Quantum walks induced by Dirichlet random walks on infinite trees

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Abstract
We consider the Grover walk on infinite trees from the viewpoint of spectral analysis. From the previous work, infinite regular trees provide localization. In this paper, we give the complete characterization of the eigenspace of this Grover walk, which involves localization of its behavior and recovers the previous work. Our result suggests that the Grover walk on infinite trees may be regarded as a limit of the quantum walk induced by the isotropic random walk with the Dirichlet boundary condition at the $n$-th depth rather than one with the Neumann boundary condition.

Keywords: quantum walk, infinite tree, eigenspace, flow, Dirichlet condition

(Some figures may appear in colour only in the online journal)

1. Introduction

A discrete-time quantum walk (QW) on a graph $G = (V,E)$ has been proposed by Gudder [10] as ‘quantum graphic dynamics’ in his book [10]; a walker jumps to neighbors with a matrix valued weight at each time step so that the time evolution of the whole state is unitary. This walk can be interpreted as a dynamics on the arcs of $G$ [23]. From this observation, it is possible to naturally connect quantum walks [11, 26] on graphs and the scatterings of a one-dimensional plane wave on the wire [8]. In this paper, we identify the discrete-time quantum walk with a pair of $U$ and $\mu$: $U$ is a unitary operator on $l^2(A) := l^2(A, C)$ with the standard inner product so that

$$\langle \delta_f, U \delta_e \rangle \neq 0 \iff t(e) = o(f)$$
and $\mu$ is the measurement $\mu : \ell^2(\mathbb{A}, \mathbb{C}) \to \ell^1(\mathbb{V}, \mathbb{R}_{\geq 0})$ such that
\[
(\mu(\psi))(u) = \sum_{e \in \mathbb{E} : e = u} |\psi(e)|^2,
\]
where $(\mu(\psi))(u)$ is interpreted as the findings probability at vertex $u$ if \(|\psi| = 1\). Here $\mathbb{A}$ is the set of symmetric arcs induced by $\mathbb{E}$, and $o(e), l(e) \in \mathbb{V}$ are the origin and terminus of arc $e \in \mathbb{A}$, respectively. We often call the unitary operator $\mathbb{U}$ simply the quantum walk. Due to the unitarity of the time evolution $\mathbb{U}$, we can define the distribution $\nu_n^{(\psi_n)} : \mathbb{V} \to [0, 1]$ at each time $n$ with the initial state $\psi_0 \in \ell^2(\mathbb{A})$ with \(|\psi_0| = 1\) such that
\[
\nu_n^{(\psi_0)} \equiv \mu(\mathbb{U}^n\psi_0).
\]
One of the main topics of the study of quantum walks is its asymptotics of $\nu_n$ for large $n$ e.g. localization, linear spreading and recurrent property and so on (see [4, 15] and their references).

The Grover walk is regarded as the induced quantum walk by the underlying isotropic random walk $\mathbb{T}$ [7, 25]. Here $\mathbb{T}$ is a self-adjoint operator on $\ell^2(\mathbb{V})$ with the standard inner product such that
\[
\langle \delta_u, \mathbb{T}\delta_v \rangle = \frac{\mathbb{1}_\mathbb{A}(u, v)}{\deg(u)\deg(v)}.
\]
We note that $\mathbb{T}$ is unitarily equivalent to the transition operator of the isotropic random walk. For a finite graph $\mathbb{G}$, the spectrum of the Grover walk $\mathbb{U}$ is simply decomposed into
\[
\sigma(\mathbb{U}) = \{e^{\pm i\arccos \sigma(\mathbb{T})} \} \cup \{1\}^{b_1} \cup \{-1\}^{b_{-1}+b_1},
\]
where $b_1$ and $b_{-1} - 1 + b_1$ are the multiplicities of the eigenvalues 1 and $-1$, respectively [12]. Here $b_1$ coincides with the first Betti number of $\mathbb{G}$, that is, $b_1 = |E| - |V| + 1$, and $b_1 = 1$ if $\mathbb{G}$ is bipartite, $b_1 = 0$ otherwise. We call the first term the inherited part from the underlying RW, and the last two terms the birth part. As is seen, the above multiplicities in the birth part reflect a homological structure of the graph. Every eigenfunction of the birth part has a finite support corresponding to fundamental cycles [12]. On the other hand, the birth part never appears for a finite tree, because no cycles exist. Let us consider whether this kind of statement still holds for an infinite graph. Naturally, if a cycle exists, then we can construct the eigenfunction with a finite support along it in the same fashion as in the finite case. This implies localization happens if the initial state has an overlap between the birth eigenspace. Indeed, even if there are no cycles in an infinite graph, the localization of the Grover walk may occur. In fact, localization on some infinite tree with some appropriate initial state can be seen in [5].

We first show in this paper that for an infinite tree whose minimal degree is at least 3, actually there are an infinite number of birth eigenfunctions (see theorem 1). The birth eigenfunction is generated by a finite energy flow [3] starting from a vertex to the infinite downstream. A one-dimensional lattice is also a tree with degree $\kappa = 2$ and we can make an infinite flow. However the 'function' generated by such a flow is $\ell^\infty(\mathbb{A})$ but no longer $\ell^2(\mathbb{A})$. From the above reason, the Grover walk on the one-dimensional lattice never exhibits localization as it is known that this walk is trivially going one way without any interactions. From the above reason, we assume that the minimal degree is at least 3 throughout this paper. Once the minimal degree $\kappa_0 + 1 \geq 3$ is assumed, then the square summability of the function generated by a flow is ensured (see lemma 1). Studies of localization has gained attention by many researchers. In previous studies, it has been known that the derivation of localization of the Grover walk is a cycle structure [12, 18] of the graph and inherited eigenspace from
underlying isotropic random walk \cite{13, 16}. Thus the positivity of such a geometric constant in corollary 3 can be said to be a new criterion for the localization.

To understand such a spectral structure of the Grover walk on infinite trees, we introduce a quantum walk induced by the random walk under the Dirichlet boundary condition at \( n \)-depth; this type of random walk may be called the Dirichlet random walk in this paper. We show that if we regard the Grover walk on the infinite tree as a limit of this induced QW for \( n \to \infty \), then the birth part naturally appears. More precisely, the eigenfunctions of the birth part of the approximate QW coincide with the eigenfunctions of the original Grover walk within the \( n \)-th depth (see theorem 4). The positivity of a kind of Cheeger constant ensures the square summability (see corollary 3). We note that the QW induced by the Dirichlet random walk has essentially appeared as a tool of several quantum spatial search algorithms on graphs; the target vertices in these algorithms correspond to the Dirichlet cut-off ones. The previous works \cite{1, 2, 24, 25} with the Dirichlet cut-off underlying random walk for a quantum search problem focused on the inherited part since the ‘uniform’ state, which is the initial state of these algorithms, has a small overlap to the birth part for a large system size. On the other hand, we propose an advantage of focusing on the birth part with the Dirichlet cut-off underlying random walk to extract a geometric structure of infinite graphs.

Connecting the Grover walk on the infinite tree to the QWs with the other construction \cite{17} is one of the interesting future problems.

This paper is organized as follows. In section 2, we provide the setting of the Grover walk on the infinite tree and introduce inherited and birth parts of the Grover walk. Section 3 is devoted to obtaining an expression of the birth eigenspace by finite energy flows on the infinite tree (theorem 1). In the previous work \cite{5} (2007), it is shown that one initial state provides localization of the Grover walk on the infinite regular tree, while the other one does not. Here a graph is called regular, if the degree is constant. We can check that the essential difference with respect to the localization between them is the overlap to such birth eigenfunctions. In the subsequent section, section 4, we introduce a QW induced by the Dirichlet random walk as an approximation of the Grover walk on the infinite tree and give the spectral mapping theorem from the Dirichlet random walk (theorem 4). As a result, the birth part of the approximate walk can be described by that of the original Grover walk. Finally in section 5, we give a summary of our results in this paper comparing with our previous sequential studies \cite{11–14} and discuss the relationship between our results and the quantum search algorithms driven by QWs \cite{6, 19, 20}.

