Localization of a multi-dimensional quantum walk with one defect

Toru Fuda [*], Daiju Funakawa [†] and Akito Suzuki [‡]

Abstract

In this paper, we introduce a multidimensional generalization of Kitagawa's split-step discrete-time quantum walk, study the spectrum of its evolution operator for the case of one defect coins, and prove localization of the walk. Using a spectral mapping theorem, we can reduce the spectral analysis of the evolution operator to that of a discrete Schrödinger operator with variable coefficients, which is analyzed using the Feshbach map.

Keywords: quantum walks, localization, eigenvalues, Feshbach map

1 Introduction

Quantum walks (QWs) have been introduced and studied in various contexts such as quantum probability [13], quantum optics [1], quantum cellular automata, [15, 28], and quantum information [2, 8] (see [4, 21, 24, 37] for more details). Among them, motivated by Grover's quantum search algorithms[14, 35, 10], researchers have proposed several types of discrete time QWs on graphs [38, 3, 22, 20, 25, 36]. Szegedy [32] introduced a bipartite walk, which is defined on a bipartite graph, to construct a quantum search algorithm. Magniez et al [29, 30] updated the notion of bipartite walks and Segawa [33] redefined an evolution operator U_G on the Hilbert space $\ell^2(D)$ of square summable functions on the set D of arcs for a digraphs $G = (V, D)$. The QW defined by U_G is now referred to as the Szgedy walk on G, which includes the Grover walk on G as a special case. The Szegedy walks have a spectral mapping property from the transition probability matrix P_G of a random walk on G to the evolution U_G, which gives a useful tool for analyzing the

[*]Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan,
E-mail: t-fuda@math.sci.hokudai.ac.jp

[†]Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan,
E-mail: funakawa@math.sci.hokudai.ac.jp

[‡]Division of Mathematics and Physics, Faculty of Engineering, Shinshu University, Wakasato, Nagano 380-8553, Japan, E-mail: akito@shinshu-u.ac.jp

spectrum of U_G (see [33, 27, 17] for more details). An extended version of the Szegedy walk, the twisted Szegedy walk, was introduced by Higuchi et al [16] to study the spectral and asymptotic properties of the Grover walks on crystal lattices. Higuchi, Segawa, and one of the authors of this paper [18] proved the spectral mapping theorem (SMT) for more general evolution $U = SC$, where S and C are unitary and self-adjoint on a Hilbert space $\mathcal{H}$ and where C is assumed to be of the form

$$C = 2d^*d - 1$$

with a coisometry d from $\mathcal{H}$ to a Hilbert space $\mathcal{K}$, i.e., dd^* is the identity $I_{\mathcal{K}}$ on $\mathcal{K}$. Observe that the Hilbert space $\mathcal{H}$ here can be taken to be arbitrary and is no longer needed to be $\ell^2(D)$. Let $T = dSd^*$. T is a self-adjoint operator on $\mathcal{K}$ and called the discriminant operator of U. Let $\mathcal{D}_\pm = \ker d \cap \ker(S \pm 1)$. The subspace $\mathcal{D}_{\rm B} = \mathcal{D}_+ \oplus \mathcal{D}_- \subset \mathcal{H}$ is called the *birth eigenspace* of U and its orthogonal complement $\mathcal{D}_{\rm I}$ the *inherited subspace* of U (see [17, 26]). As shown elsewhere [34], the restriction $U_{\rm I} := U|_{\mathcal{D}_{\rm I}}$ to the inherited subspace is unitarily equivalent to

$$\exp(+i \arccos T) \oplus \exp(-i \arccos T)$$

and the restriction $U_{\rm B} := U|_{\mathcal{D}_{\rm B}}$ to the birth eigenspace is $I_{\mathcal{D}_+} \oplus (-I_{\mathcal{D}_-})$. Thus, the spectral analysis of U is reduced to two parts: (1) the spectral analysis of T and (2) the calculation of $\dim \mathcal{D}_{\rm B}$. This reduction leads the SMT from T to U (Theorem 2.1), which allows us to use it for QWs other than the Szegedy walk. As evident below, such an abstract theorem is applicable for a class of d-dimensional QWs, which is not the Szegedy walk on $\mathbb{Z}^d$. In forthcoming papers [11, 12], we will consider a unified model that includes a split-step QW introduced by Kitagawa et al [23] and traditional one-dimensional QWs [2, 13, 28] as special cases. The evolution of the walk is a unitary operator on $\ell^2(\mathbb{Z}; \mathbb{C}^2)$ defined as $U = S_1 C$, where

$$(S_1\psi)(x) = \begin{pmatrix} p\psi_1(x) + q\psi_2(x+1) \\ q^*\psi_1(x-1) - p\psi_2(x) \end{pmatrix}, \quad x \in \mathbb{Z}, \ \psi \in \ell^2(\mathbb{Z}; \mathbb{C}^2).$$

Taking $(p, q) \in \mathbb{R} \times \mathbb{C}$ as $p^2 + |q|^2 = 1$ ensures S_1 is unitary and self-adjoint. C is a multiplication operator by unitary matrices $C(x) \in U(2)$. If $C(x)$ is in addition hermitian and $\dim \ker(C(x) - 1) = 1$ for all $x \in \mathbb{Z}$, then C is written as $2d^*d - 1$ with a coisometry $d : \ell^2(\mathbb{Z}; \mathbb{C}^2) \to \ell^2(\mathbb{Z})$ (see Example 2.2). Thus the SMT is applicable.

Models In this paper, we consider a multi-dimensional generalization of the aforementioned model, which is a $2d$-state QW on $\mathbb{Z}^d$ with a position dependent coin $C(\boldsymbol{x}) \in U(2d)$ and $d \geq 2$. However, for conceptual and notational simplicity, we first concentrate on the case of $d = 2$. The case of $d \geq 3$ is dealt with in the subsequent sections. Let $\mathcal{H} = \ell^2(\mathbb{Z}^2; \mathbb{C}^4)$ be the Hilbert space of states. As usual, the evolution operator $U = SC$ is defined as the product of a shift S and a coin C. To define the shift operator, we introduce a set

$$D = \{(\boldsymbol{p}, \boldsymbol{q}) = (p_1, p_2, q_1, q_2) \in \mathbb{R}^2 \times \mathbb{C}^2 : p_j^2 + |q_j|^2 = 1 \ (j = 1, 2)\}$$

and use $\{\boldsymbol{e}_j\}_{j=1}^2$ to denote the standard basis of $\mathbb{Z}^2$. We define operators S_j $(j = 1, 2)$ on $\ell^2(\mathbb{Z}^2; \mathbb{C}^2)$ as

$$(S_j\Psi)(\boldsymbol{x}) = \begin{pmatrix} p_j\psi_1(\boldsymbol{x}) + q_j\psi_2(\boldsymbol{x} + \boldsymbol{e}_j) \\ q_j^*\psi_1(\boldsymbol{x} - \boldsymbol{e}_j) - p_j\psi_2(\boldsymbol{x}) \end{pmatrix}, \quad \boldsymbol{x} \in \mathbb{Z}^2,$$

for all $\Psi = {}^t(\psi_1, \psi_2) \in \ell^2(\mathbb{Z}^2; \mathbb{C}^2)$. The shift S on $\mathcal{H}$ is defined as a diagonal operator $S = S_1 \oplus S_2$ on $\mathcal{H} \simeq \oplus^2\ell^2(\mathbb{Z}^2; \mathbb{C}^2)$. The condition $(\boldsymbol{p}, \boldsymbol{q}) \in D$ ensures that S_j is self-adjoint and unitary on $\ell^2(\mathbb{Z}^2; \mathbb{C}^2)$ and so is S on $\mathcal{H}$. The coin operator is a multiplication by unitary and self-adjoint square matrices $C(\boldsymbol{x}) \in U(4)$. In general, a unitary and self-adjoint operator is an involution; hence, it can only have eigenvalues ± 1 as its spectrum. We impose the following on the coin operator C.

