarrow 3 \bullet\rangle \overset{\text{def}}{=} |0; a_{12} = 1\rangle |0; a_{23} = 1\rangle |1; a_{33} = 1\rangle \prod_{k=4}^{N} |0; a_{kk} = 1\rangle.$$  \hspace{1cm} (5)

In each of the $(N - 1)$ terms in equation (5) a different vertex is visited. $|g(1)\rangle$ is a normalised state by construction. However, $\hat{S}(1)$ is not a unitary operator:

$$\hat{S}(1)^* \hat{S}(1) \neq \mathbb{1}$$

But it can be shown that
\[ \hat{S}(1)^* |g(1)\rangle = \hat{S}(1)^* \hat{S}(1) |g(0)\rangle = |g(0)\rangle. \]  

Equation (6) shows that \( \hat{S}(1)^* \) reverses the action of \( \hat{S}(1) \) when \( \mathcal{G} \) is initially in the state \( |g(0)\rangle \). Although \( \hat{S}(1) \) and \( \hat{S}(1)^* \) are not inverses of each other, they behave as inverses when they act on \( |g(0)\rangle \).

For the second step of the tour we define the step operator \( \hat{S}(2) \) which will operate on \( |g(1)\rangle \) to produce \( |g(2)\rangle \).

\[ |g(2)\rangle = \hat{S}(2) |g(1)\rangle, \]

where

\[ \hat{S}(2) = \frac{1}{\sqrt{N-2}} \sum_{i,j=1}^{N} A_{ij} \hat{v}_i \hat{a}_{ii}^* \hat{a}_{jj}^* \hat{a}_{jj} \hat{v}_j^* \].

\( \hat{S}(2) \) is identical to \( \hat{S}(1) \) except that it contains a new operator combination \( \hat{a}_{jj}^* \hat{a}_{jj} \) and a normalisation factor of \((N-2)^{-1/2}\) not \((N-1)^{-1/2}\). The role of the additional operator combination is described presently. \( \hat{S}(2) \) will act on the \((N-1)\) terms of \( |g(1)\rangle \) in equation (5) to produce many more terms. Let us look at \( \hat{S}(2) \) acting on just the first term of \( |g(1)\rangle \), namely \( |1 \rightarrow 2 \rangle \). In the sum over \( i \) the only term that survives is the one with \( i = 2 \) as all others are annihilated by the action of \( \hat{v}_i \). From \( N^2 \) terms we are reduced to \( N \). 

\[ \hat{S}(2) |1 \rightarrow 2 \rangle = \frac{1}{\sqrt{N-2}} \sum_{j=1}^{N} A_{2j} \hat{v}_2 \hat{a}_{22} \hat{a}_{jj}^* \hat{a}_{jj} \hat{v}_j^* |1 \rightarrow 2 \rangle. \]

The term with \( j = 2 \) does not contribute because \( A_{22} = 0 \) so the sum over \( j \) produces at most \((N-1)\) terms. The term with \( j = 1 \) corresponds to visiting \( V_1 \) from \( V_2 \) which would certainly not be a legal step since \( V_1 \), being the starting vertex, has already been visited. But the operator for this step contains \( \hat{a}_{11}^* \) which will produce \( 0 \) because in this state \( a_{11} = 0 \). So the term with \( j = 1 \) does not survive meaning that \( V_1 \) is not visited from \( V_2 \) in the second step. So the sum over \( j \) produces just \((N-2)\) terms. Since there is nothing special about \( V_2 \), the same argument holds for all other vertices. Therefore, from each term of \( |g(1)\rangle \) in equation (5), the action of \( \hat{S}(2) \) will produce \((N-2)\) terms to give

\[ |g(2)\rangle = \hat{S}(2) \hat{S}(1) |g(0)\rangle = \frac{1}{\sqrt{(N-1)(N-2)}} \sum_{i,j=1}^{N} \sum_{j=1}^{N} |1 \rightarrow i \rightarrow j \rangle. \]

\( |g(2)\rangle \) is normalised. The operator \( \hat{S}(2)^* \) reverts \( |g(2)\rangle \) to \( |g(1)\rangle \).