### 2. Grover walk on the infinite tree

To define the Grover walk on the infinite tree \( \mathbb{T} = (V, A) \), we prepare two boundary operators \( d_T, d_O : \ell^2(A) \to \ell^2(V) \),

\[
(d_T \psi)(u) = \sum_{e \in (e) = u} 1/\sqrt{\text{deg}(t(e))} \psi(e),
\]

\[
(d_O \psi)(u) = \sum_{e \in (e) = u} 1/\sqrt{\text{deg}(o(e))} \psi(e), \quad (u \in V),
\]

respectively. Here \( \text{deg}(u) \) is the degree of \( u \in V \). Putting \( S : \ell^2(A) \to \ell^2(A) \) as a permutation operator denoted by

\[
(S \psi)(e) = \psi(\bar{e}),
\]
we have $d_0 = dT$. Here $\bar{e}$ is the inverse arc of $e$. The adjoint operators are

$$(d^*_T f)(e) = \frac{1}{\sqrt{\deg(t(e))}} f(t(e)), \quad (d^*_O f)(e) = \frac{1}{\sqrt{\deg(o(e))}} f(o(e)), \quad (e \in A),$$

respectively. Remark that

$$d_T d^*_T = dO d^*_O = 1_V,$$

where $1_V$ is the identity operator on $V \equiv \ell^2(V)$. We define the self-adjoint operator $T$ on $V$ by

$$T = dT d^*_O = dO d^*_T;$$

for $f \in V$,

$$(Tf)(u) = \sum_{e, t(e) = u} \frac{1}{\sqrt{\deg(t(e)) \deg(o(e))}} f(o(e)).$$

We remark that $T$ is unitarily equivalent to the transition operator $P$ of the isotropic random walk on $\mathbb{T}$, that is, $T = D^{-1} PD$, where $(Df)(u) = \sqrt{\deg(u)} f(u)$.

**Definition 1.** The Grover walk on a connected tree is defined as follows:

1. total space: $\mathcal{A} \equiv \ell^2(A)$;
2. time evolution: $U : \ell^2(A) \to \ell^2(A)$ such that

$$U = S(2d_T^* d_T - 1_A).$$

Here $1_A$ is the identity operator on $\mathcal{A}$.

We read

$$\langle \delta_f, U \delta_e \rangle = 1_{\{o(f) = o(e)\}}(e,f) \left( \frac{2}{\deg(t(e))} - \delta_{e,f} \right)$$

as the amplitude associated with the one-step moving from $e$ to $f$. We also define an important invariant subspace $\mathcal{L} \subset \mathcal{A}$ and its orthogonal complement $\mathcal{L}^\perp$; we call them the inherited and birth subspaces, respectively. Here

$$\mathcal{L} = d_T^*(V) + d_O^*(V).$$

**Proposition 1.** It holds that

$$U = U|_\mathcal{L} \oplus U|_{\mathcal{L}^\perp}.$$ 

**Proof.** It is sufficient to show $U(\mathcal{L}) = \mathcal{L}$. First we show $U(\mathcal{L}) \subset \mathcal{L}$. For any $\psi \in \mathcal{L}$, there exist $f, g \in V$ such that $\psi = d_T^* f + d_O^* g$. By equation (2.5), we have

$$U\psi = -(d_T^* g + d_O^* (f - 2Tg)),

which implies $U\psi \in \mathcal{L}$. Conversely, it is easily checked that for any $f, g \in V$,

$$d_T^* f + d_O^* g = U(d_T^* (g - 2Tf) - d_O^* f) \in U(\mathcal{L}).$$

In our previous works [14, 21, 22], we have the general result on the spectrum of a generalized QW on infinite graphs including the Grover walk as follows:
(1) the spectrum $\sigma(U|_{\mathcal{L}})$ of $U$ which restricted to a subspace $\mathcal{L}$ coincides with the image of the inverse Joukowski transform of the spectrum $\sigma(T)$ of an underlying random walk:

$$\sigma(U|_{\mathcal{L}}) = J^{-1}(\sigma(T)),$$

where $\sigma(\cdot)$ is the set of spectrum and $J(z) = (z + z^{-1})/2$;

(2) the continuous spectrum $\sigma_c(U)$ of the induced QW is completely derived from the continuous one $\sigma_c(T)$ of the underlying random walk: $\sigma_c(U) = J^{-1}(\sigma_c(T))$.

Moreover it is well known that the spectrum of the isotropic random walk $T$ on the infinite $\kappa$-regular tree consists of the continuous spectrum:

$$\sigma(T) = \sigma_c(T) = [-2\sqrt{\kappa - 1/\kappa}, 2\sqrt{\kappa - 1/\kappa}].$$

Thus, we can conclude that the eigenspace of the Grover walk on the infinite regular tree derives from the birth part $\mathcal{L}^\perp$. In the next section, we present a construction of this eigenspace by investigating a graph structure of the infinite tree; in other words, we will construct a kind of combinatorial flow with finite energy on the tree.

### 3. Construction of the eigenspace of the Grover walk on $\mathbb{T}$

We take a choice of a fixed arbitrary vertex $o$ as the root of $\mathbb{T}$. For each $u \in V$, we take the connected infinite subtree $\mathbb{T}^{(u)} = (V^{(u)}, A^{(u)})$ which is the induced subgraph of $\mathbb{T}$ by

$$V^{(u)} = \{v \in V : \text{dist}(o, v) = \text{dist}(o, u) + \text{dist}(u, v)\};$$

equivalently, $\mathbb{T}^{(u)}$ is the subtree of $\mathbb{T}$ consisting of all the descendants of $u$, which is considered as the root of $\mathbb{T}^{(u)}$. See figure 1. Here dist$(x, y)$ is the usual graph-distance between two vertices $x$ and $y$. The set of vertices $\{v \in V : \text{dist}(o, v) = n\}$ is often called the $n$-th depth (from $o$) of $\mathbb{T}$. In particular, we define $\mathbb{T}^{(o)} = \mathbb{T}$. Let $\{e^{(u)}_0, \ldots, e^{(u)}_{m-1}\} \subset A^{(u)}$ be the set of arcs $e$ such that $o(e) = u$ and $t(e) \in V^{(u)}$, where

$$m(u) = \begin{cases} \deg(u) : u = o, \\ \deg(u) - 1 : u \neq o. \end{cases}$$

(3.6)

Thus $m(u)$ is number of children of $u$.

Now we define important functions by the recurrent way as follows, which corresponds to a kind of combinatorial flow:

**Definition 2.** Assume $\deg(v) \geq 2$. Let $\varphi^{(\pm)} : \{(u, j) ; u \in V, j \in \{1, \ldots, m(u) - 1\}\} \to \mathbb{C}^A$ be defined as follows.

For $e, f \in \{g \in A^{(u)} : \text{dist}(o(g), u) < \text{dist}(t(g), u)\}$, $\varphi^{(\pm)}(u, j) := \varphi^{(\pm)}_{u, j}$ denotes

$$\varphi^{(\pm)}_{u, j}(e) = \begin{cases} \omega_j/m(o(e)) : e = t_k^{(u)}, & (k = 0, \ldots, m(u) - 1), \\
\pm \varphi^{(\pm)}_{u, j}(f)/m(o(e)) : t(f) = o(e), o(e) \neq u, \end{cases}$$

(3.7)

$$\varphi^{(\pm)}_{u, j}(e) = \mp \varphi^{(\pm)}_{u, j}(e).$$

(3.8)

For $e \notin A^{(u)}$, $\varphi^{(\pm)}_{u, j}(e) = 0$. Here $\omega_j = e^{2\pi ik/m(u)}$ and $i = \sqrt{-1}$. 

In the following, \( \varphi^{(\pm)}_{u,j} \) denotes \( \varphi^{(\pm)}(u,j) \).

**Remark 1.** Let \( \kappa_0 + 1 \) be the minimum degree of \( \mathbb{T} \). For \( \kappa_0 \geq 2 \), we have \( \varphi^{(\pm)}_{u,j} \in \ell^2(A) \) as shown by the following lemma.