- (**Simplicity**) $\dim\ker(C(\boldsymbol{x}) - 1) = 1, \quad \boldsymbol{x} \in \mathbb{Z}^2$.
- (**One defect**) $C(\boldsymbol{x}) = \begin{cases} C_1, & \boldsymbol{x} \in \mathbb{Z}^2 \setminus \{\boldsymbol{0}\} \\ C_0, & \boldsymbol{x} = \boldsymbol{0} \end{cases}$ with some $C_0, C_1 \in U(4)$.

We here comment on the aforementioned conditions. The simplicity condition means that $C(\boldsymbol{x})$ is a Grover-type coin. Indeed, by $\dim\ker(C(\boldsymbol{x}) - 1) = 1$, we can take a unique normalized eigenvector $\chi(\boldsymbol{x}) \in \ker(C(\boldsymbol{x}) - 1)$ up to a constant factor. As seen in Lemma 3.1, we can write $C = 2d^*d - 1$ with a coisometry $d : \mathcal{H} \to \mathcal{K} := \ell^2(\mathbb{Z}^2)$ defined as

$$(d\Psi)(\boldsymbol{x}) = \langle \chi(\boldsymbol{x}), \Psi(\boldsymbol{x}) \rangle_{\mathbb{C}^2}, \quad \boldsymbol{x} \in \mathbb{Z}^2 \quad \text{for all } \Psi \in \mathcal{H}.$$

The one defect condition means that $\chi(\boldsymbol{x})$ can be written as

$$\chi(\boldsymbol{x}) = \begin{cases} \Phi = {}^t(\Phi_1, \Phi_2) \text{ with } \Phi_j \in \mathbb{C}^2 \ (j = 1, 2), & \boldsymbol{x} \in \mathbb{Z}^2 \setminus \{\boldsymbol{0}\}, \\ \Omega = {}^t(\Omega_1, \Omega_2) \text{ with } \Omega_j \in \mathbb{C}^2 \ (j = 1, 2), & \boldsymbol{x} = \boldsymbol{0}, \end{cases}$$

where $\Phi \in \ker(C_1 - 1)$ and $\Omega \in \ker(C_0 - 1)$ are normalized vectors. In Grover's search algorithm on a graph $G = (V, E)$, the coin operator $C(\boldsymbol{x})$ differs only at a vertex $\boldsymbol{x} = \boldsymbol{x}_0$, which is a unique solution to the search problem . This is a one-defect condition. Moreover, finding the marked vertex $\boldsymbol{x}_0$ with non-zero probability is closely related to localization of the corresponding QW. Motivated by Grover's search algorithm, we study localization of the one defect model on $\mathbb{Z}^d$.

Results Let $\Psi_0 \in \mathcal{H}$ be the initial state of a quantum walker, and let $\Psi_t = U^t\Psi_0$ $(t = 1, 2, \ldots)$ be the state of the walker at time t. The position X_t of the walker at time t follows $P(X_t = \boldsymbol{x}) = \|\Psi_t(\boldsymbol{x})\|_{\mathbb{C}^2}^2$ $(\boldsymbol{x} \in \mathbb{Z}^2)$. As shown in [34], if the initial state Ψ_0 has a overlap with an eigenvector of U, then localization occurs, i.e.,

$$\limsup_{t\to\infty} P(X_t = \boldsymbol{x}) > 0 \text{ with some } \boldsymbol{x} \in \mathbb{Z}^2.$$

Thus the problem is reduced to proving the existence of eigenvalues for U.

We are now in a position to state our result. Let $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, and $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We set $a_\Omega(\boldsymbol{p}) = \sum_{j=1}^{2} p_j \langle \Omega_j, \sigma_3 \Omega_j \rangle_{\mathbb{C}^2}$, $a_\Phi(\boldsymbol{p}) = \sum_{j=1}^{2} p_j \langle \Phi_j, \sigma_3 \Phi_j \rangle_{\mathbb{C}^2}$, $\lambda(\boldsymbol{q}) = 2 \sum_{j=1}^{2} |q_j \langle \Phi_j, \sigma_+ \Phi_j \rangle_{\mathbb{C}^2}|$, and $D_j = \{(\boldsymbol{p}, \boldsymbol{q}) \in D \colon p_j q_j \neq 0\}$ $(j = 1, 2)$. Let $\mathbb{T}_- = [-1, -\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}))$, $\mathbb{T}_+ = (\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}), 1]$, and $g_\pm(\lambda) = e^{\pm i \arccos \lambda}$. We use $\cdot$ to denote the scalar product.

Theorem 1.1. *Let $U = SC$ as above. Suppose that the following conditions hold.*

(1) $\Phi_j \cdot (\sigma_1 \Omega_j) = 0$ for all $j \in \{1, 2\}$ and $\langle \Phi_l, \sigma_+ \Omega_l \rangle_{\mathbb{C}^2} \neq 0$ with some $l \in \{1, 2\}$;

(2) $a_\Omega(\boldsymbol{p}_0) \neq a_\Phi(\boldsymbol{p}_0)$ with some $\boldsymbol{p}_0 \in \{-1, 1\} \times \{-1, 1\}$.

If $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$ and $\|(\boldsymbol{p}, \boldsymbol{q}) - (\boldsymbol{p}_0, \boldsymbol{0})\|_{\mathbb{R}^2 \times \mathbb{C}^2}$ is sufficiently small , U has two eigenvalues in $\{g_-(\lambda), g_+(\lambda) \mid \lambda \in \mathbb{T}_-\}$ or $\{g_-(\lambda), g_+(\lambda) \mid \lambda \in \mathbb{T}_+\}$.

This is a special case of Theorem 3.7. See Figure 1 for the location of the eigenvalues and the continuous spectrum. The criteria for U_{I} to have eigenvalues in $\{g_-(\lambda), g_+(\lambda) \mid \lambda \in \mathbb{T}_-\}$ and $\{g_-(\lambda), g_+(\lambda) \mid \lambda \in \mathbb{T}_+\}$ are obtained in Theorem 3.5.

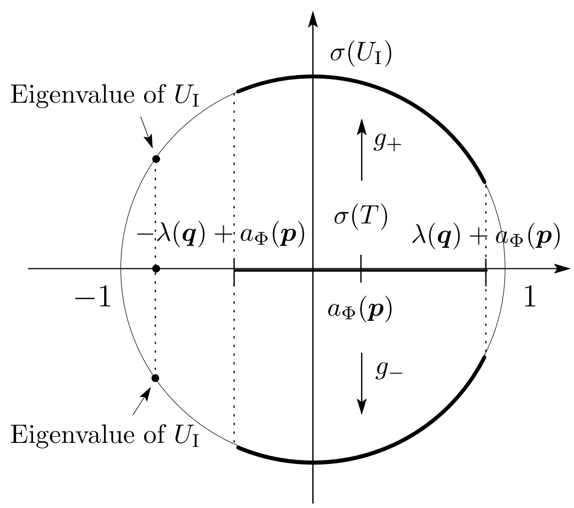

Figure 1: Location of the spectrum $\sigma(U_{\mathrm{I}})$ for $a_\Omega(\boldsymbol{p}_0) < a_\Phi(\boldsymbol{p}_0)$. $g_\pm(\lambda) = e^{\pm i \arccos \lambda}$ map $\sigma(T) = [-\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}), \lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p})]$ onto $\sigma(U_{\mathrm{I}}) \subset S^1$. The difference $\sigma(U) \setminus \sigma(U_{\mathrm{I}})$ is at most $\sigma(U_{\mathrm{B}}) \subset \{-1, +1\}$. See Theorem 3.7 for more details.