\[ \hat{S}(2)^* \hat{S}(2) |g(2)\rangle = \frac{1}{\sqrt{N-1}} \frac{1}{\sqrt{N-2}} \sum_{i=2}^{N} (N-2) |1 \rightarrow i \rangle \]

\[ = \frac{1}{\sqrt{N-1}} \sum_{i=2}^{N} |1 \rightarrow i \rangle. \]

It is convenient then, to define the adjacency operator \( \hat{A}_{ij}(T) \)

\[ \hat{A}_{ij}(T) = \frac{1}{\sqrt{N-T}} A_{ij} \hat{v}_i \hat{a}_{ii}^* \hat{a}_{jj}^* \hat{a}_{jj}, \quad T = 1, 2, \ldots, (N-1) \]

(7)

where \( i = 1, 2, \ldots, N \), and from which we can define a sequence of step operators, \( \hat{S}(T) \), for the \( N \) steps of the tour.

\[ \hat{S}(T) = \begin{cases} \sum_{i,j=1}^{N} \hat{v}_i \hat{A}_{ij}(T) \hat{v}_j, & \text{if } T = 1, 2, \ldots, (N-1) \\ \sum_{i=1}^{N} \hat{v}_i \hat{a}_{ii}^* \hat{v}_i^*, & \text{if } T = N. \end{cases} \]

(8)
The operator for the last step, $\hat{S}(N)$, does not produce new terms. Its effect is to visit $V_1$ for the second time. After the action of $\hat{S}(N)$ every term in the superposition will have $v_1 = 1$. Starting from the initial state $|g(0)\rangle$ we produce a final state $|g(N)\rangle$ where

$$|g(N)\rangle = \hat{S}(N)\hat{S}(N-1)\cdots\hat{S}(1)|g(0)\rangle.$$

(9)

$|g(N)\rangle$ is a superposition of $(N-1)!$ basis states and is normalised by construction. Each of these corresponds to a distinct Hamiltonian tour. All terms in the superposition have the same probability amplitude of $1/\sqrt{(N-1)!}$.

As has been noted, $\hat{S}(T)$ is not a unitary operator. Although the operators used in Feynman’s description are unitary, the following weaker condition is sufficient.

$$\hat{S}(T)^*\hat{S}(T)|g(T-1)\rangle = |g(T-1)\rangle$$

This implies that the computation is meaningful only starting from the special state $|g(0)\rangle$.

3 The cost of a tour

In the simulation just described all tours have the same quantum amplitude. If a measurement is made on $|g(N)\rangle$, one tour is as likely as another. This can be improved by taking into account the cost of a tour. Let $w_{ij}$ be the weight of the edge $(i,j)$ defined as follows.

$$w_{ij} = 0 \quad \text{if} \quad i = j; \quad 0 < w_{ij} < 1 \quad \text{if} \quad i \neq j.$$

(10)

The $w_{ij}$ are non-negative real numbers which are normalised.

$$\sum_{j=1}^{N} w_{ij}^2 = 1, \quad (i = 1, 2, \ldots, N).$$

(11)

The $w_{ij}$ are taken to be symmetric: $w_{ij} = w_{ji}$. We can always impose on the $w_{ij}$ the $N$ conditions in equation (11) because there are $N(N-1)/2$ $w_{ij}$. In equation (7) we defined $\hat{A}_{ij}(1)$ the operator for the first step

$$\hat{A}_{ij}(1) = \frac{1}{\sqrt{N-1}} A_{ij} \hat{a}_{ii} \hat{a}_{ij}^* \hat{a}_{jj} \hat{a}_{jj}, \quad i, j = 1, 2, \ldots, N.$$

We replace this with a new definition

$$\hat{A}_{ij}(1) = w_{ij} \hat{a}_{ii} \hat{a}_{ij}^* \hat{a}_{jj} \hat{a}_{jj}.$$

(12)

For the first step the operator $\hat{S}(1)$ will use this new $\hat{A}_{ij}(1)$ rather than the one defined in equation (7). Acting on $|g(0)\rangle$ with the new $\hat{A}_{ij}(1)$ gives

$$|g(1)\rangle = \hat{S}_{1}|g(0)\rangle = \sum_{i=2}^{N} w_{1i} |1 \rightarrow i \bullet\rangle.$$