**Lemma 1.** Assume \( \kappa_0 \geq 2 \). We have
\[
\| \varphi^{(\pm)}_{u,j} \| = c_{u,j},
\]
where \( c_{u,j} > 0 \) is a uniformly bounded constant, that is, there exists \( c_0 < \infty \) such that \( \sup_{u,j} c_{u,j} \leq c_0 \). Moreover, \( \{ \varphi^{(\epsilon)}(u) : u \in V, j \in 0, \ldots, m(u) - 1, \epsilon \in \{ \pm \} \} \) are linearly independent. In particular, when \( \mathbb{T} \) is \( \kappa \)-regular tree, then they are orthogonal to each other, that is, for every \( \epsilon, \epsilon' \in \{ \pm \} \), \( u, u' \in V, j \in 1, \ldots, m(u) - 1 \) and \( j' \in 1, \ldots, m(u') - 1 \),
\[
\langle \varphi^{(\epsilon)}_{u,j}, \varphi^{(\epsilon')}_{u',j'} \rangle = \frac{2(\kappa - 1)}{m(u)(\kappa - 2)} \delta_{\epsilon,\epsilon'} \delta_{u,u'} \delta_{j,j'}.
\]

**Proof.** Let \( \mathcal{H}^{(\pm)} \) be eigenspaces of eigenvalues \( \{ \pm 1 \} \) of \( \mathcal{S} \), respectively, that is,
\[
\mathcal{H}^{(\pm)} = \{ \psi \in \mathcal{A} : \psi(e) = \pm \psi(e) \ (e \in A) \}.
\]

First we show that the linear independence. Assume that \( \varphi^{(+)}_{u,j} \) is expressed by a linear combination of \( \varphi^{(\epsilon)}_{u',j'} \)s with \( u' \in V, j' \in 1, \ldots, m(u') - 1 \):
\[
\varphi^{(+)}_{u,j} = \sum_{(u',j') \neq (u,j)} r^{(+)}_{u',j'} \varphi^{(+)}_{u',j'} + \sum_{(u',j')} r^{(-)}_{u',j'} \varphi^{(-)}_{u',j'}.
\]

We will show the contradiction step by step as follows:

1. From the definition, we have \( \varphi^{(+)}_{u,j} \in \mathcal{H}^{(-)} \) and \( \varphi^{(-)}_{u',j'} \in \mathcal{H}^{(+)} \). Thus \( \varphi^{(+)}_{u,j} \perp \varphi^{(-)}_{u',j'} \). Therefore, any \( \varphi^{(\epsilon)}_{u',j'} \)s with \( u' \in V, j' \in 1, \ldots, m(u') - 1 \) are not contained in the linear combination (3.10), that is, \( r^{(-)}_{u',j'} = 0 \) for every \( u' \in V, j' \in 1, \ldots, m(u') - 1 \).

2. Note that if \( V^{(u') \cap V^{(u')}} = 0 \), then \( \varphi^{(\epsilon)}_{u,j} \perp \varphi^{(\epsilon')}_{u',j'} \) holds since their supports are disjoint, where the support of \( \psi \in \mathcal{A} \) is denoted by \( \text{supp}(\psi) = \{ a \in A : \psi(a) \neq 0 \} \). Therefore,
any \( \varphi^{(+)}_{u',j} \)'s with \( V(\omega') \cap V(\omega) = \emptyset \) are not contained in the linear combination (3.10), that is, \( r^{(+)}_{u',j} = 0 \) for every \( u' \) with \( V(\omega') \cap V(\omega) = \emptyset \), \( j' \in \{1, \ldots, m(\omega') - 1\} \).

(3) Remark that \( V(\omega) \cap V(\omega') = \emptyset \) if and only if \( T^{(\omega)} \supseteq T^{(\omega')} \) or \( T^{(\omega')} \subseteq T^{(\omega)} \). If \( T^{(\omega)} \supseteq T^{(\omega')} \), then

\[
\text{supp}(\varphi_{\omega \omega}) \setminus \text{supp}(\varphi_{\omega' \omega}) \supseteq \{ a \in A^{(\omega)} : t(a) = u, \text{ or } o(a) = u \}.
\]

Therefore, \( \varphi_{\omega \omega}^{(+)} \) cannot be described by the linear combination only using

\[
\{ r^{(+)}_{\omega' \omega, j' \omega' : u' \in V(\omega) \setminus \{ u \}, j' \in \{1, \ldots, m(\omega') - 1\} \}.
\]

(4) The shortest path from \( o \) to \( u \) is denoted by \( (e_1, e_2, \ldots, e_n) \) with \( o(e_1) = o \) and \( t(e_n) = u \). By (1)–(3), we have

\[
\varphi_{\omega \omega}^{(+)} = \sum_{(u', j') \in Q} r^{(+)}_{u', j', \omega' \omega} \varphi_{u', j'}^{(+)}.
\]

Here

\[
Q = \{(u', j') : u' \in \{o, t(e_1), \ldots, t(e_{n-1})\} \cup V(\omega), j' \in \{1, \ldots, m(\omega') - 1\}\}.
\]

Assume that \( \varphi_{\omega \omega}^{(+)} \) is contained in the linear combination. However, the values of the linear combination function on all arcs \( e \) with \( o(e) = o \) or \( t(e) = o \) come from only \( \varphi_{\omega \omega}^{(+)} \). Therefore any \( \varphi_{\omega' \omega}^{(+)} (j' \in \{1, \ldots, m(o) - 1\}) \) are not contained in the linear combination, that is, \( r_{\omega \omega}^{(+)} \)'s are 0. By taking the same argument recursively, we conclude that any \( \varphi_{\omega' \omega}^{(+)} \)'s with \( u' \in \{o, t(e_1), \ldots, t(e_{n-1})\}, j' \in \{1, \ldots, m(\omega') - 1\} \) are not contained in the linear combination (3.10). Thus

\[
\varphi_{\omega \omega}^{(+)} = \sum_{j' \neq j} r^{(+)}_{\omega \omega, j', \omega' \omega} \varphi_{\omega \omega, j'}^{(+)} + \sum_{u' \in V(\omega) \setminus \{ u \}, j' \in \{1, \ldots, m(\omega') - 1\}} r^{(+)}_{u', j', \omega' \omega} \varphi_{u', j'}^{(+)}.
\]

(5) For \( u = u' \), since \( T[1, \omega, \ldots, \omega^{m(\omega') - 1}] \) and \( T[1, \omega', \ldots, \omega^{m(\omega') - 1}] \) are orthogonal to each other \((j' \neq j)\) with respect to \( \mathbb{C}^{m(\omega')-1} \)-inner product, then \( \varphi_{\omega \omega, j'}^{(+)} \) and \( \varphi_{\omega \omega, j'}^{(+)} \) are linearly independent. Therefore \( r_{\omega \omega, j'} \)'s with \( j' \in \{1, \ldots, m(u) - 1\} \setminus \{j\} \) are 0 which implies the contradiction to the statement of (3).

Then we have shown the linear independence of \( \{ \varphi_{\omega \omega, j'}^{(+)} : u \in V, j \in \{1, \ldots, m(u) - 1\}\} \).

Next we show if \( k_0 \geq 2 \), then \( \varphi := \varphi_{\omega \omega}^{(\omega)} \in \mathcal{A} \). Let \( \partial A^{(\omega)}_{\omega} \) be the set of \( n \)-th depth of arcs in \( T^{(\omega)} \), that is,

\[
\partial A^{(\omega)}_{\omega} = \{ e \in A^{(\omega)} : \text{dist}(u, o(e)) = n, \text{ dist}(u, t(e)) = n + 1 \}.
\]

We have

\[
|| \varphi \|_{\partial A^{(\omega)}_{\omega}}^2 = 2/m(u) \leq 2/k_0 \quad \text{and}
\]

\[
|| \varphi \|_{\partial A^{(\omega)}}^2 = 2 \times \sum_{k=0}^{m(u)-1} \frac{1}{m^2(u)m^2(t(e_k^{(\omega)}))} \leq 2/k_0^3.
\]

Here for any subset \( A' \subseteq A \) and \( \psi \in \mathcal{A} \), \( \psi_{A'} \) denotes
We set \((u, \bar{v}_1^{(w)}, \ldots, \bar{v}_h^{(w)}, w)\) as the shortest path between \(u\) and \(w\) for \(w \in A^{(w)}\). Now we show that \(\| \varphi |_{\partial A^{(w)}} \|^2 \leq \frac{2}{k^0} \) by induction with respect to \(s\):

\[
\| \varphi |_{\partial A^{(w)}_s} \|^2 = \sum_{x \in \partial A^{(w)}_s} \prod_{i=1}^{s+1} \frac{1}{m^2(u)m^2(v_i)}
\]

\[
= \sum_{y \in \partial A^{(w)}_s} \prod_{i=1}^{s} \frac{1}{m^2(u)m^2(v_i)}
\]

\[
\leq \frac{1}{k^0} \sum_{y \in \partial A^{(w)}_s} \prod_{i=1}^{s} \frac{1}{m^2(u)m^2(v_i)} = \frac{1}{k^0} \| \varphi |_{\partial A^{(w)}_s} \|^2 \leq \frac{1}{k^0} \times \frac{2}{k^0 + 2}.
\]

Then we have

\[
\| \varphi \|^2 \leq \sum_{s=0}^{\infty} \frac{2}{k^0 + 2} = \frac{2}{k^0(k^0 - 1)} < \infty. \tag{3.11}
\]

Finally, under the assumption that \(T\) is the \(\kappa\)-regular tree, we prove the orthogonality. We put \(\varphi^{(\epsilon)}_{u,w} := \varphi\) and \(\varphi^{(\epsilon)}_{u',w'} := \varphi'\). Remark that

\[
\langle \varphi^{(\epsilon)}_{u,w}, \varphi^{(\epsilon)}_{u',w'} \rangle = \langle \varphi, \varphi' \rangle.
\]

