Pseudo-Hermitian continuous-time quantum walks

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Abstract
In this paper we present a model exhibiting a new type of continuous-time quantum walk (as a quantum-mechanical transport process) on networks, which is described by a non-Hermitian Hamiltonian possessing a real spectrum. We call it pseudo-Hermitian continuous-time quantum walk. We introduce a method to obtain the probability distribution of walk on any vertex and then study a specific system. We observe that the probability distribution on certain vertices increases compared to that of the Hermitian case. This formalism makes the transport process faster and can be useful for search algorithms.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction
In recent years, the studies of quantum random walks have suggested that they may display different behavior from their classical counterpart [1, 2]. One of the promising features of quantum random walks is that they provide an intuitive framework on which one can build novel quantum algorithms. Since many classical algorithms can be formulated in terms of random walks, one can hope that some of them may be translated into quantum algorithms which run faster than their classical counterparts. However, Shenvi et al [3] have shown that the quantum search algorithm can be derived from a certain kind of quantum random walks. Also, Childs et al [4] have presented a general approach to the Grover problem using a continuous-time quantum walk (CTQW) on a graph.

Quantum walk is generally divided into two standard versions: discrete-time quantum walk (DTQW) and CTQW [5–12]. In the past years, CTQW has been studied on the line [13–15], distance regular graphs [16], n-cube [17], star graphs [18, 19], quotient graphs [20], circulant Bunkbeds [21], decision trees [22, 23], odd graphs [24], Apollonian network [25] and dendrimers [26]. In all of the above-mentioned works, CTQW has been described by...
Hermitian Hamiltonians on networks. In this paper we describe a model exhibiting a new type of CTQW (as a quantum-mechanical transport process) on networks, which is described by a non-Hermitian Hamiltonian possessing a real spectrum. In recent years, we have witnessed a growing interest in the study of \( PT \)-symmetric Hamiltonian. These operators are specific by their \( PT \)-symmetry, i.e. \( [PT, H] = 0 \), where \( P \) is the space reflection and \( T \) is the time reversal, and can be covered by a broad class of pseudo-Hermitian operators which satisfy the following operator equation:
\[
H^\dagger = \Theta H \Theta^{-1},
\]
where the operator \( \Theta \) is required to be Hermitian, invertible and bounded [27–36]. One of the first application of the apparently non-Hermitian Hamiltonian with real spectra appeared in nuclear physics [37]. Also, in the recent works, attention has been paid to the extension of the phenomenological scope as well as the practical feasibility of the use of the Hamiltonians \( H \) which are made Hermitian only after the introduction of sophisticated, Hamiltonian-dependent \textit{ad hoc} metrics [38, 39], and studied for non-Hermitian matrices Hamiltonian \( 2 \times 2 \) and \( 3 \times 3 \) on Hilbert spaces with dimensions 2 and 3 [40, 41], respectively.

Here, we consider that kind of graphs whose Hamiltonians are pseudo-Hermitian. Using pseudo-Hermitian quantum mechanics, we obtain the probability distribution (transition probability) of walk on any vertex. The results show that the probability distribution on certain vertices increases in comparison with that of Hermitian CTQW. Therefore, we can increase the probability distribution on any arbitrary vertex. Noting the fact that the Grover search algorithm is a quantum random walk search algorithm [3, 42–45], pseudo-Hermitian quantum walk is a better candidate than Hermitian quantum walk for the search algorithm. Also, by noting the increasing and decreasing of the probability distribution on any arbitrary vertex, this formalism gives a faster transport on networks than that of the Hermitian case. This paper is organized as follows. In section 2 we first review CTQW on general graphs. Then, we describe the pseudo-Hermitian formalism and define pseudo-Hermitian CTQW (PHCTQW) and obtain probability distribution for PHCTQW on general graphs. In section 3 we derive PHCTQW for an example. The conclusion is given in section 4.