Methods and related work Localization of the one defect model of traditional one-dimensional QWs was solved by Cantero et al [7], who used the CGMV method, which is not applicable for multidimensional cases. In the present work, we use the SMT. Several studies on the birth eigenspace $\mathcal{D}_{\mathrm{B}}$ have been reported. As shown by Higuchi et al [16], multi-dimensional models are likely to have eigenvalues ± 1 due to the existence of cycles, which makes $\mathcal{D}_{\mathrm{B}}$ non trivial. For the one-dimensional split-step QW, the birth eigenspace is characterized elsewhere [12]. However, the eigenspace contained in the inherited subspace $\mathcal{D}_{\mathrm{I}}$ is study only for the Grover walk case, in which the discriminant T is unitarily equivalent to the transition probability matrix P_G of the symmetric random walk on G. In our case, T becomes a discrete Schrödinger operator with variable coefficients:

$$T = a(\boldsymbol{p}, \cdot) + \sum_{j=1}^{2} \{ q_j \langle \chi_j, L_j \sigma_+ \chi_j \rangle + (q_j \langle \chi_j, L_j \sigma_+ \chi_j \rangle)^* \},$$

where $\chi(\boldsymbol{x}) = {}^t(\chi_1(\boldsymbol{x}), \chi_2(\boldsymbol{x}))$, $a(\boldsymbol{p}, \boldsymbol{x}) = \sum_{j=1}^{2} p_j \langle \chi_j(\boldsymbol{x}), \sigma_3 \chi_j(\boldsymbol{x}) \rangle$, and L_j is the shift by $\boldsymbol{e}_j$ on $\mathcal{K}$. To analyze the above operator T, we employ the Feshbach map [9]:

$$F(\lambda) = \Pi^\perp (T - \lambda) \Pi^\perp - \Pi^\perp T \Pi (\Pi (T - \lambda) \Pi)^{-1}_{\mathrm{ran}\Pi} \Pi T \Pi^\perp, \quad \lambda \in \mathbb{C} \setminus \{a_\Omega(\boldsymbol{p})\},$$

where Π is the projection onto $\{\psi \in \mathcal{K} \mid \psi(\boldsymbol{x}) = 0 \text{ except for } \boldsymbol{x} = 0\}$ and λ is a spectral parameter. The isospectral property of this map implies that λ is an eigenvalue of T if $\ker F(\lambda)$ is non-trivial (Proposition 4.2). The Feshbach map was used in a study of nuclear reactions [9] and was used for constructing a renormalization map [6]. To our best knowledge, this is the first application of the Feshbach map to analyze the spectrum of an evolution operator for a QW. The one defect condition yields the following formula:

$$F(\lambda) = \Pi^\perp \left(T_0 - \lambda - \frac{1}{a_\Omega(\boldsymbol{p}) - \lambda} |\varphi_{\boldsymbol{q}}\rangle \langle \varphi_{\boldsymbol{q}}| \right) \Pi^\perp, \tag{1.1}$$

where $\varphi_{\boldsymbol{q}} \in \mathcal{K}$. This is a one rank perturbation of a constant coefficient discrete Laplacian T_0. The spectral analysis of an operator $(1/\sqrt{d}) \sum_{j=1}^{d} (L_j + L_j^*) + v |\delta_{\boldsymbol{0}}\rangle \langle \delta_{\boldsymbol{0}}|$ (with v a coupling constant and $\delta_{\boldsymbol{0}}$ the delta function at the origin) similar to the right-hand side in (1.1) is treated elsewhere [19]. Because the nonlinearity of the spectral parameter λ, the analysis of the kernel of $F(\lambda)$ becomes more involved. This task is reduced to finding zeros of a function

$$\mathfrak{f}(\lambda) = \lambda - a_\Omega(\boldsymbol{p}) + \langle \varphi_{\boldsymbol{q}}, (T_0 - \lambda)^{-1} \varphi_{\boldsymbol{q}} \rangle_{\mathcal{K}}, \quad \lambda \in [-1, 1] \setminus \sigma(T_0) \neq \emptyset.$$

The rest of this paper is constructed as follows. In Sec. 2, we review the SMT, which plays an important role in this work. The precise definitions of our evolution U and the discriminant T are given in Sec. 3. We thereafter give the essential spectrum of T, which is mapped onto the essential spectrum of U_{I} by the SMT. We also give a criterion for T to have an eigenvalue in terms of the Feshbach map $F(\lambda)$ (Theorem 3.4). We then present the main results. Theorem 3.5 gives criteria for U to have eigenvalues and Theorem 3.7 shows the existence of eigenvalues for U. We prove Theorem 3.7 using Theorem 3.5. Sec. 4 is devoted to the precise definition of the Feshbach map $F(\lambda)$ and its properties. Sec. 5 is devoted to the analysis of $\mathfrak{f}(\lambda)$ and the proof of Theorem 3.5.

2 Preliminaries

In this section, we briefly review the spectral mapping theorem (SMT). Readers can consult [18, 34] for more details. We use $\sigma(A)$, $\sigma_{\mathrm{p}}(A)$, $\sigma_{\mathrm{ac}}(A)$, $\sigma_{\mathrm{sc}}(A)$ to denote the spectrum, the set of all eigenvalues, the absolutely continuous spectrum, and the singular continuous spectrum of an operator A, respectively. Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces and $d : \mathcal{H} \to \mathcal{K}$ be a coisometry, i.e.,

$$dd^* = I_{\mathcal{K}},$$

where $d^* : \mathcal{K} \to \mathcal{H}$ is the adjoint of d and $I_{\mathcal{K}}$ is the identity on $\mathcal{K}$. Then, d is an isometry and d^*d is a othogonal projection on $\mathcal{H}$, because d^*d is idempotent and self-adjoint, i.e., $(d^*d)^2 = d^*d$ and $(d^*d)^* = d^*d$. The operator

$$C := 2d^*d - 1$$

is a self-adjoint unitary operator, because $C^2 = 1$. Let S be a self-adjoint unitary operator on $\mathcal{H}$ and set $U = SC$. The discriminant operator T of U is defined as

$$T = dSd^*,$$

which is a bounded self-adjoint operator on $\mathcal{K}$ and $\|T\| \le 1$. Hence, $\sigma(T)$ is a closed set contained in the interval $[-1, 1]$. Let $\mathcal{D}_\pm = \ker d \cap \ker(S \pm 1) \subset \mathcal{H}$. The subspaces

$$\mathcal{D}_{\mathrm{B}} := \mathcal{D}_+ \oplus \mathcal{D}_- \quad \text{and} \quad \mathcal{D}_{\mathrm{I}} := \mathcal{D}_{\mathrm{B}}^\perp$$

are called the *birth eigenspace* of U and *inherited subspace* of U, respectively. The restriction $U_{\mathrm{I}} := U|_{\mathcal{D}_{\mathrm{I}}}$ to the inherited subspace is unitarily equivalent to

$$\exp(+i \arccos T) \oplus \exp(-i \arccos T) \quad \text{on } \mathrm{ran}(d^*d).$$

See [34] for the precise meaning of the above decomposition. On the other hand, the restriction $U_{\mathrm{B}} := U|_{\mathcal{D}_{\mathrm{B}}}$ to the birth eigenspace coincides with $I_{\mathcal{D}_+} \oplus (-I_{\mathcal{D}_-})$. The SMT from T to U is given as follows.