Since the orthogonality of \(\epsilon \neq \epsilon'\) case has been already shown, so we consider \(\epsilon = \epsilon'\) case. We should remark that for any \(e \in \partial A^{(w)}\) there uniquely exists \(k \in \{0, \ldots, m(u) - 1\}\) such that

\[
\phi(e) = \frac{\omega_j^k}{m(u)(\kappa - 1)^{m+\alpha}}. \tag{3.12}
\]

By (3.12), then if \(u \neq u'\),

\[
\sum_{e \in \partial A^{(w)}_{u'}} \phi'(e) \overline{\phi(e)} = \frac{\omega_j^{-k}}{m(u)(\kappa - 1)^{m+\alpha}} \sum_{e \in \partial A^{(w)}_{u'}} \phi'(e) = 0. \tag{3.13}
\]

Here the fact \(\sum_{k=0}^{m(u) - 1} \omega_j^k = 0\) leads the second equality. If \(u = u'\) case, we have

\[
\sum_{e \in \partial A^{(w)}_{u'}} \phi'(e) \overline{\phi(e)} = \left( \frac{1}{\kappa - 1} \right)^{2m(u')} \sum_{k=0}^{m(u')} \frac{\omega_j^k \omega_j^k}{m^2(u')} = \frac{\delta_{j,j}}{m(u')} \left( \frac{1}{\kappa - 1} \right)^{2m(u')} \cdot \tag{3.14}
\]

Therefore (3.13) and (3.14) imply if \(j \neq j'\), then

\[
\sum_{e \in \partial A^{(w)}_{u'}} \phi'(e) \overline{\phi(e)} = \sum_{e \in \partial A^{(w)}_{u'}} \overline{\phi(e)} \phi'(e) = 0, \quad (n' \geq 0). \tag{3.15}
\]
The second equality derives from (3.8). Then if \( \phi \neq \varphi' \), we have
\[
\langle \phi, \varphi' \rangle = \sum_{n'=0}^{\infty} \sum_{e \in \partial A_{(\varphi')}} \left( \phi(e) \varphi'(e) + \bar{\phi}(\bar{e}) \varphi'(\bar{e}) \right) = 0. \tag{3.16}
\]

On the other hand, if \( \phi = \varphi' \), that is, \( \varphi_{u,j}^{(\pm)} = \varphi_{u',j'}^{(\pm)} \) then from (3.14),
\[
\|\varphi'\|^2 = \sum_{n'=0}^{\infty} \sum_{e \in \partial A_{(\varphi')}} \left( \frac{1}{m(u')} \left( \frac{1}{\kappa - 1} \right)^{2n'} \right) = \frac{2(\kappa - 1)}{m(u')(\kappa - 2)}. \tag{3.17}
\]

This completes the proof. \( \square \)

We set the following subspace of \( A \) spanned by \( \varphi_{u,j}^{(\pm)} \) as
\[
\mathcal{F}^{(\pm)} = \text{span} \left\{ \varphi_{u,j}^{(\pm)} : u \in V, j \in \{1, \ldots , m(u) - 1\} \right\}, \tag{3.18}
\]
which is the finite span of \( \{ \varphi_{u,j}^{(\pm)} \} 's \), that is,
\[
\mathcal{F}^{(\pm)} = \left\{ \sum_{u \in V'} \sum_{j=1}^{m(u) - 1} c_{u,j} \varphi_{u,j}^{(\pm)} : c_{u,j} \in \mathbb{C}, |V'| < \infty \right\}.
\]

By lemma 1, \( \{ \varphi_{u,j}^{(\pm)}/\sqrt{c_{0}} : u \in V, j \in \{1, \ldots , m(u) - 1\} \} \) is a complete system of \( \mathcal{F}^{(\pm)} \).
In particular, if \( T \) is a \( \kappa \)-regular tree with \( \kappa \geq 3 \), then it becomes a complete orthogonal normalized system. Here for \( K \subset A \), \( \overline{K} \) is the closed linear span of \( K \) such that \( \{ \psi \in A : \forall \epsilon > 0, \exists \varphi \in K \text{ s.t., } \| \psi - \varphi \| < \epsilon \} \),
where \( \| \cdot \| \) is the \( \ell^2 \)-norm.

**Lemma 2.**
\[
\ker(d_T) \cap \mathcal{H}^{(\pm)} = \ker(d_O) \cap \mathcal{H}^{(\pm)} \tag{3.19}
\]

and
\[
\mathcal{L}^\perp = \left( \ker(d_O) \cap \mathcal{H}^{(+)\perp} \right) \oplus \left( \ker(d_O) \cap \mathcal{H}^{(-)} \right). \tag{3.20}
\]

Under this decomposition we have
\[
U|_{\mathcal{L}^\perp} = -1 \oplus 1. \tag{3.21}
\]

**Proof.** For any \( \psi \in \mathcal{H}^{(\pm)} \), we have \( d_O \psi = d_T S \psi = \pm d_T \psi \), which implies \( \ker(d_T) \cap \mathcal{H}^{(\pm)} = \ker(d_O) \cap \mathcal{H}^{(\pm)} \). Since \( \mathcal{L}^\perp = \ker(d_T) \cap \ker(d_O) \) and \( \mathcal{H}^{(+)\perp} \oplus \mathcal{H}^{(-)} = A \),
\[
\mathcal{L}^\perp = \left( \ker(d_T) \cap \ker(d_O) \cap \mathcal{H}^{(+)\perp} \right) \oplus \left( \ker(d_O) \cap \ker(d_T) \cap \mathcal{H}^{(-)} \right) = \left( \ker(d_O) \cap \mathcal{H}^{(+)\perp} \right) \oplus \left( \ker(d_O) \cap \mathcal{H}^{(-)} \right),
\]

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which follows from (3.19). For any $\psi \in \ker d_T$, it holds that $U\psi = SC\psi - S\psi$. Then we immediately obtain (3.21).

It follows from lemma 1 that $F^+$ and $F^-$ are orthogonal.

**Theorem 1.** Assume $\mathbb{T}$ is a tree with minimum degree $\kappa_0 + 1 \geq 3$. Then $\{\pm 1\} \subset \sigma(U|_{\mathcal{L}^-})$, which are eigenvalues. Moreover, the birth eigenspace $\mathcal{L}^\perp$ is the infinite dimensional subspace of $\ell^2(A)$ which can be expressed as

$$\mathcal{L}^\perp = F^+ \oplus F^-.$$  

(3.22)

Here $F^\pm$ is (3.18).

**Remark 2.** If $\mathbb{T} = \mathbb{Z}$, then $\mathcal{L}^\perp = \emptyset$.

**Proof.** It is sufficient to show that $F^+ = \ker(d_o) \cap \mathcal{H}^-$ and $F^- = \ker(d_o) \cap \mathcal{H}^+$. By definition of $F^\pm$, it is obvious that

$$F^\pm \subset \ker(d_o) \cap \mathcal{H}^\mp.$$  

Since $\mathcal{H}^\pm$ and $\ker d_o$ are closed sets, we have $F^\pm \subset \ker(d_o) \cap \mathcal{H}^\mp$.

Now we will show $F^+ \subset \ker(d_o) \cap \mathcal{H}^+$. We define a subtree $\mathbb{T}_\psi = (V_\psi, A_\psi)$ induced by $\psi \in \ker(d_o) \cap \mathcal{H}^+$ as

$$V_\psi = \{o(e) \in V : e \in \text{supp}(\psi)\}, \quad A_\psi = \text{supp}(\psi),$$  

where $\text{supp}(\psi) = \{e \in A : \psi(e) \neq 0\}$ for $\psi \in A$. Since $\psi \in \ker(d_o)$, for any $e \in \text{supp}(\psi)$, we have $\deg(o(e)) > 2$, which means that $\mathbb{T}_\psi$ is decomposed into disjoint infinite connected subtrees which have no leaves. Then $\psi$ can be decomposed into $\psi = \psi_1 \oplus \psi_2 \oplus \cdots$. Here $\text{supp}(\psi_i) \cap \text{supp}(\psi_j) = \emptyset$ ($i \neq j$), and for any $e \in \text{supp}(\psi_i)$, there exists at least one arc $e' \in \text{supp}(\psi_i) \setminus \{e\}$ such that $\tau(e) = o(e')$.