2. Pseudo-Hermitian continuous-time quantum walk

CTQW was introduced by Farhi and Gutmann [2] as a quantum-mechanical transport process on discrete structures, generally called graphs. A graph is a pair of two sets, \( G = (V, E) \), where \( V \) is a non-empty set and \( E \) is a subset of \( \{(i, j) : i, j \in V, i \neq j \} \). The elements of \( V \) and \( E \) are called vertices and edges, respectively. The adjacency matrix of \( G \) is defined as
\[
A_{ij} = \begin{cases} 
1 & \text{if } (i, j) \in V, \\
0 & \text{otherwise} 
\end{cases} \quad (i, j \in V). \tag{2.1}
\]

We assume that states \( |k\rangle \), associated with localized excitation at the vertex \( k \), form an orthonormal basis set and span the whole accessible Hilbert space. The Hamiltonian of quantum walk is defined as the Laplacian of the graph, \( H = A - D \), where \( D \) is a diagonal matrix with entries \( D_{jj} = \text{deg}(j) \), where \( \text{deg}(j) \) is the degree of the vertex \( j \) which is the number of proper edges incident on \( j \). Time evolution of quantum walk on graphs obtained by using the Schrödinger equation:
\[
i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle. \tag{2.2}
\]
The solution of this equation is $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$, where we assume $\hbar = 1$, and $|\psi(0)\rangle$ is the initial wavefunction amplitude of the particle. The transition probability of quantum walk at the vertex $k$ at time $t$ is given by

$$p_q^k(t) = |\langle k|\psi(t)\rangle|^2,$$

where '$q'$ stands for quantum walk. Also, by using Kolmogorov’s equation one can obtain the transition probability for classical random walk as

$$p_c^k(t) = |\langle k|e^{-Ht}|\psi(0)\rangle|^2,$$

(2.3)

where 'c' refers to classical walk. To solve equations (2.2) and (2.4) exactly, we need to know all the eigenvalues and eigenvectors of the Hermitian Hamiltonian $H$. Let $E_n$ and $|q_n\rangle$ be the $n$th eigenvalue and the corresponding orthonormalized eigenvector of $H$, respectively. Hence, the classical- and quantum-mechanical transition probabilities at the vertex $k$ at time $t$ are given by

$$p_q^k(t) = \sum_{n,l} e^{-i(t(E_n - E_l))}\langle k|q_n\rangle \langle q_n|\psi(0)\rangle \langle \psi(0)|q_l\rangle,$$

$$p_c^k(t) = \sum_{n} e^{-iE_n t}\langle k|q_n\rangle \langle q_n|\psi(0)\rangle,$$

(2.5, 2.6)

respectively.

Here, we consider a model exhibiting a new type of quantum-mechanical transport processes on networks described by a non-Hermitian Hamiltonian possessing a real spectrum. Let $\mathcal{H}$ be a Hilbert space and $H : \mathcal{H} \rightarrow \mathcal{H}$ be a diagonalizable linear Hamiltonian operator. $H$ is said to be pseudo-Hermitian if there exists a positive-definite operator $\Theta : \mathcal{H} \rightarrow \mathcal{H}$ such that

$$H^\dagger = \Theta H \Theta^{-1}.$$ 

(2.7)

It can be shown that $H$ is a Hermitian operator with respect to some positive-definite inner product $\langle , \rangle_+$ on $\mathcal{H}$ (which is generally different from its defining inner product $\langle , \rangle$). A specific choice for $\langle , \rangle_+$ is $\langle \cdot | \Theta \cdot \rangle$. Therefore, one can consider the set of the $H$ eigenvectors as a basis for $\mathcal{H}$. If $E_n$ and $|\psi_n\rangle$ are the $n$th eigenvalue and the corresponding eigenvector of $H$, respectively, we have

$$H|\psi_n\rangle = E_n|\psi_n\rangle.$$ 

(2.8)

One can construct another basis $\{|\phi_n\rangle\}$ of $\mathcal{H}$ satisfying

$$H^\dagger|\phi_n\rangle = E_n|\phi_n\rangle,$$

$$\langle \phi_n|\psi_m\rangle = \delta_{nm},$$

$$\sum_n |\psi_n\rangle \langle \psi_n| = 1.$$ 

(2.9)

In other words, the set $\{|\psi_n\rangle, |\phi_n\rangle\}$ forms a biorthonormal system, and we have

$$H = \sum_n E_n|\psi_n\rangle \langle \phi_n|,$$

$$H^\dagger = \sum_n E_n|\phi_n\rangle \langle \psi_n|.$$ 

(2.10)