Theorem 2.1 (Spectral mapping theorem [18, 34])**.** *Let $U = SC$ be as above. Then, U is decomposed into $U = U_{\mathrm{I}} \oplus U_{\mathrm{B}}$ on $\mathcal{H} = \mathcal{D}_{\mathrm{I}} \oplus \mathcal{D}_{\mathrm{B}}$ and the following hold:*

(1) $\sigma_\sharp(U) = \sigma_\sharp(U_{\mathrm{I}})$ *for* $\sharp = \mathrm{ac}, \mathrm{sc}$ *and* $\sigma_{\mathrm{p}}(U) = \sigma_{\mathrm{p}}(U_{\mathrm{I}}) \cup \sigma_{\mathrm{p}}(U_{\mathrm{B}})$*;*

(2) $\sigma_\sharp(U_{\mathrm{I}}) = \exp(+i \arccos \sigma_\sharp(T)) \cup \exp(-i \arccos \sigma_\sharp(T))$ *for* $\sharp = \mathrm{p}, \mathrm{ac}, \mathrm{sc}$*;*

(3) $\sigma_\sharp(U_{\mathrm{B}}) = \emptyset$ *for* $\sharp = \mathrm{ac}, \mathrm{sc}$ *and* $\sigma_{\mathrm{p}}(U_{\mathrm{B}}) = \begin{cases} \{1, -1\} & \textit{if } \mathcal{D}_+ \neq \emptyset \textit{ and } \mathcal{D}_- \neq \emptyset, \\ \{\pm 1\} & \textit{if } \mathcal{D}_\pm \neq \emptyset \textit{ and } \mathcal{D}_\mp = \emptyset, \\ \emptyset & \textit{otherwise.} \end{cases}$

Theorem 2.1 is widely applicable for the evolutions of quantum walks. Here we give two examples. The first one is the Szegedy walk. See [16] for the twisted Szegedy walk.

Example 2.1 ([16, 18])**.** *Let D be the set of arcs of a symmetric digraph $G = (V, D)$ (possibly not bipartite) and $\mathcal{H} = \ell^2(D)$ be the Hilbert space of square summable functions $\psi : D \to \mathbb{C}$. Define a unitary operator U_G on $\ell^2(D)$ as the product*

$$U_G = S_{\mathrm{f}} C_\chi$$

of a shift $S_{\rm f}$ *and coin* C_χ*. The shift* $S_{\rm f}$ *is defined as* $(S_{\rm f}\psi)(e) = \psi(\bar{e})$ *for* $e \in D$*, where* $\bar{e}$ *stands for the inverse arc of* e*. The coin* C_χ *is defined as*

$$C_\chi = \bigoplus_{x \in V} (2|\chi(x)\rangle\langle\chi(x)| - 1)\,,$$

where we have used an identification $\ell^2(D) \simeq \bigoplus_{x\in V} \mathcal{H}_x$ *with* $\mathcal{H}_x = \overline{\mathrm{Span}}\{\psi\colon \psi(e) = 0, o(e) \neq x\}$ *and* $\chi(x) = \sum_{e\in D; o(e)=x} \sqrt{p_{t(e),x}}\delta_e \in \ell^2(D)$ *is a normalized vector. Here* $p_{u,v}$ *is the transition probability of a (classical) random walk from* v *to* u $(u, v \in V)$*. The QW with this evolution* U_G *is now referred to as the Szegedy walk on* G*, which is called the Grover walk on* G *in particular if* $p_{u,v} = 1/\mathrm{deg}x$*. In the case of the Szegedy evolution operator* U_G*, Theorem 2.1 is applicable for any symmetric digraph* $G = (V, D)$*, because* $S_{\rm f}$ *is self-adjoint and unitary and* $C_\chi = 2d_\chi^* d_\chi - 1$ *with a coisometry* $d_\chi : \ell^2(D) \to \ell^2(V)$ *defined as*

$$(d_\chi\psi)(x) := \langle\chi(x), \psi\rangle, \quad x \in V.$$

Moreover, the discriminant operator T_G *of* U_G *is unitary equivalent to the transition probability matrix* $P_G = (p_{u,v})$ *and the birth eigenspace can be characterized by the structure of* G*.*

The next example is a one-dimensional QW but not the Szegedy walk on $\mathbb{Z}$. This is a unified model including a split-step QW introduced by Kitagawa et al [23] and traditional one-dimensional QWs [2, 13, 28] as special cases. In the subsequent sections, we consider a multidimensional extension of this model.

Example 2.2 (Split-step QWs)**.** *The evolution of a split-step QW is a unitary operator on* $\ell^2(\mathbb{Z}; \mathbb{C}^2)$ *defined as* $U = S_1 C$*, where*

$$(S_1\psi)(x) = \begin{pmatrix} p\psi_1(x) + q\psi_2(x+1) \\ q^*\psi_1(x-1) - p_2\psi(x) \end{pmatrix}, \quad x \in \mathbb{Z}.$$

We suppose that $(p, q) \in \mathbb{R} \times \mathbb{C}$ *satisfy* $p^2 + |q|^2 = 1$*, which ensure* S_1 *is unitary and self-adjoint.* C *is a multiplication operator by unitary matrices* $C(x) \in U(2)$*. When* $p = 0$ *and* $q = 1$*, it becomes a QW on* $\mathbb{Z}$ *with a flip-flop shift [5], which is unitarily equivalent to traditional QWs (see [31] for more information). The evolutions with* $p = 0$ *and* $p \neq 0$ *are not unitarily equivalent and these walks have weak limit measures different from usual one [11]. If* $C(x)$ *is self-adjoint unitary and* $\dim\ker(C(x) - 1) = 1$ *for all* $x \in \mathbb{Z}$*, then* C *is written as* $2d_\chi^* d_\chi - 1$ *with a coisometry* $d_\chi : \ell^2(\mathbb{Z}; \mathbb{C}^2) \to \ell^2(\mathbb{Z})$ *defined as*

$$(d_\chi\Psi)(x) = \langle\chi(x), \Psi(x)\rangle_{\mathbb{C}^2}, \quad x \in \mathbb{Z},$$

where $\chi(x) \in \ker(C(x) - 1)$*. Thus the SMT is applicable for this model. In [12], the birth eigenspace of this model is characterized.*

3 Multi-dimensional models and main results

3.1 Definition of models

From now on, we consider a QW on $\mathbb{Z}^d$, which is a generalization of the split-step QW defined in Example 2.2. Let $n \in \mathbb{N}$ and use $\ell^2(\mathbb{Z}^d; \mathbb{C}^n)$ to denote the Hilbert space of the square-summable functions $\Psi : \mathbb{Z}^d \to \mathbb{C}^n$. If $n = 1$, we simply denote $\ell^2(\mathbb{Z}^d; \mathbb{C})$ by $\ell^2(\mathbb{Z}^d)$. Hereafter, we set $\mathcal{H} = \ell^2(\mathbb{Z}^d; \mathbb{C}^{2d})$ and $\mathcal{K} = \ell^2(\mathbb{Z}^d)$. We fist define an evolution operator U on $\mathcal{H}$ as a product $U = SC$ of a shift operator S and coin operator C, then introduce a coisometry $d : \mathcal{H} \to \mathcal{K}$, and give an explicit formula of the discriminant operator $T = dSd^*$ on $\mathcal{K}$.