Because of the condition in equation (11), $|g(1)\rangle$ is normalised and it is still the case that

$$\hat{S}_{1}^* |g(1)\rangle = \hat{S}_{1}^* \hat{S}_{1} |g(0)\rangle = |g(0)\rangle.$$

The amplitude for the step $V_1 \rightarrow V_i$, which was previously $(N-1)^{-1/2}$, is now $w_{1i}$. For the second step, suppose we could define an operator that is identical to $\hat{A}_{ij}(1)$ in equation (12).

$$\hat{A}_{ij}(2) = \hat{A}_{ij}(1)$$

and operate on $|g(1)\rangle$. As before $|g(2)\rangle$ will contain $(N-1)(N-2)$ terms because we have changed only the amplitudes and not the dynamics. After the second step the path $V_1 \rightarrow V_{i_1} \rightarrow V_{i_2}$ will have quantum
amplitude $w_{1i_1}w_{i_1i_2}$. But recall that in the second step, starting from $V_{i_1}$, we do not visit $V_1$ or $V_{i_1}$ itself. That is, only $(N-2)$ other vertices are visited not $(N-1)$. In any step, starting from a given vertex, the total probability of all terms produced must be unity. The total probability of all terms produced by travelling from $V_{i_1}$ to $(N-2)$ other vertices is produced by summing over $i_2$ — the index of the vertices visited from $V_{i_1}$.

\[ \sum_{i_2 \neq 1}^N w_{i_1i_2}^2 = (1 - w_{i_11}^2) < 1. \]

Therefore $|g(2)\rangle = \hat{S}(2)|g(1)\rangle$ is not a normalised state. We are missing a probability of $w_{i_11}^2$. We can get around this situation by using a modified operator for the second step

\[ \hat{A}_{ij}(2) = \frac{w_{ij}}{\sqrt{1 - w_{i_11}^2}} \hat{a}_{ii}^* \hat{a}_{jj}^* \hat{a}_{jj}. \quad (13) \]

This is exactly the same as $\hat{A}_{ij}(1)$ in equation (12) except that all weights have been rescaled. In terms of the rescaled weights, in the second step, the total probability of all terms produced by starting from $V_{i_1}$ is now

\[ \sum_{i_2 \neq 1}^N \frac{w_{i_1i_2}^2}{(1 - w_{i_11}^2)} = \frac{1}{(1 - w_{i_11}^2)} \sum_{i_2 \neq 1}^N w_{i_1i_2}^2 = 1 \]

as required. The probability of all paths starting from $V_1$ is produced by summing over $i_1$ and $i_2$.

\[ \sum_{i_1,i_2,i_2 \neq 1}^N w_{i_1i_2}^2 \frac{w_{i_1i_2}^2}{(1 - w_{i_11}^2)} = \sum_{i_1=1}^N \frac{w_{i_1i_1}^2}{(1 - w_{i_11}^2)} \sum_{i_2 \neq 1}^N w_{i_1i_2}^2 = \sum_{i_1=1}^N w_{i_1i_1}^2. \]

This produces, from equation (14), unity proving that $|g(2)\rangle$ is normalised.

The rescaling of weights works in step 2 because in this step, every vertex, $V_{i_1}$, visited in the first step was visited from the fixed vertex $V_1$. At the end of the first step, every path has the same history — all start at $V_1$. This is not the case in subsequent steps. In the third step look for example, at the path $V_1 \rightarrow V_2 \rightarrow V_3 \rightarrow V_4$. In going from $V_3$ to $V_4$, neither $V_1$ nor $V_2$ is visited from $V_3$, the missing probability is $(w_{31}^2 + w_{32}^2)$ which means all amplitudes for the step starting from $V_3$ must be scaled by $(1 - (w_{31}^2 + w_{32}^2))^{-1/2}$. Now look at the path $V_1 \rightarrow V_3 \rightarrow V_4 \rightarrow V_6$. Here the missing probability in going from $V_4$ to $V_6$ is $(w_{41}^2 + w_{43}^2)$. So for this path the scaling factor is $(1 - (w_{41}^2 + w_{43}^2))^{-1/2}$. For the second and subsequent steps every path has a distinct history which cannot be accounted for by the technique used in step 2.