From now on, we assume $\psi \in \ker(d_o) \cap \mathcal{H}^+$ so that $\mathbb{T}_\psi$ is connected. We put $o_\psi \in V_\psi$ as the most closest vertex from the origin vertex $o$. We define $e^{(a)}_k$ ($k = 0, \ldots, m(u) - 1$) by $o(e^{(a)}_k) = u$ with $\tau(o(e^{(a)}_k)) \leq \tau(o(e^{(a)}_{k-1}))$, where $m(u)$ is defined by (3.6): in other words, they are arcs from $u$ to its children. For every $u \in V_\psi \setminus \{o_\psi\}$, we also define $e^{(a)}_k \in A_\psi$ by the arc such that $o(e^{(a)}_k) = u$ with $\tau(o(e^{(a)}_k)) > \tau(o(e^{(a)}_{k-1}))$: in other words, it is the one from $u$ to its parent. For each $u \in V_\psi$, we set subspaces $A_u, V_u$ and $W_u$ by

$$A_u = \{\phi \in A : o(e) \neq u \Rightarrow \phi(e) = 0\},$$

$$V_u = \begin{cases} 0 & : u = o_\psi, \\ \{\phi \in A_u : \phi(e^{(a)}_0) = \cdots = \phi(e^{(a)}_{m(u)-1}) = -\phi(e^{(a)}_{m(u)})/m(u)\} & : u \neq o_\psi, \end{cases}$$

$$W_u = \begin{cases} \{\phi \in A_u : \sum_{k=0}^{m(u)-1} \phi(e^{(a)}_k) = 0\} & : u = o_\psi, \\ \{\phi \in A_u : \phi(e^{(a)}_0) = \sum_{k=0}^{m(u)-1} \phi(e^{(a)}_k) = 0\} & : u \neq o_\psi, \end{cases}$$
where $\emptyset$ is the set whose element is only 0-constant function.

**Remark 3.** Put $\mathcal{X}_a = \{ \phi \in A : \phi(e_u(0)) = \phi(e_u(1)) = \cdots = \phi(e_u(m_u-1)) \}$. Then by definition, $A_a = V_a \oplus W_a \oplus \mathcal{X}_a$.

Moreover, for any $\phi \in V_a \oplus W_a$, we have $\sum_{e \in V} \phi(e) = 0$ which means $\phi \in \ker(d_0)$ while for any $\phi' \in \mathcal{X}_a$, it is obvious that $\phi' \in \ker(d_0)^\perp$.

Consider $T^{(a)} = (V^{(a)}, A^{(a)})$, which is the subtree of $T$ with the root $o_a$. Then $T_{\psi}$ is a subtree of it. Moreover, we set $V_i = \{ v \in V^{(a)} : \text{dist}(o_a, v) = i \text{ in } T^{(a)} \}$ and $A_i = \{ e \in A^{(a)} : o(e) \in V_i \text{ and } t(e) \in V_{i+1} \}$ for $i = 0, 1, 2, \ldots$. Naturally $V_0 = \{ o_a \}$ and $A_0 = \{ e \in A_{o_a} : o(e) = o_a, t(e) \in V_1 \}$.

Since $\ker(d_0) \cap A_a = V_{a} \oplus W_{a}$ from the above remark, we have

$$
\psi|_{A_a} = f_a \oplus g_a,
$$

where $f_a \in V_a$ and $g_a \in W_a$. Here $\psi|_{A_a}$ is the projection of $\psi$ onto $A_a$, that is,

$$
\psi|_{A_a}(a) = \begin{cases}
\psi(a) : o(a) = u_a, \\
0 : \text{otherwise. (}u \in V) 
\end{cases}
$$

Let us construct a sequence $\{ \phi_a \}$ for approximating $\psi \in \ker(d_0) \cap A_a$.

For $u = o_{a}$, we have $\psi|_{A_{o_a}} = g_{o_a}$. Thus there exists a unique system of complex coefficients $\{ C_{o_a} \}$ such that

$$
g_{o_a} = \sum_{j=1}^{m(o_a)-1} C_{o_a,j} \cdot \varphi_{o_a,j}^{(\pm)}|_{A_{o_a}};
$$

we set

$$
\phi_0 = \sum_{j=1}^{m(o_a)-1} C_{o_a,j} \cdot \varphi_{o_a,j}^{(\pm)}.
$$

We should remark that $\psi(e) = \phi_0(e)$ for every $e \in A \setminus \bigcup_{j=1}^{\infty} (A_j \cup \bar{A}_j)$. Here $E = \{ e \mid \bar{e} \in E \}$ for the set of arcs $E$. Moreover, if there exists an arc $e_0 \in A_0$ such that $\psi(e_0) = 0$, then $\phi(e) = 0$ for every arc $e$ in $T^{(a)}$, since $T_{\psi}$ is assumed to be connected. On the other hand, we can easily check $\phi_0(e) = 0$ for every arc $e$ in $T^{(a)}$ by our construction in definition 2. We have $\psi = \phi_0$ in $T^{(a)}$.

Next we focus on $V_1$ and $A_1$. From our observation stated above, we only have to treat $V_1 \cap \{ t(e) : \psi(e) \neq 0 \}$ on $A_0$. It follows from remark 2 that, for $u = t(e) \in V_1$ such that $e \in A_0$,

$$
\psi|_{A_e} = f_a \oplus g_a;
$$

we can set $f_a = \phi_0|_{A_e}$, since $f_a$ is the unique function in $V_a \oplus W_a$ such that $f_a(e) \neq o_a$. Obviously it holds that $\sum_{e \in A_0} \psi(e) = \sum_{e \in A_0} \phi_0(e)$. We remark again that we assume $\psi(e) \neq 0$ for $e \in A_0$ and $t(e) = u$ here. Then there exists a unique system of complex coefficients $\{ C_{u,e} \}$ such that

\[ \text{...} \]
we set

$$\phi_1 = \phi_0 + \sum_{e \in V_1 \cap \{t(e) : \psi(e) \neq 0 \text{ for } e \in A_0\}} \sum_{j=1}^{m(u)-1} c_{uj} \cdot \varphi^{(\pm)}_{ujj}.$$  

Recursively we can set, for any $n = 1, 2, \ldots$,

$$\phi_n = \phi_{n-1} + \sum_{e \in V_n \cap \{t(e) : \psi(e) \neq 0 \text{ for } e \in A_{n-1}\}} \sum_{j=1}^{m(u)-1} c_{uj} \cdot \varphi^{(\pm)}_{ujj}$$

as in the same fashion stated above. It is easy to see that $\psi(e) = \phi_u(e), e \in A \setminus \cup_{i=n+1}^{\infty} (A_i \cup \bar{A}_i)$ and that $\phi_u(e) \in F(+) \forall n = 1, 2, \ldots$

Now let us show $\psi \in F(+)$. Let $\psi_m = \psi|_{\cup_{i=n+1}^{\infty} (A_i \cup \bar{A}_i)}$ and $\phi_m = \phi_m|_{\cup_{i=n+1}^{\infty} (A_i \cup \bar{A}_i)}$. Since $\psi \in A = t^2(A)$ by the assumption, for any $\epsilon > 0$, there exists $k$, such that

$$\|\psi_k\|^2 < \epsilon.$$  

On the other hand, it holds that

$$\|\psi_k\|^2 = 2(\|\psi_k\|^2 + \|\phi_k\|^2) \leq 2(\epsilon + \sum_{e \in A_k} \frac{|\psi(e)|^2}{m^2(t(e))} \|\varphi^{(\pm)}_{e\pm}\|^2)$$

$$\leq 2\epsilon \left(1 + \frac{2\epsilon_0}{n_0}\right).$$

Then we have $\psi \in F(+)$. When $T_\psi$ is a union of disjoint infinite subtrees, we take a linear combination of the above $\psi$’s and take a similar estimation. Then we have $\psi \in F(+)$. Now we arrive at $\ker(d_0) \cap H^{- \epsilon} \subset F(+)$. In a similar way, we obtain $\ker(d_0) \cap H^{(\epsilon)} \subset F(-)$. \hfill \Box

We close this section to illustrate examples. The first one recovers some previous results in [5]. We define $\tilde{\nu}(J) : V(T_\infty) \to [0, 1] \{J \in \{A, B\}\}$ by

$$\tilde{\nu}(J)(u) := \lim_{I \to \infty} \frac{1}{I} \sum_{n=0}^{I-1} \left\{ \sum_{e(t(e)) = u} \left| (U^e \psi_0(J))(e)\right|^2 \right\}.$$  

**Corollary 1.** If $\sigma(T) = \sigma_c(T)$, then

$$\tilde{\nu}(J)(u) = \sum_{e(t(e)) = u} \left| (\Pi_{F^+} \psi_0(J))(e)\right|^2.$$  

(3.27)
In particular, if $T$ is $\kappa$-regular, for the following initial states introduced by [5]

\[
\langle \psi_0^{(A)}(e) \rangle = \begin{cases} 1 & : e = e_k, (k = 0, \ldots, \kappa - 1), \\ 0 & : \text{otherwise}, \end{cases}
\]

\[
\langle \psi_0^{(B)}(e) \rangle = \begin{cases} e^{2\pi i e/k} & : e = e_k, (k = 0, \ldots, \kappa - 1), \\ 0 & : \text{otherwise}, \end{cases}
\] (3.28)

we have

\[
\tilde{\mu}^{(J)}(u) = \begin{cases} 0 & : J = A, \\ \left(\frac{\kappa - 2}{k - 1}\right)^{\delta_{\text{out}}(a) + 1 - \delta_{\text{in}}(a)} & : J = B, \end{cases}
\]

which agrees with the previous result on [5]. The essential difference between initial states $\psi_0^{(A)}$ and $\psi_0^{(B)}$ is that $\psi_0^{(A)} \in \mathcal{F}^1_k$ while $\psi_0^{(B)} \notin \mathcal{F}^1_k$.