Therefore, by using equation (2.7) one can define the pseudo-metric operator $\Theta$ associated with the operator $H$ as

$$\Theta = \sum_n |\phi_n\rangle \langle \phi_n|,$$

$$\Theta^{-1} = \sum_n |\psi_n\rangle \langle \psi_n|.$$ 

(2.11)

Using the inner product $\langle , \rangle_+$, we can introduce a new vector space called the physical Hilbert space $\mathcal{H}_{\text{phys}}$. This space is actually the same as $\mathcal{H}$, but with different inner product.
To conserve the total transition probability of PHCTQW, we must consider time evolution of the vector state \( |\psi(t)\rangle \) determined by the Schrödinger equation in physical Hilbert space \( H_{\text{phys}} \) with respect to the inner product \( \langle \cdot, \cdot \rangle_{+} \). In this case, to solve the Schrödinger equation (2.2) for PHCTQW we have

\[
|\psi(t)\rangle = \sum_{n} e^{-iE_{n}t} |\psi_{n}\rangle \langle \phi_{n}| \psi_{0}\rangle, \tag{2.12}
\]

where we use the completeness relations of the basis in equation (2.9). The norm of the state should be conserved, so

\[
\langle \psi(t)|\psi(t)\rangle_{+} = \sum_{m,n} e^{-iE_{m}t} \langle \psi_{m}|\Theta|\psi_{n}\rangle \langle \phi_{m}| \psi_{0}\rangle \langle \phi_{n}| \psi_{0}\rangle
\]

\[
= \sum_{n} \langle \phi_{n}| \psi_{0}\rangle \langle \psi_{0}| \phi_{n}\rangle = \langle \psi_{0}| \sum_{n} |\phi_{n}\rangle \langle \phi_{n}| \psi_{0}\rangle = \langle \psi_{0}| \Theta \psi_{0}\rangle = 1, \tag{2.13}
\]

where \( |\psi_{0}\rangle = \frac{\langle \psi(0)| \psi(0)\rangle}{\sqrt{\langle \psi(0)| \psi(0)\rangle}} \) and we used the definition of \( \Theta \) in equation (2.11). Therefore, by using equations (2.12) and (2.13), the transition probability of quantum walk at the vertex \( k \) and the time \( t \) for the state \( |\psi(t)\rangle \) is given by

\[
p_{sq}^{k}(t) = |\langle k|\Omega|\psi(t)\rangle|^{2}. \tag{2.14}
\]

where \( \Omega \) need not in general be Hermitian and is defined as \( \Theta = \Omega^{\dagger} \Omega [46–50] \). In this paper we consider \( \Omega \) to be a Hermitian operator and defined as \( \Omega = \sqrt{\Theta} \), and ‘sq’ stands for pseudo-Hermitian quantum walk. To obtain the operator \( \Omega \) it is necessary to have the eigenvalues and eigenvectors of operator \( \Theta \). Denoting the eigenvalues and eigenvectors of \( \Theta \) by \( \epsilon_{n} \) and \( |\epsilon_{n}\rangle \), respectively, we have

\[
\Theta |\epsilon_{n}\rangle = \epsilon_{n} |\epsilon_{n}\rangle, \quad \langle \epsilon_{m}| \epsilon_{n}\rangle = \delta_{mn}, \quad \sum_{n} |\epsilon_{n}\rangle \langle \epsilon_{n}| = 1. \tag{2.15}
\]

These in turn imply

\[
\Omega = \sum_{n} \sqrt{\epsilon_{n}} |\epsilon_{n}\rangle \langle \epsilon_{n}|. \tag{2.16}
\]

3. Example

As an example, we consider PHCTQW on the graph in figure 1. As can be seen, in this example, vertex 3 has preference to other vertices. The Hamiltonian \( H = D - A \), where \( D \) is
the diagonal matrix defined before and $A$ is the adjacency matrix, is non-Hermitian possessing a real spectrum which satisfies equation (2.7). Considering the graph, $H$ is as follows:

$$H = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & 0 & 2 \end{pmatrix}. \quad (3.1)$$