We need an operator to rescale the weights. Let us look at this one.

\[ \hat{w}_1 = \sum_{j=1}^N w_{ij}^2 \hat{a}_{jj}^* \hat{a}_{jj}. \quad (14) \]

This is a real, linear operator which has every basis state of $G$ as an eigenvector. Let us apply $\hat{w}_3$ to the path $V_1 \rightarrow V_2 \rightarrow V_3$.

\[ \hat{w}_3 |1 \rightarrow 2 \rightarrow 3 \bullet \rangle = (w_{31}^2 + w_{32}^2) |1 \rightarrow 2 \rightarrow 3 \bullet \rangle. \]

So $\hat{w}_3$ picks out the total probability along all edges from $V_3$ leading vertices already visited along the path $V_1 \rightarrow V_2 \rightarrow V_3$. In general, if along some path, $V_i$ is the vertex being visited and we operate on that state with $w_i$, the eigenvalue will be the sum of the squares of weights from $V_i$ to all vertices which have already
been visited along the path. However the operator we really want is one related to \( \hat{w}_i \). Look at the rescaling operator

\[
\hat{W}_i = \left(1 - \sum_{j=1}^{N} w_{ij}^{2} \hat{a}_{jj}^{*} \hat{a}_{jj}\right)^{-1/2}
\]

which we can write as a power series

\[
\hat{W}_i = c_0 + c_1 \sum_{j=1}^{N} w_{ij}^{2} \hat{a}_{jj}^{*} \hat{a}_{jj} + c_2 \left(\sum_{j=1}^{N} w_{ij}^{2} \hat{a}_{jj}^{*} \hat{a}_{jj}\right)^2 + \cdots.
\]

where the \((c_0, c_1, \ldots)\) are real numbers. This is a power series of commuting operators \( \hat{a}_{ii}^{*} \hat{a}_{ii} \). So \( \hat{W}_i \) is a linear operator and can be used to renormalize weights along the edges. The problem is that the \( \hat{W}_i \) are highly degenerate and have a large number of eigenvalues which are infinite. Any state corresponding to a Hamiltonian tour — in which all vertices have been visited — will be a state with an infinite eigenvalue. A Hamiltonian tour is a state in which \( a_{jj} = 0 \) for every \( j \). In this state, for any fixed \( i \) and distinct \( i_1, i_2, \ldots, i_{(N-1)} \),

\[
(1 - \sum_{j=1}^{N} w_{ij}^{2} \hat{a}_{jj}^{*} \hat{a}_{jj}) |1 \rightarrow i_1 \to \cdots \to i_{(N-1)} \rightarrow 1\rangle = (1 - \sum_{j=1}^{N} w_{ij}^{2}) |1 \rightarrow i_1 \to \cdots \to i_{(N-1)} \rightarrow 1\rangle = 0.
\]

To avoid this we redefine the scaling operator.

\[
\hat{W}_i = \left(1 - \hat{v}_1 \hat{v}_1^{*} \sum_{j=1}^{N} w_{ij}^{2} \hat{a}_{jj}^{*} \hat{a}_{jj}\right)^{-1/2}
\]

(15)

The infinite eigenvalues are avoided because the action of \( \hat{v}_1 \hat{v}_1^{*} \) in equation (15) will produce 0 for any state in which \( v_1 = 1 \). At both the start and end of a tour the second term in equation (15) vanishes to produce a scaling of unity which is exactly what is required.

The adjacency operator for the graph is now

\[
\hat{A}_{ij} = w_{ij} \hat{a}_{ii} \hat{a}_{ij}^{*} \hat{a}_{jj} \hat{a}_{jj} \hat{W}_i.
\]

The step operators are

\[
\hat{S}(T) = \begin{cases} 
\sum_{i,j=1}^{N} \hat{v}_1 \hat{A}_{ij}(T) \hat{v}_1^{*}, & \text{if } T = 1, 2, \ldots (N-1) \\
\sum_{i=2}^{N} \hat{v}_1 \hat{a}_{ii} \hat{a}_{ij}^{*} \hat{v}_1, & \text{if } T = N.
\end{cases}
\]

(16)

These will produce all Hamiltonian tours as desired. The amplitude for the last step is always unity. This is because in the last step we must return to the starting vertex. But in fact it is unity even in step \((N-1)\). Scaling increases the weights along the edges which is expected since after each step there are fewer edges along which to leave a given vertex. The amplitude for the tour \( V_1 \to V_{i_1} \to V_{i_2} \to V_{i_3} \to \cdots \to V_{i_N} \to V_1 \) will be

\[
\frac{w_{i_{1}i_{2}}}{\sqrt{1 - w_{i_{1}i_{1}}^{2}}} \frac{w_{i_{2}i_{3}}}{\sqrt{1 - (w_{i_{2}i_{1}}^{2} + w_{i_{2}i_{3}}^{2})}} \cdots 1.
\]

(17)

where each term in the product is the factor produced in each step. Each factor is a ratio that approaches unity as the tours progresses.