Let us give another type of example, in which we show the spectrum $\sigma(U)$ of $U$ consists of only eigenvalues for a special class of trees. In other words, only localization of the Grover walk occurs on such trees. As is seen in section 2, if $T$ is the $\kappa$-regular tree, $\sigma(U)$ can be expressed as

\[
\sigma(U) = J^{-1}(\sigma(T)) \cup \{\pm 1\},
\]

where $\sigma(T) = \sigma_c(T) = [-2\sqrt{\kappa - 1}/\kappa, 2\sqrt{\kappa - 1}/\kappa], J(z) = (z + z^{-1})/2$ and each of eigenvalues $\pm 1$ has infinite multiplicity. It is obvious to see $\sigma_c(U) = J^{-1}(\sigma(T)) \neq \emptyset$.

Now we put, for the root $o$ of a tree $T$,

\[
K(r) = \inf\{\deg(x) ; x \in \mathcal{V}(T), \text{dist}(o, x) \geq r\}.
\]

Obviously $\lim_{r \to \infty} K(r) = \kappa < \infty$ for the $\kappa$-regular tree. On the other hand, if $T$ is a tree with $\lim_{r \to \infty} K(r) = \infty$, then it is called rapidly branching. For the discrete Laplacian, equivalently, the transition operator $T$ for isotropic random walks, it is shown in [9] that any rapidly branching tree has no continuous spectrum:

**Theorem 2 ([9]).** Let $T$ be a rapidly branching tree. Then the continuous spectrum $\sigma_c(T) = \emptyset$, the essential one of $\sigma(T)$ coincides $\{0\}$ and every $\lambda \in \sigma(T) \setminus \{0\}$ is an eigenvalue with finite multiplicity. Moreover, if 0 is an eigenvalue, then it has infinite multiplicity.

For a kind of family of trees, it can be decided whether 0 is an eigenvalue or not. For details, refer to [9]. Combining the theorem above, the spectral mapping theorem with $J(z)$ and theorem 1, we can easily obtain the following:

**Corollary 2.** Let $T$ be a rapidly branching tree. Then $\sigma(U)$ consists of only eigenvalues and their accumulating points. In addition, if $\lambda \in \sigma(U) \setminus \{\pm 1\}$, then it is an eigenvalue of finite multiplicity; if $\lambda = \pm 1$, then it is an eigenvalue of infinite multiplicity; if $\lambda = \pm i$, then it is the accumulating point of eigenvalues or an eigenvalues of infinite multiplicity.

4. **An approximation of the Grover walk on $T$**

In this section, we consider a QW induced by a random walk with the Dirichlet boundary condition. Almost all topics in this paper are discussed on trees, but the concept of this QW is defined not only for a tree but for a general graph. Thus we firstly, in section 4.1, construct such a QW on a general graph, which applied to a quantum search algorithm with some
marked elements on it [2, 24, 25]. After that, in section 4.2, we return to the case where a graph is a tree and a QW is the Grover walk on T. This observation gives some information on the structure of the birth eigenspace discussed in theorem 1.

4.1. QW induced by Dirichlet random walk on graphs

Let $G' = (V', A')$ be a connected graph, and $M \subset V'$ be the set of marked elements. The total Hilbert space of this QW is $A' = L^2(A')$ and we set $V'$ by $L^2(V')$. We assign a weight to each arc $\alpha : A' \to \mathbb{C}$ so that $\sum_{v \in \alpha(a) = v} |\alpha(a)|^2 = 1$ for all $v \in V'$. Define $d_{T,M}, d_{O,M} : A' \to V'$ by

$$(d_{T,M}\psi)(v) = \begin{cases} \sum_{t(e) = v} \alpha(e)\psi(e) & : v \in M^c, \\ 0 & : v \in M. \end{cases}$$

$$(d_{O,M}\psi)(v) = \begin{cases} \sum_{t(e) = v} \alpha(e)\psi(e) & : v \in M^c, \\ 0 & : v \in M. \end{cases}$$

We define $A_M^{(+)} \subset A'$ by $\{ e \in A' : t(e) \in M^c \}$ and $A_M^{(-)} \subset A'$ by $\{ e \in A' : o(e) \in M^c \}$. The adjoint operators are

$$(d_{T,M}^* f)(e) = \begin{cases} \overline{\alpha(e)}f(t(e)) & : e \in A_M^{(+)}; \\ 0 & : e \notin A_M^{(+)}. \end{cases}$$

$$(d_{O,M}^* f)(e) = \begin{cases} \overline{\alpha(e)}f(o(e)) & : e \in A_M^{(-)}; \\ 0 & : e \notin A_M^{(-)}. \end{cases}$$

We have the following lemma.

**Lemma 3.**

1. $d_{T,M}S' = d_{O,M}$, where $(S'\psi)(e) = \psi(\bar{e})$;

2. $d_{T,M}^* d_{T,M} = d_{O,M}^* d_{O,M} = \Pi_{\mathcal{V}_M}$, where $\mathcal{V}_M = \{ f \in V' : v \in M \Rightarrow f(v) = 0 \}$. Here $\Pi_{\mathcal{K}}$ is the projection operator onto $\mathcal{K} \subset V'$;

3. $d_{T,M}^* d_{O,M} = d_{O,M}^* d_{T,M}$ is a self-adjoint operator $T_M$ such that

$$\langle \delta_u, T_M^* \delta_v \rangle = \begin{cases} \sum_{e \in \alpha(a) = u, t(e) = v} \overline{\alpha(e)}\alpha(e) & : u, v \in M^c, \\ 0 & : \text{otherwise}, \end{cases}$$

that is, $T_M$ is the cut off of the self-adjoint operator of $T'$ at the target vertices $M$:

$$T_M = \Pi_{\mathcal{V}_M} \Pi_{\mathcal{V}_M}' T' \Pi_{\mathcal{V}_M}$$

where $T'$ is

$$\langle \delta_u, T' \delta_v \rangle = \sum_{e \in \alpha(a) = u} \overline{\alpha(e)}\alpha(e);$$

4. $\sigma(T_M) \subset (-1, 1)$.

**Definition 3.** Let $U' : A' \to A'$ be the time evolution of the QW induced by $T_M'$:

$$U' = S' C_M',$$  

where $C_M = 2d_{T,M}^* d_{T,M} - 1_{A'}$. 


Put \( U' = S' C' \) by the time evolution of the QW with \( M = \emptyset \). Then

\[
\langle \delta_f, U' \delta_e \rangle = \mathbf{1}_{\{t(e) = o(f)\}} \left( \frac{2 \alpha(t)}{\alpha(e) - \delta_e} \right).
\]

We have

\[
\langle \delta_f, U' \delta_e \rangle = \begin{cases} 
\langle \delta_f, U' \delta_e \rangle : t(e) \notin M, \\
-\delta_e : t(e) \in M.
\end{cases}
\]

**Lemma 4.** It holds that

\[
d_{M}^T(V') \cap d_{0,M}^V(V') = 0.
\] (4.30)

**Proof.** Assume that \( \psi \in d_{M}^T(V') \cap d_{0,M}^V(V') \neq 0 \). For any \( \psi \in d_{M}^T(V') \cap d_{0,M}^V(V') \), there exists \( f \in V' \) such that \( d_{M}^T(V') = \gamma d_{0,M}^V(V') \) which implies \( \gamma = \pm 1 \) since \( d_{M}^T(V') \) should be an eigenfunction of \( S \). Taking operation \( d_{M}^T \) to both sides, we have \( f = \pm f' \). However \( \sigma(T'_M) \subset (-1, 1) \) holds because \( T'_M \) is a cut-off operator of \( T' \). Thus \( \psi \in d_{M}^T(V') \cap d_{0,M}^V(V') = 0 \).