The eigenvalues and eigenvectors (see equations (2.8) and (2.9)) of $H$ and $H^\dagger$ can easily be calculated:

$$E_1 = 0, \quad E_2 = 2, \quad E_3 = 3, \quad |\psi_1\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix},$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, \quad |\psi_3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix},$$

$$|\phi_1\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad |\phi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \quad |\phi_3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} -2 \\ 1 \\ 1 \end{pmatrix}. \quad (3.2)$$

Using equations (2.11) and (2.16) the operators $\Theta$ and $\Omega$ are obtained as

$$\Theta = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Omega = \begin{bmatrix} -\frac{i}{2} & \sqrt{5} & 0 \\ -\frac{i}{2} & -\frac{i}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (3.3)$$

Therefore, the solution of the Schrödinger equation (2.12) is

$$|\psi(t)\rangle = \frac{1}{\sqrt{12}} |\psi_1\rangle + \frac{1}{\sqrt{2}} e^{-i2t} |\psi_2\rangle - \frac{2}{\sqrt{6}} e^{-it} |\psi_3\rangle. \quad (3.4)$$

where we consider $|\psi(0)\rangle = |1\rangle$ as the starting point of the walk. Then using equations (2.14) and (3.3) we obtain the transition probability as

$$p_k^{(t)} = \begin{cases} \frac{1}{20} [18 + 8 \cos(t) + 2 \cos(2t) + 8 \cos(3t)] & \text{for } k = 1, \\ \frac{1}{20} [17 + 12 \cos(t) - 12 \cos(2t) - 8 \cos(3t)] & \text{for } k = 2, \\ \frac{1}{20} [26 - 24 \cos(t) + 6 \cos(2t) - 8 \cos(3t)] & \text{for } k = 3. \end{cases} \quad (3.5)$$

Figure 2 shows the transition probability on the network in figure 1, where the starting point of the walk is the node $|1\rangle$. Figure 2(a) illustrates the probability of returning to the starting point ($|1\rangle$). As can be seen, in returning to the starting point, the walk spends most of the time with the probability between 0.3 and 0.5. However, in the Hermitian version (CTQW on the complete graph $K_3$) the probability on vertex 1 is homogeneous for all time. Figure 2(b) shows that the probability of observing the walk in vertex 2 is more than that of the Hermitian version. The same happens for vertex 3, but, as shown in figure 2(c), the difference between the probabilities for the two cases (Hermitian and non-Hermitian) at vertex 3 is much more than that at vertex 2. In fact, one can apply the PHCTQW for increasing the probability of observing the walk at an arbitrary vertex, which is very useful to make the transport faster on a network.

Now, let vertex 2 be the starting point of the walk. The transition probability is obtained as

$$p_k^{(t)} = \begin{cases} \frac{1}{20} [3 + 2 \cos(t) - \cos(2t) - 2 \cos(3t)] & \text{for } k = 1, \\ \frac{1}{20} [14 + 6 \cos(t) + 12 \cos(2t) + 4 \cos(3t)] & \text{for } k = 2, \\ \frac{1}{20} [14 - 12 \cos(t) - 6 \cos(2t) + 4 \cos(3t)] & \text{for } k = 3. \end{cases} \quad (3.6)$$

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Figure 2. The probability distribution of the walk on vertices when the starting point is on vertex 1: (a) the return probability of the walk to the starting point (vertex 1), (b) the probability distribution of walk on vertex 2 and (c) the probability distribution of walk on vertex 3 for PHCTQW (higher probability = blue line) and its Hermitian version (lower probability = red line).

Figure 3 shows the behavior of $p_k^m(t)$ with respect to the time $t$. Figure 3(a) shows the probability distribution of finding the walk at vertex 1. Although the distribution is not as
Figure 3. The probability distribution of the walk on the vertices of the graph when the starting point of the walk is on vertex 2 of figure 1: (a) the probability distribution of walk on vertex 1 in terms of $t$, (b) the probability of returning to the starting point (vertex 2) and (c) the probability distribution of walk on vertex 3 of the graph for PHCTQW (higher probability = blue line) and its Hermitian version (lower probability = red line).
homogeneous as in the Hermitian case, the value of the probability has not generally changed so much. The return probability distribution to vertex 2 (starting point) is illustrated in figure 3(b). As can be seen, it changes periodically due to the special property of the graph. In figure 3(c) we see that the transition probability of the walk is increased in comparison with its transition probabilities on other vertices.