Shift operators Let

$$D = \{(\boldsymbol{p}, \boldsymbol{q}) = (p_1, \ldots, p_d, q_1, \ldots, q_d) \in \mathbb{R}^d \times \mathbb{C}^d \colon p_j^2 + |q_j|^2 = 1 \ (j = 1, \ldots, d)\}$$

and use $\{\boldsymbol{e}_j\}_{j=1}^d$ to denote the standard basis of $\mathbb{Z}^d$. Henceforth $(\boldsymbol{p}, \boldsymbol{q}) \in D$ is assumed unless otherwise specified. To define a shift operator S on $\mathcal{H}$, we introduce an operator S_j on $\ell^2(\mathbb{Z}^d; \mathbb{C}^2)$ $(j = 1, \ldots, d)$ as follows.

$$(S_j\psi)(\boldsymbol{x}) = \begin{pmatrix} p_j\psi_1(\boldsymbol{x}) + q_j\psi_2(\boldsymbol{x} + \boldsymbol{e}_j) \\ q_j^*\psi_1(\boldsymbol{x} - \boldsymbol{e}_j) - p_j\psi_2(\boldsymbol{x}) \end{pmatrix} \quad \text{for all } \boldsymbol{x} \in \mathbb{Z}^d \text{ and } \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \in \ell^2(\mathbb{Z}^d; \mathbb{C}^2).$$

Using the identification $\mathcal{H} \simeq \oplus_{j=1}^d \ell^2(\mathbb{Z}^d; \mathbb{C}^2)$, we define the shift S on $\mathcal{H}$ as $S = S_1 \oplus \ldots \oplus S_d$, i.e.,

$$(S\Psi)(\boldsymbol{x}) = \begin{pmatrix} (S_1\Psi_1)(\boldsymbol{x}) \\ \vdots \\ (S_d\Psi_d)(\boldsymbol{x}) \end{pmatrix} \quad \text{for all } \boldsymbol{x} \in \mathbb{Z}^d \text{ and } \Psi = \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_d \end{pmatrix} \in \mathcal{H} \ (\Psi_j \in \ell^2(\mathbb{Z}^d; \mathbb{C}^2)).$$

The condition $(\boldsymbol{p}, \boldsymbol{q}) \in D$ ensures S_j is self-adjoint and unitary on $\ell^2(\mathbb{Z}^d; \mathbb{C}^2)$, and so is S on $\mathcal{H}$. Let $\{C(\boldsymbol{x})\}_{\boldsymbol{x} \in \mathbb{Z}^d} \subset U(2d)$ be a family of unitary and self-adjoint square matrices of order $2d$.

Coin operators We define a coin operator C on $\mathcal{H}$ as a multiplication operator by $C(x)$, i.e.,

$$(C\Psi)(\boldsymbol{x}) = C(\boldsymbol{x})\Psi(\boldsymbol{x}) \quad \text{for all } \boldsymbol{x} \in \mathbb{Z}^d \text{ and } \Psi \in \mathcal{H}.$$

By definition, C is unitary on $\mathcal{H}$. Throughout this paper, the following two conditions are imposed on C unless otherwise specified.

- (**Simplicity**) Each $C(\boldsymbol{x})$ has 1 as a simple eigenvalue, i.e.,

$$\dim \ker(C(\boldsymbol{x}) - 1) = 1, \quad \boldsymbol{x} \in \mathbb{Z}^d.$$

- (**One defect**) There exist matrices C_0 and $C_1 \in U(2d)$ such that

$$C(\boldsymbol{x}) = \begin{cases} C_1, & \boldsymbol{x} \in \mathbb{Z}^d \setminus \{\boldsymbol{0}\}, \\ C_0, & \boldsymbol{x} = \boldsymbol{0}. \end{cases}$$

Because $\dim \ker(C(\boldsymbol{x}) - 1) = 1$, we can take a unique normalized vector (up to a constant factor):

$$\chi(\boldsymbol{x}) = \begin{pmatrix} \chi_1(\boldsymbol{x}) \\ \vdots \\ \chi_d(\boldsymbol{x}) \end{pmatrix} \in \ker(C(\boldsymbol{x}) - 1), \quad \chi_j(\boldsymbol{x}) = \begin{pmatrix} \chi_{j,1}(\boldsymbol{x}) \\ \chi_{j,2}(\boldsymbol{x}) \end{pmatrix} \in \mathbb{C}^2 \ (j = 1, \cdots, d).$$

The spectral decomposition of $C(\boldsymbol{x})$ implies $C(\boldsymbol{x}) = 2|\chi(\boldsymbol{x})\rangle\langle\chi(\boldsymbol{x})| - 1$. By the one defect condition of C, $\chi(\boldsymbol{x})$ is written as follows.

$$\chi(\boldsymbol{x}) = \begin{cases} \Phi = \begin{pmatrix} \Phi_1 \\ \vdots \\ \Phi_d \end{pmatrix} \text{ with } \Phi_j = \begin{pmatrix} \phi_{j,1} \\ \phi_{j,2} \end{pmatrix} \in \mathbb{C}^2 \ (j = 1, \cdots, d), & \boldsymbol{x} \in \mathbb{Z}^d \setminus \{\boldsymbol{0}\}, \\ \Omega = \begin{pmatrix} \Omega_1 \\ \vdots \\ \Omega_d \end{pmatrix} \text{ with } \Omega_j = \begin{pmatrix} \omega_{j,1} \\ \omega_{j,2} \end{pmatrix} \in \mathbb{C}^2 \ (j = 1, \cdots, d), & \boldsymbol{x} = \boldsymbol{0}. \end{cases} \tag{3.1}$$

Evolutions and their discriminants Let S and C be as above and define an evolution operator U on $\mathcal{H}$ as

$$U = SC.$$

S and C are unitary, and so is U. We define a coisometry $d : \mathcal{H} \to \mathcal{K}$ as

$$(d\Psi)(\boldsymbol{x}) = \langle \chi(\boldsymbol{x}), \Psi(\boldsymbol{x}) \rangle_{\mathbb{C}^{2d}} \quad \text{for all } \boldsymbol{x} \in \mathbb{Z}^d \text{ and } \Psi \in \mathcal{H}.$$

Lemma 3.1. *(1) The adjoint $d^* : \mathcal{K} \to \mathcal{H}$ of d is a multiplication operator by $\chi(\boldsymbol{x})$, i.e.,*

$$(d^* f)(\boldsymbol{x}) = \chi(\boldsymbol{x}) f(\boldsymbol{x}) \quad \textit{for all } \boldsymbol{x} \in \mathbb{Z}^d \textit{ and } f \in \mathcal{K}.$$

(2) $d^* d = \bigoplus_{\boldsymbol{x} \in \mathbb{Z}^d} |\chi(\boldsymbol{x})\rangle\langle\chi(\boldsymbol{x})|$ *and* $dd^* = I_{\mathcal{K}}$.

(3) $C = 2d^*d - 1$.

Proof. (1) For all $f \in \mathcal{K}$, since $\sum_{\boldsymbol{x} \in \mathbb{Z}^d} \|\chi(\boldsymbol{x}) f(\boldsymbol{x})\|^2_{\mathbb{C}^{2d}} = \sum_{\boldsymbol{x} \in \mathbb{Z}^d} |f(\boldsymbol{x})|^2 = \|f\|^2_{\mathcal{K}} < \infty$, then the multiplication operator $\chi : \mathcal{K} \ni f \mapsto \chi f \in \mathcal{H}$ is bounded. For all $\Psi \in \mathcal{H}$ and $f \in \mathcal{K}$, $\langle f, d\Psi \rangle_{\mathcal{K}} = \sum_{\boldsymbol{x} \in \mathbb{Z}^d} f(\boldsymbol{x})^* \langle \chi(\boldsymbol{x}), \Psi(\boldsymbol{x}) \rangle_{\mathbb{C}^{2d}} = \langle \chi f, \Psi \rangle_{\mathcal{H}}$. Thus we have $d^* f = \chi f$.