We introduce new boundary operators as follows.

**Definition 4.** We define \( d_{\pm,M} : \mathcal{A'} \rightarrow V' \) and its adjoint operator \( d_{\pm,M}^* : V' \rightarrow \mathcal{A'} \) by

\[
d_{M}^\pm = \frac{1}{\sqrt{2(1 - T'_M)}} \left( d_{M}^T - \frac{1}{\alpha(t)} \right),
\] (4.31)

\[
d_{M}^* = \left( d_{M}^T - d_{0,M}^V \right) \frac{1}{\sqrt{2(1 - T'_M)}}.
\] (4.32)

For \( f' \in \ker(\nu - T'_M) \), we have

\[
\langle d_{M}^\pm f', \psi \rangle = \frac{1}{\sqrt{2(1 - \nu^2)}} \left\{ \alpha(t) f'(t(e)) - \sqrt{1 - \nu^2} \alpha(t) f'(o(e)) \right\}.
\] (4.33)

We can easily check that

**Lemma 5.**

1. \( \|d_{M}^\pm f\| = \|f\| \)
2. Let \( \mathcal{L}_M \subset \mathcal{A'} \) denote \( d_{M}^T(V') + d_{0,M}^V(V') \). Then \( \mathcal{L}_M = d_{+M}(V') \oplus d_{-M}(V') \).

**Theorem 3.** It holds that

\[
\sigma(U'_M |_{\mathcal{L}_M}) = J^{-1}(\sigma(T'_M)).
\] (4.34)

Moreover the generator of \( U'_M |_{\mathcal{L}_M} \) can be expressed by

\[
d_{+M}(\arccos T'_M) d_{+M}^* \oplus d_{-M}(\arccos T'_M) d_{-M}^*.
\]

that is,

\[
U'_M |_{\mathcal{L}_M} = d_{+M} e^{i \arccos T'_M} d_{+M}^* \oplus d_{-M} e^{-i \arccos T'_M} d_{-M}^*.
\] (4.35)
Proof. By lemma 5, for any $\psi \in L^M$, $\psi = d^+_M d^+_M \psi \oplus d^-_M d^-_M \psi$ holds. We can easily check that
\begin{equation}
U d^+_M = d^+_M e^{i \arccos(T)},
\end{equation}
\begin{equation}
U d^-_M = d^-_M e^{-i \arccos(T)}.
\end{equation}
Then we have
\begin{equation}
U \psi = U (d^+_M d^+_M + d^-_M d^-_M) \psi
\end{equation}
\begin{equation}
= \left( d^+_M e^{i \arccos(T') M} d^+_M + d^-_M e^{-i \arccos(T') M} d^-_M \right) \psi.
\end{equation}
\hfill $\square$

4.2. Tree case

Let $T = (V, A)$ be an infinite tree, and induced Hilbert spaces are $A$ and $V$. Let $V_n \subset V$ be all the vertices within the $n$-th depth that is,
\begin{equation}
V_n = \{ v \in V : \text{dist}(o, v) \leq n \}.
\end{equation}
Put $A_n$ and $A_n^{(\pm)} \subset L^2(A)$ as
\begin{equation}
A_n = \text{span}\{ \delta_e : e \in A_n \},
A_n^{(\pm)} = \text{span}\{ \delta_e : e \in A, t(e) \in V_n \},
A_n^{(-)} = \text{span}\{ \delta_e : e \in A, o(e) \in V_n \}
\end{equation}
and $V_n \subset L^2(V)$ by
\begin{equation}
V_n = \text{span}\{ \delta_v : v \in V_n \}.
\end{equation}
We set the marked vertices $M$ by $V_n^c$. Define $d^{(n)}_T := d^{(n)}_{T, M}, d^{(n)}_O := d_{O, M}$ by
\begin{equation}
d^{(n)}_T = \Pi_{V_n} d_T, d^{(n)}_O = \Pi_{V_n} d_O.
\end{equation}
These adjoint operators are $d^{(n), *}_T = d^{(n)}_T \Pi_{V_n}$ and $d^{(n), *}_O = d^{(n)}_O \Pi_{V_n}$. The cut-off self-adjoint operator $T$ under the Dirichlet boundary condition outside of the $n$-th depth is denoted by $T_n$ and defined as
\begin{equation}
T_n = \Pi_{V_n} T \Pi_{V_n}.
\end{equation}
In this setting, we can observe the following properties on restricted boundary operators $d_T$ and $d_O$ and their adjoints.

Remark 4.
\begin{enumerate}
\item $d^{(n)}_T = \Pi_{V_n} d_T = d^{(n)}_T \Pi_{A^{(\pm)}_n}$, $d^{(n)}_O = \Pi_{V_n} d_O = d^{(n)}_O \Pi_{A^{(-)}_n}$
\end{enumerate}
or equivalently, $d^{(n), *}_T = d^{(n)}_T \Pi_{V_n}$ and $d^{(n), *}_O = d^{(n)}_O \Pi_{V_n} = \Pi_{A^{(-)}_n} d^{(n), *}_O$.
\begin{enumerate}
\item $T_n = d^{(n)}_T d^{(n), *}_T = d^{(n)}_O d^{(n), *}_O$.
\end{enumerate}
We define a unitary operator on $L^2(A)$ induced by $T_n$ as follows.
Definition 5. For given $n \in \mathbb{N}$, we define

$$U^{(n)} = S(2d_T^{(n)}d_T^{(n)*} - I_A).$$ \hfill (4.40)

We call the cut-off QW for this $U^{(n)}$ with the standard measurement $\mu$. Remark that

$$\langle \delta_f, U^{(n)} \delta_e \rangle = \begin{cases} \langle \delta_f, U^{(n)} \delta_e \rangle : t(e) \in V_n, \\ -\delta_f \delta_e : \text{otherwise.} \end{cases}$$ \hfill (4.41)

The following properties of $U^{(n)}$ can be easily seen.

Remark 5.\hfill (1)

$U^{(n)}$ is a unitary operator on $A = \ell^2(A)$.

$\Pi_{A_n+1} U^{(n)} = U^{(n)} \Pi_{A_n+1}$.

The cut-off QW $U^{(n)}$ is an approximation of $U$ in the following mean.

Proposition 2. For every $\psi \in \ell^2(A)$, we have

$$\lim_{n \to \infty} \|U\psi - U^{(n)}\psi\|_{\ell^2(A)}^2 = 0.$$ \hfill (4.42)

Proof. By (4.41), putting $U\psi = \phi$ and $U^{(n)}\psi = \phi_n$,

$$\|\phi - \phi_n\|^2 = \sum_{e \in A} |(U\psi)(e) - (U^{(n)}\psi)(e)|^2,$$

$$= \sum_{e \in \delta(e) \in V_n} |(U\psi)(e) - (-S\psi)(e)|^2.$$ \hfill (4.43)

Since $U = 2d_T^*d_T - S$,

$$\|\phi - \phi_n\|^2 / 4 = \|1_A - \Pi_{A_n+1} d_T^*d_T\psi\|_{A_n+1}^2.$$ \hfill (4.44)

By remark 4,

$$\|d_T^*d_T\psi\|^2 = \langle d_T^*d_T\psi, d_T^*d_T\psi \rangle = \langle d_T\psi, d_T\psi \rangle$$ \hfill (4.46)

$$= \|d_T\psi\|^2,$$ \hfill (4.47)

$$\|\Pi_{A_n+1} d_T^*d_T\psi\|^2 = \langle d_T^*d_T\psi, d_T^*d_T\psi \rangle = \langle d_T\psi, \Pi_{V_n}d_T\psi \rangle$$ \hfill (4.48)

$$= \|\Pi_{V_n}d_T\psi\|^2.$$ \hfill (4.49)

Combining (4.47) and (4.49) with (4.45), we have

$$\|\phi - \phi_n\|^2 / 4 = \|(1\psi - \Pi_{V_n})d_T\psi\|_{A_n+1}^2.$$ \hfill (4.44)

Therefore we have $\|U\psi - U^{(n)}\psi\| \to 0$, \hfill (n \to \infty).\hfill \Box$