To connect with the classical result, let \( c_{ij} \) be the classical cost of travelling along the edge \((i,j)\). Each \( c_{ij} \) is a positive real number with \( c_{ij} = c_{ji} \) and \( c_{ii} = 0 \). Let
\[(C_i)^2 = \sum_{j=1, j\neq i}^{N} e^{-2c_{ij}} \tag{18}\]

An obvious choice for \(w_{ij}\) is

\[
w_{ij} = \begin{cases} 0, & \text{if } i = j; \\ \frac{e^{-c_{ij}}}{C_i}, & \text{if } i \neq j. \end{cases} \tag{19}\]

These \(w_{ij}\) satisfy the condition in equation (11) and can be treated as quantum amplitudes. Smaller classical costs \(c_{ij}\) will produce larger quantum amplitudes for a step along the corresponding edge.

In terms of the \(c_{ij}\) equation (17) is

\[
e^{-c_{i1}} \frac{e^{-c_{i12}}}{C_1} \sqrt{C_{i1}^2 - e^{-2c_{i1}}} \frac{e^{-c_{i23}}}{\sqrt{C_{i2}^2 - (e^{-2C_{i21}} + e^{-2c_{i21}}) \cdots e^{-c_{iN1}}}}. \]

But for scaling, which is an effect of the simulation, the quantum amplitude is the exponential of the sum of the classical costs of the edges in the tour.

The scaling factors have two quite different effects. In the classical analysis, the Hamiltonian tour \(V_1 \rightarrow V_2 \rightarrow V_3 \cdots \rightarrow V_N \rightarrow V_1\) has the same cost as the tour in the reverse direction. In this quantum simulation these two tours will generally have different quantum amplitudes because the scaling factors will be different for each.

In the classical case the optimal paths are those with the smallest total cost. In this simulation the optimal paths are those with the largest quantum amplitude. Due to scaling, Hamiltonian tours with the largest quantum amplitudes may not be the same as the classical tours with the smallest classical cost. The two results are expected to be the same in the majority of cases but this is based on the general notion that the classical optimal path will play the leading role even in the quantum domain. Numerical simulations on small problems and a few choices of edge-costs seem to support this claim.

### 4 Summary

By doing quantum mechanics on a graph I have described a simulation which can efficiently traverse all Hamiltonian tours and only the Hamiltonian tours. It is expected that in the majority of cases, tours with the smallest classical cost will have the largest quantum amplitude. There will certainly be cases in which the two differ. One can take this to mean that this simulation does not always produce a final superposition containing the correct — classically defined — results. On the other hand the final state contains basis states which represent the quantum optimal paths. Computing either is equally difficult.

It will take \(O(N(N - 1)/2)\) measurements on the final state to reduce it to a basis state corresponding to a Hamiltonian tour. In general the amplitude for any give tour is \(O(1/\sqrt{(N - 1)})\) so as expected, the simulation will have to be executed many times to find the optimal paths. This simulation will therefore be effective in those cases where the optimal tours have much larger quantum amplitudes than the sub-optimal tours.

The scaling operators \(\hat{W}_i\) have additional infinities. States with \(v_1 = 0\) and all \(a_{ii} = 0\) are states with an infinite eigenvalue. However these states are never reached in this simulation.

The marking scheme described in section 2 is by no means unique. There is plenty of room for different choices of basis states and the step operators. The one described here is natural because of the central role of the adjacency matrix. It is also one of the simplest. The marking scheme described in section 2 is an efficient way to traverse all Hamiltonian tours without any scaling.

One of the objectives of this simulation was to make quantum amplitudes depend in some way on the classical cost of travelling along an edge. Other simulations are possible in which the classical costs are used in different ways.
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