(2) For all $\Psi \in \mathcal{H}$ and $\boldsymbol{x} \in \mathbb{Z}^d$, $(d^*d\Psi)(\boldsymbol{x}) = \chi(\boldsymbol{x})(d\Psi)(\boldsymbol{x}) = \langle\chi(\boldsymbol{x}), \Psi(\boldsymbol{x})\rangle\chi(\boldsymbol{x})$ holds. Then we have $d^*d = \bigoplus_{\boldsymbol{x}\in\mathbb{Z}^d} |\chi(\boldsymbol{x})\rangle\langle\chi(\boldsymbol{x})|$. On the other hand, for all $f \in \mathcal{K}$ and $\boldsymbol{x} \in \mathbb{Z}^d$, $(dd^*f)(\boldsymbol{x}) = \langle\chi(\boldsymbol{x}), (d^*f)(\boldsymbol{x})\rangle_{\mathbb{C}^{2d}} = \langle\chi(\boldsymbol{x}), f(\boldsymbol{x})\chi(\boldsymbol{x})\rangle_{\mathbb{C}^{2d}} = f(\boldsymbol{x})$. Then $dd^* = I_{\mathcal{K}}$ holds.
(3) Obviously, the result follows from $d^*d = \bigoplus_{\boldsymbol{x}\in\mathbb{Z}^d} |\chi(\boldsymbol{x})\rangle\langle\chi(\boldsymbol{x})|$. □

Lemma 3.1 implies that Theorem 2.1 is applicable for the above evolution U. In what follows, we give an explicit form of the discriminant operator T of U, defined as

$$T = dSd^*.$$

Let L_j be a shift on $\mathcal{K}$ by $\boldsymbol{e}_j$ ($j \in \{1, \cdots, d\}$), i.e.,

$$(L_j f)(\boldsymbol{x}) = f(\boldsymbol{x} + \boldsymbol{e}_j), \quad \text{for all } \boldsymbol{x} \in \mathbb{Z}^d \text{ and } f \in \mathcal{K},$$

by which S_j can be expressed as a matrix form

$$S_j = \begin{pmatrix} p_j I_{\mathcal{K}} & q_j L_j \\ q_j^* L_j^* & -p_j I_{\mathcal{K}} \end{pmatrix}.$$

We use the following notations:

$$a_\Omega(\boldsymbol{p}) = \sum_{j=1}^d p_j \langle\Omega_j, \sigma_3\Omega_j\rangle_{\mathbb{C}^2}, \quad a_\Phi(\boldsymbol{p}) = \sum_{j=1}^d p_j \langle\Phi_j, \sigma_3\Phi_j\rangle_{\mathbb{C}^2},$$

$$\text{and} \quad a(\boldsymbol{p}, \boldsymbol{x}) = \sum_{j=1}^d p_j \langle\chi_j(\boldsymbol{x}), \sigma_3\chi_j(\boldsymbol{x})\rangle_{\mathbb{C}^2},$$

where $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Observe that

$$a(\boldsymbol{p}, \boldsymbol{x}) = a_\Omega(\boldsymbol{p})\mathbb{1}_{\{\boldsymbol{0}\}}(\boldsymbol{x}) + a_\Phi(\boldsymbol{p})\mathbb{1}_{\mathbb{Z}^d\setminus\{\boldsymbol{0}\}}(\boldsymbol{x}), \tag{3.2}$$

where $\mathbb{1}_A$ is the characteristic function of a set A. As seen in Section 2, the discriminant operator $T = dSd^*$ of U is a bounded self-adjoint on $\mathcal{K}$ and $\|T\| \leq 1$.

Lemma 3.2. *T is expressed as*

$$T = a(\boldsymbol{p}, \cdot) + \sum_{j=1}^d \left\{ q_j\chi_{j,1}^* L_j \chi_{j,2} + (q_j\chi_{j,1}^* L_j \chi_{j,2})^* \right\}, \tag{3.3}$$

where $\chi_{j,1}, \chi_{j,2}$ and $a(\boldsymbol{p}, \cdot)$ denote multiplication operators.

Remark 3.1. *In Section 1, we abbreviate the expression* (3.3) *as*

$$T = a(\boldsymbol{p}, \cdot) + \sum_{j=1}^2 \{q_j\langle\chi_j, L_j\sigma_+\chi_j\rangle + (q_j\langle\chi_j, L_j\sigma_+\chi_j\rangle)^*\} \ \textit{with } \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Proof. For all $f \in \mathcal{K}, j \in \{1, \cdots, d\}$, we set $(d^* f)_j = \chi_j f \in \ell^2(\mathbb{Z}^d; \mathbb{C}^2)$. Since $d^* f = \begin{pmatrix} (d^*f)_1 \\ \vdots \\ (d^*f)_d \end{pmatrix}$, we have $Sd^* f = \begin{pmatrix} S_1(d^*f)_1 \\ \vdots \\ S_d(d^*f)_d \end{pmatrix}$. By definition of T, the following holds for all $f \in \mathcal{K}$ and $\boldsymbol{x} \in \mathbb{Z}^d$:

$$\begin{aligned}
(Tf)(\boldsymbol{x}) &= \langle \chi(\boldsymbol{x}), (Sd^*f)(\boldsymbol{x})\rangle_{\mathbb{C}^{2d}} = \sum_{j=1}^{d} \langle \chi_j(\boldsymbol{x}), (S_j(d^*f)_j)(\boldsymbol{x})\rangle_{\mathbb{C}^2} \\
&= \sum_{j=1}^{d} \left\langle \begin{pmatrix} \chi_{j,1} \\ \chi_{j,2} \end{pmatrix}(\boldsymbol{x}), \left(\begin{pmatrix} p_j & q_j L_j \\ q_j^* L_j^* & -p_j \end{pmatrix} \begin{pmatrix} f\chi_{j,1} \\ f\chi_{j,2} \end{pmatrix} \right)(\boldsymbol{x}) \right\rangle_{\mathbb{C}^2} \\
&= \left(\left(a(\boldsymbol{p}, \cdot) + \sum_{j=1}^{d} \left\{ q_j \chi_{j,1}^* L_j \chi_{j,2} + (q_j \chi_{j,1}^* L_j \chi_{j,2})^* \right\} \right) f \right)(\boldsymbol{x}).
\end{aligned}$$

□

We close this subsection by characterizing the essential spectrum of the discriminant T. To this ends, we introduce a self-adjoint operator T_0 and constant $\lambda(\boldsymbol{q})$ by

$$T_0 = a_\Phi(\boldsymbol{p}) + \sum_{j=1}^{d} (\alpha_j L_j + \alpha_j^* L_j^*) \quad \text{and} \quad \lambda(\boldsymbol{q}) = 2\sum_{j=1}^{d} |\alpha_j|,$$

where $\alpha_j = q_j \phi_{j,1}^* \phi_{j,2}$ $(j = 1, \cdots, d)$. In Sec. 1, we set $\lambda(\boldsymbol{q}) = 2\sum_{j=1}^{2} |q_j \langle \Phi_j, \sigma_+ \Phi_j \rangle_{\mathbb{C}^2}|$, because $\alpha_j = q_j \langle \Phi_j, \sigma_+ \Phi_j \rangle_{\mathbb{C}^2}$.