In this example we saw that the non-Hermitian property of the Hamiltonian is responsible for increasing the probability of observing a particle on any vertex.

Also, one can generalize this method to obtain PHCTQW on the graph shown in figure 4. Figure 4 illustrates a cycle graph with \( n \) vertices such that the edge between the vertices \( n-1 \) and \( n \) is directed, in other words, the vertex \( n \) has preference to the other vertices. As an example, we consider the above-mentioned graph with four vertices. The Hamiltonian is given by

\[
H = \begin{pmatrix}
2 & -1 & 0 & -1 \\
-1 & 2 & -1 & 0 \\
0 & -1 & 1 & -1 \\
-1 & 0 & 0 & 2
\end{pmatrix}.
\]

The eigenvalues and eigenvectors (see equations (2.8) and (2.9)) of \( H \) and \( H^\dagger \) can be obtained as

\[
E_1 = 0, \quad E_2 = 2, \quad E_3 = \frac{1}{2}(5 + \sqrt{5}), \quad E_4 = \frac{1}{2}(5 - \sqrt{5}),
\]

\[
|\psi_1\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 2 \\ 3 \\ 4 \\ 1 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix},
\]

\[
|\psi_3\rangle = \frac{i}{\sqrt{\frac{5}{2}(3 + \sqrt{5})}} \begin{pmatrix} \frac{1}{2}(1 + \sqrt{5}) \\ -\frac{1}{2}(1 + \sqrt{5}) \\ 1 \\ -1 \end{pmatrix}, \quad |\psi_4\rangle = \frac{i}{\sqrt{\frac{5}{2}(3 - \sqrt{5})}} \begin{pmatrix} \frac{1}{2}(1 - \sqrt{5}) \\ \frac{1}{2}(-1 + \sqrt{5}) \\ 1 \\ -1 \end{pmatrix},
\]

\[
|\phi_1\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad |\phi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ -1 \\ 1 \\ 1 \end{pmatrix}, \quad |\phi_3\rangle = \frac{i}{\sqrt{\frac{5}{2}(3 + \sqrt{5})}} \begin{pmatrix} -(1 + \sqrt{5}) \\ \frac{1}{2}(3 + \sqrt{5}) \\ 1 \\ -1 \end{pmatrix},
\]
\[ |\phi_4 \rangle = \frac{i}{\sqrt{\frac{5}{2}(3 - \sqrt{5})}} \begin{pmatrix} \frac{1}{2}(3 - \sqrt{5}) \\ -1 \\ \frac{1}{2}(3 - \sqrt{5}) \end{pmatrix}. \] (3.8)

In this case, by using equation (2.11), we obtain the operator \( \Theta \) as follows:

\[ \Theta = \begin{pmatrix} \frac{11}{5} & \frac{1}{5} & -\frac{4}{5} & -\frac{4}{5} \\ \frac{1}{5} & 6 & 5 & \frac{1}{5} \\ -\frac{4}{5} & -\frac{4}{5} & \frac{5}{5} & \frac{1}{5} \\ -\frac{4}{5} & \frac{1}{5} & \frac{1}{5} & \frac{5}{5} \end{pmatrix}. \] (3.9)

Therefore, one can investigate PHCTQW for this graph as was done for the previous example.

### 4. Conclusions

In this paper we have introduced a model exhibiting a new type of CTQW on networks, which is described by a non-Hermitian Hamiltonian possessing a real spectrum. The model is called PHCTQW. Then we introduced a method to obtain the probability distribution of walk on any vertex. We have applied this model to a network and saw that the probability distribution on certain vertices increased compared to its Hermitian counterpart. Indeed by choosing a non-Hermitian Hamiltonian for CTQW one can increase the probability distribution on an arbitrary vertex which can help to make the transport faster and can be useful for search algorithms. One can generalize this method to perfect quantum state transfer over some special networks, which is under investigation now.

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