The cut-off QW at the $n$-th depth satisfies that $U^{(n)}(A_{n+1}) = A_{n+1}$ and it is a unitary operator on $A_{n+1}$. From remark 5, we have
where \( A^\perp_n = \text{span}\{\delta_e : e \in A'_n\} \). The rhs of the second term means that \( U^{(n)} \) ‘freezes’ the dynamics at the outside of the \( n \)-th depth acting as a trivial reflection operator in the same edge, that is, \( (U^{(n)}|_{A^\perp_{n+1}}) \psi(e) = -\psi(e) \), for every \( e \in A'_n \). So we focus on the first term which gives a non-trivial dynamics of the walk from now on. From remark 5, we have \( U^{(n)} = U^{(n)}|_{A_{n+1}} \oplus U^{(n)}|_{A_n} \) with \( U^{(n)}|_{A_{n+1}} = -S|_{A_{n+1}} \). The second term which has a non-trivial structure, \( U^{(n)}|_{A_n} \), is decomposed as follows. Putting for \( \varphi_{u,j}^{(\pm)} \in \mathbb{C}^A \) in definition 2, which is not necessary to be \( \ell^2 \)-summable, \( \varphi_{u,j}^{(\pm)} := \Pi_{A_u} \varphi_{u,j}^{(\pm)} \):

\[
\mathcal{F}^{(\pm)}_n = \text{span}\left\{\varphi_{u,j}^{(\pm)} : (u,j) \in \bigcup_{v \in V_{n-1}} (\{v\} \times \{1, \ldots, m(v) - 1\})\right\}.
\]

**Theorem 4.** Assume that there are no leaves, \( \kappa_0 \geq 1 \), in \( T \). It holds that

\[
U^{(n)}|_{A_{n+1}} = U^{(n)}|_{\mathcal{L}_n} \oplus U^{(n)}|_{\mathcal{F}^{(\pm)}_n} \oplus U^{(n)}|_{\mathcal{F}^{(-)}_n}.
\]  

Here

\[
U^{(n)}|_{\mathcal{L}_n} = d^{(\pm)}_+ e^{-i \arccos T_n d^{(\pm)}_+} \oplus d^{(-)}_+ e^{-i \arccos T_n d^{(-)}_+}.
\]  

**Proof.** The proof of the inherited part has been already shown. So we will prove the birth part. The dimension of \( \mathcal{L}_n \) is \( \dim(\mathcal{L}_n) = 2|V_n| \) while the dimension of the total state space of \( A_{n+1} \) is \( \dim(A_{n+1}) = 2|E_{n+1}| = 2(|V_{n+1}| - 1) \) which implies

\[
\dim(\mathcal{L}^\perp_n \cap A_{n+1}) = 2(|V_{n+1}| - |V_n|) - 1.
\]

Therefore the remaining spaces \( \mathcal{L}^\perp_n \cap A_{n+1} \) exist. By the way,

\[
\dim(\mathcal{F}^{(\pm)}_n) = \dim(\mathcal{F}^{(\pm)}_n) = \left| \bigcup_{u \in V_n} \{u\} \times \{1, \ldots, m(u) - 1\} \right| = |E_{n+1}| - |V_n| = |V_{n+1}| - 1 - |V_n| = \frac{1}{2}\dim(\mathcal{L}^\perp_n \cap A_{n+1}).
\]

It holds that

\[
\mathcal{L}^\perp_n \cap A_{n+1} = \left( \ker(d^{(\pm)}_n) \cap \mathcal{H}^{(-)} \cap A_{n+1} \right) \oplus \left( \ker(d^{(\pm)}_n) \cap \mathcal{H}^{(+)} \cap A_{n+1} \right).
\]

Since \( \varphi_{u,j}^{(\pm)} \in \ker(d^{(\pm)}_n) \cap \mathcal{H}^{(\pm)} \cap A_{n+1} \) and \( \{\varphi_{u,j}^{(\pm)} : j \in V_{n-1}, j \in \{1, \ldots, m(u) - 1\}\} \) are orthogonal to each other, we obtain \( \mathcal{F}^{(\pm)}_n = \ker(d^{(\pm)}_n) \cap \mathcal{H}^{(\pm)} \cap A_{n+1} \).
Finally, we compute the density of the birth part. We set $B_n = |V_n|$, $\partial B_n = |V_{n+1}| - |V_n|$.

**Corollary 3.** Assume that there are no leaves in $\mathbb{T}$. Let $\rho_n(\pm)$ be the density of $\ker(\pm 1 - U(n))$, that is, $\rho_n(\pm) = \dim(\ker(\pm 1 - U(n))) / \dim(A_{n+1})$. Put $h_+ := \limsup_{n \to \infty} \partial B_n / B_n$ and $h_- := \liminf_{n \to \infty} \partial B_n / B_n$. If $h_- > 0$, then

$$0 < \frac{h_-}{2(1 + h_-)} = \liminf_{n \to \infty} \rho_n(\pm) \leq \limsup_{n \to \infty} \rho_n(\pm) = \frac{h_+}{2(1 + h_+)} \leq 1/2.$$  

In particular, if $\lim_{n \to \infty} \partial B_n / B_n =: h$ exists, then

$$\lim_{n \to \infty} \rho_n(\pm) = \frac{h}{2(1 + h)}.$$  

5. Summary and discussion

We have here determined the localization properties of a special type of quantum walk (QW), the Grover walk, on the tree, which is a general type of Bethe lattices. This localization is induced by the birth eigenspace of the Grover walk, which can be characterized by all of the finite energy flows. In this section, we first give the significant feature of this result by comparing with our previous results in [11–14]. In [11], the authors have shown that the QW can be expressed by the formulation as a dynamics among arcs through the quantum graph describing a dynamics of transmission and reflection of the plane wave on a metric graph at each vertex; this formulation helps us to discuss the nature of the birth eigenspace. In [12], the existence of the cycles ensures the localization on a general class of the integer lattices. On the other hand, it is shown in [13] that the derivation of the localization on some type of the integer lattices without cycles is also the eigenvalues of the the underlying isotropic random walk. Now let us focus on trees, which is the general class of graphs without cycles. We have already known that the Grover walk on a finite tree has no birth eigenspace [12]. Moreover, the authors in [14] have shown that the orthogonal complement of the inherited Hilbert space from the isotropic random walk on general connected graphs, which possibly may be infinite, is the birth eigenspace, and the spectrum of the birth eigenspace, if it exists, consists of eigenvalues. Thus we can naturally raise a question whether the localization of the Grover walk on an infinite tree occurs or not, equivalently whether it has eigenvalues or not. Since the infinite Bethe lattices have no cycles and the underlying isotropic random walk on these has no eigenvalues, it seems, at first glance, no localization on such an acyclic graph occurs. However, under an appropriate initial state, the localization of the Grover walk on Bethe lattices has been observed [5]. In this paper, concerning Bethe lattices, we have given the complete answer to the above question and visualize this birth eigenspace of the Grover walk using the finite energy flow, which is discussed on cycles in [14]. As a by-product of this, one of the useful ways to determine whether an infinite given graph provides the localization is to check that the graph has a cycle or the positivity of a kind of Cheeger constant in the sense of corollary 3.

We next explain the physical relevance comparing with some previous researches. In this paper, we have shown that the Grover walk on an infinite tree has the birth eigenspaces of infinite dimensions while that on a finite tree has no birth eigenspace. In addition, to understand this gap, we took a modification to the dynamics at the leaves of the finite tree of the original Grover walk; this walk is equivalent to a QW induced by the isotropic random walk with the Dirichlet boundary condition at the $n$-th revel set. Then we could naturally obtain the birth eigenspace generated by all the finite energy flows with the sinks at the leaves. This kind of
QW induced by the Dirichlet boundary condition has already appeared in the context of the quantum search algorithm, for example, [2, 20, 25]; the leaves correspond to the target vertices for our case. Philipp et al [19] address to a quantum search driven by a continuous-time QW on finite trees. They reduce the problem to a continuous-time QW on an appropriate quotient graph from a given tree and its target vertices. It is one of the interesting future problems to extend this idea to the discrete-time QWs. Dimcovic et al [6] study a kind of resolvent of a QW driven by a different kind of quantum coin from Grover’s coin on an infinite tree using a path counting method by the identification of the vertices in the same level set, which is similar to [5]. Since this problem is reduced to a QW on the semi-infinite one-dimensional lattice, the explicit expression for the resolvent can be obtained. Thus it becomes possible to numerically examine the efficiency of a ‘hitting time’ of a quantum walker at the origin starting from the n-th level set for large n and to see a kind of quantum speed-up comparing with a classical random walker. Here their identification is restricted to a special invariant subspace of the whole system of the QW, so a kind of localization effect on the hitting time controlled by the initial state seems to be observed. Though we restricted the quantum coin to Grover’s coin in this paper, we believe that, under an extension of the Grover coin so that a kind of spectral mapping theorem like theorem 3 is conserved, to study how the birth eigenspace behaves is also one of the interesting future problems in the context of the quantum search algorithm.

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