Lemma 3.3. *It follows that*

$$\sigma_{\mathrm{ess}}(T) = \sigma_{\mathrm{ess}}(T_0) = \sigma(T_0) = [-\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}), a_\Phi(\boldsymbol{p}) + \lambda(\boldsymbol{q})]. \tag{3.4}$$

Moreover, the following conditions are equivalent:

(1) $\sigma(T_0) = [-1, 1]$*;*

(2) $\lambda(\boldsymbol{q}) = 1$*;*

(3) $p_j = 0$ *and* $|\phi_{j,1}| = |\phi_{j,2}|$ *for all* $j \in \{1, \cdots, d\}$*.*

Remark 3.2. *Let* $g_\pm(\lambda) = e^{\pm i \arccos \lambda}$*. The spectral mapping theorem (Theorem 2.1) concludes that*

$$\sigma_{\mathrm{ess}}(U) = \{g_-(\lambda) \mid \lambda \in \sigma(T_0)\} \cup \{g_+(\lambda) \mid \lambda \in \sigma(T_0)\}.$$

See Figure 1.

Proof. Let $W = T - T_0$. Then $T = T_0 + W$ and

$$W = a(\boldsymbol{p}, \boldsymbol{x}) - a_\Phi(\boldsymbol{p}) + \sum_{j=1}^{d} q_j(\chi_{j,1}(\boldsymbol{x})^* \chi_{j,2}(\boldsymbol{x} + \boldsymbol{e}_j) - \phi_{j,1}^* \phi_{j,2}) L_j$$

$$+ \sum_{j=1}^{d} q_j^*(\chi_{j,2}(\boldsymbol{x})^* \chi_{j,1}(\boldsymbol{x} - \boldsymbol{e}_j) - \phi_{j,2}^* \phi_{j,1}) L_j^*.$$

Because, by (3.1) and (3.2), $(Wf)(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \neq \pm \boldsymbol{e}_j, \boldsymbol{0}$ and $f \in \mathcal{K}$,

$$W = \beta_0 \mathbb{1}_{\{\boldsymbol{0}\}} + \sum_{j=1}^{d} \left\{ \beta_j^+ \mathbb{1}_{\{\boldsymbol{e}_j\}} + \beta_j^- \mathbb{1}_{\{-\boldsymbol{e}_j\}} \right\}$$

with some constants β_0 and $\beta_j^\pm$ $(j = 1, \dots, d)$. Because W is compact, $\sigma_{\mathrm{ess}}(T) = \sigma_{\mathrm{ess}}(T_0)$.

Let $\mathcal{F} : \mathcal{K} \to L^2([0, 2\pi]^d, d\boldsymbol{k}/(2\pi)^d)$ be the Fourier transformation defined as the unitary extension of

$$(\mathcal{F}f)(\boldsymbol{k}) = \hat{f}(\boldsymbol{k}) = \sum_{\boldsymbol{x} \in \mathbb{Z}^d} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{for all } f \in \mathcal{K} \text{ with finite support.}$$

Because $\mathcal{F} L_j \mathcal{F}^*$ and $\mathcal{F} L_j^* \mathcal{F}^*$ are multiplication operators by e^{ik_j} and e^{-ik_j}, the Fourier transform $\mathcal{F} T_0 \mathcal{F}^*$ of T_0 is also a multiplication operator by

$$\hat{T}_0(\boldsymbol{k}) = a_\Phi(\boldsymbol{p}) + 2 \sum_{j=1}^{d} |\alpha_j| \cos(k_j + \theta_j), \tag{3.5}$$

where each $\theta_j \in [0, 2\pi)$ is an argument of α_j, i.e., $\alpha_j = |\alpha_j| e^{i\theta_j}$ (if $\alpha_j = 0$, we define $\theta_j = 0$). Because $\hat{T}_0([0, 2\pi]^d) = [-\lambda_{\boldsymbol{q}} + a_\Phi(\boldsymbol{p}), a_\Phi(\boldsymbol{p}) + \lambda_{\boldsymbol{q}}]$, we have (3.4).

(3.4) implies that $a_\Phi(\boldsymbol{p}) = 0$ if $\lambda(\boldsymbol{q}) = 1$ and hence that $\sigma(T_0) = [-1, 1]$ if and only if $\lambda(\boldsymbol{q}) = 1$. On the other hand, $|q_j| \leq 1$ and the inequality of arithmetic and geometric means yield the inequality

$$\lambda(\boldsymbol{q}) \leq 2 \sum_{j=1}^{d} |\phi_{j,1} \phi_{j,2}| \leq \sum_{j=1}^{d} (|\phi_{j,1}|^2 + |\phi_{j,2}|^2) = 1$$

with equality if and only if $|q_j| = 1$ and $|\phi_{j,1}| = |\phi_{j,2}|$ for all $j \in \{1, \cdots, d\}$. This completes the proof. □

3.2 Main results

In what follows, we prove the existence of discrete eigenvalues of U_{I}. To this end, we impose the following on the coin operator, which corresponds to (1) in Theorem 1.1 for the case of $d = 2$. Let $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. We use $\cdot$ to denote the scalar product, i.e., $\Psi \cdot \Phi = \psi_1 \phi_1 + \psi_2 \phi_2$ for $\Psi = {}^t(\psi_1, \psi_2)$, $\Phi = {}^t(\phi_1, \phi_2) \in \mathbb{C}^2$.

Assumption 1. *(a)* $\Phi_j \cdot (\sigma_1 \Omega_j) = 0$ *for all* $j \in \{1, \cdots, d\}$*;*

(b) $\langle \Phi_l, \sigma_+ \Omega_l \rangle_{\mathbb{C}^2} \neq 0$ *with some* $l \in \{1, \cdots, d\}$*.*

Let l be as in Assumption 1 and set

$$D_l = \{(\boldsymbol{p}, \boldsymbol{q}) \in D \colon p_l q_l \neq 0\}.$$

Lemma 3.3 shows that if $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$, then $\sigma_{\mathrm{ess}}(T) = \sigma(T_0) \subsetneq [-1, 1]$. Hence, there can exist discrete eigenvalues of T in $[-1, 1] \setminus \sigma(T_0) \neq \emptyset$. In order to find the discrete eigenvalue, we introduce a function $\mathfrak{f} : [-1, 1] \setminus \sigma(T_0) \to \mathbb{R}$ as follows. Let

$$\varphi_{\boldsymbol{q}} = \sum_{j=1}^{d} \left(q_j \omega_{j,2} \phi_{j,1}^* \mathbb{1}_{\{-\boldsymbol{e}_j\}} + q_j^* \omega_{j,1} \phi_{j,2}^* \mathbb{1}_{\{\boldsymbol{e}_j\}} \right) \in \mathcal{K}.$$

For $\lambda \in [-1, 1] \setminus \sigma(T_0) \neq \emptyset$, we define

$$\mathfrak{f}(\lambda) = \lambda - a_\Omega(\boldsymbol{p}) + \langle \varphi_{\boldsymbol{q}}, \psi_\lambda \rangle_{\mathcal{K}},$$

where

$$\psi_\lambda = (T_0 - \lambda)^{-1} \varphi_{\boldsymbol{q}} \in \mathcal{K}. \tag{3.6}$$

Let $\sigma_- = \sigma_+^*$. Because $\varphi_{\boldsymbol{q}}$ is written as

$$\varphi_{\boldsymbol{q}} = \sum_{j=1}^{d} \left(q_j \langle \Phi_j, \sigma_+ \Omega_j \rangle \mathbb{1}_{\{-\boldsymbol{e}_j\}} + q_j^* \langle \Phi_j, \sigma_- \Omega_j \rangle \mathbb{1}_{\{\boldsymbol{e}_j\}} \right), \tag{3.7}$$

$(\boldsymbol{p}, \boldsymbol{q}) \in D_l$ ensures that $\varphi_{\boldsymbol{q}} \not\equiv 0$ and $\psi_\lambda \not\equiv 0$.

The next theorem plays an important role to show the eigenvalue of T.

Theorem 3.4. *Suppose that Assumption 1 holds and* $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$*. If* $\mathfrak{f}$ *has a zero* $\lambda_\star \in [-1, 1] \setminus (\sigma(T_0) \cup \{a_\Omega(\boldsymbol{p})\})$*, then* $\lambda_\star$ *is a discrete eigenvalue of* T*.*

Remark 3.3. *By Lemma 5.2 (3),* $a_\Omega(\boldsymbol{p})$ *can not be a zero of* $\mathfrak{f}$ *even if* $a_\Omega(\boldsymbol{p}) \in [-1, 1] \setminus \sigma(T_0)$*. Hence,* $\mathfrak{f}$ *has a zero* $\lambda_\star \in [-1, 1] \setminus (\sigma(T_0) \cup \{a_\Omega(\boldsymbol{p})\})$ *(if it exists) and Theorem 3.4 concludes that* $\lambda_\star \in \sigma_{\mathrm{p}}(U)$*. The SMT and Theorem 3.4 imply that* $g_\pm(\lambda_\star) \in \sigma_{\mathrm{p}}(U)$ *are discrete eigenvalues of* U*. See Figure 1.*

The proof of Theorem 3.4 is based on the Feshbach projection method [9, 6]. This reduces the spectral analysis of T to that of the Feshbach map $F(T, P, \lambda)$, which is an operator defined by T, a projection P suitably chosen, and a spectral parameter λ. Let $\Pi = |\mathbb{1}_{\{\mathbf{0}\}}\rangle\langle\mathbb{1}_{\{\mathbf{0}\}}|$ be the projection onto the subspace $\{\alpha \mathbb{1}_{\{\mathbf{0}\}} \mid \alpha \in \mathbb{C}\} \subset \mathcal{K}$ and $\Pi^\perp = I_{\mathcal{K}} - \Pi$. Here we chose $P = \Pi^\perp$ as the projection defining the Feshbach map and set $F(\lambda) = F(T, \Pi^\perp, \lambda)$. See Sec. 4 for the precise definition of $F(\lambda)$ and propositions used in the following proof.

Proof of Theorem 3.4. By Proposition 4.3, $F(\lambda)$ is written as

$$F(\lambda) = \Pi^\perp \left(T_0 - \lambda - \frac{1}{a_\Omega(\boldsymbol{p}) - \lambda} |\varphi_{\boldsymbol{q}}\rangle\langle\varphi_{\boldsymbol{q}}| \right) \Pi^\perp, \quad \lambda \in \mathbb{C} \setminus \{a_\Omega(\boldsymbol{p})\}.$$

Let $\lambda_\star \in [-1,1] \setminus (\sigma(T_0) \cup \{a_\Omega(\boldsymbol{p})\})$ be a zero of $\mathfrak{f}$, i.e., $\mathfrak{f}(\lambda_\star) = 0$, and let $\psi_{\lambda_\star}$ be defined in (3.6) with $\lambda = \lambda_\star$. Because by Proposition 4.4, $\psi_{\lambda_\star} \in \mathrm{ran}\Pi^\perp \setminus \{0\}$,

$$\begin{aligned} F(\lambda_\star)\psi_{\lambda_\star} &= \Pi^\perp \left(T_0 - \lambda_\star - \frac{1}{a_\Omega(\boldsymbol{p}) - \lambda_\star} |\varphi_{\boldsymbol{q}}\rangle\langle\varphi_{\boldsymbol{q}}| \right) \psi_{\lambda_\star} \\ &= \left(1 - \frac{\langle \varphi_{\boldsymbol{q}}, \psi_{\lambda_\star}\rangle}{a_\Omega(\boldsymbol{p}) - \lambda} \right) \varphi_{\boldsymbol{q}} = -\frac{\mathfrak{f}(\lambda_\star)}{a_\Omega(\boldsymbol{p}) - \lambda_\star} \varphi_{\boldsymbol{q}} = 0. \end{aligned}$$

This completes the proof, because by Proposition 4.2, $\lambda_\star \in \sigma_{\mathrm{p}}(T)$ is equivalent that $\ker F(\lambda_\star)$ is non trivial, which is confirmed by Proposition 4.4 again. □

The following is a criterion for $\mathfrak{f}$ to have a zero.

Theorem 3.5. *Suppose that Assumption 1 holds and* $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$*.*

(1) $\mathfrak{f}$ *has a zero* $\lambda_\star \in \mathbb{T}_- := [-1, -\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}))$ *if*

$$\lambda(\boldsymbol{q})(\lambda(\boldsymbol{q}) + a_\Omega(\boldsymbol{p}) - a_\Phi(\boldsymbol{p})) < \|\varphi_{\boldsymbol{q}}\|^2 \le (1 + a_\Omega(\boldsymbol{p}))\frac{(1 + a_\Phi(\boldsymbol{p}))^2 - \lambda(\boldsymbol{q})^2}{1 + a_\Phi(\boldsymbol{p})}; \tag{3.8}$$

(2) $\mathfrak{f}$ *has a zero* $\lambda_\star \in \mathbb{T}_+ = (\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}), 1]$ *if*

$$\lambda(\boldsymbol{q})(\lambda(\boldsymbol{q}) - a_\Omega(\boldsymbol{p}) + a_\Phi(\boldsymbol{p})) < \|\varphi_{\boldsymbol{q}}\|^2 \le (1 - a_\Omega(\boldsymbol{p}))\frac{(1 - a_\Phi(\boldsymbol{p}))^2 - \lambda(\boldsymbol{q})^2}{1 - a_\Phi(\boldsymbol{p})}. \tag{3.9}$$

Thanks to Lemma 3.6 below, the right-hand sides of (3.8) and (3.9) make sense. The proof of Theorem 3.5 will be stated in the last section.

Lemma 3.6. *Suppose that Assumption 1 holds and* $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$*. Then,*

$$a_\Phi(\boldsymbol{p}) \ne \pm 1 \quad \textit{and} \quad a_\Omega(\boldsymbol{p}) \ne \pm 1.$$

Proof. Suppose $a_\Phi(\boldsymbol{p}) = -1$. By the definition of $a_\Phi(\boldsymbol{p})$ and $\|\Phi\|^2 = 1$,

$$-1 = \sum_{j \notin A} p_j(|\phi_{j,1}|^2 - |\phi_{j,2}|^2) \quad \text{and} \quad 1 = \sum_{j\notin A}(|\phi_{j,1}|^2 + |\phi_{j,2}|^2),$$

where $A = \{j \in \{1, \cdots, d\} \mid \phi_{j,1} = \phi_{j,2} = 0\}$. Summing the above two equations, we get $0 = \sum_{j\notin A} \{(1 + p_j)|\phi_{j,1}|^2 + (1 - p_j)|\phi_{j,2}|^2\}$, which, combined with $1 \pm p_j \ge 0$, implies that for $j \notin A$,

$$(1 - p_j)|\phi_{j,2}|^2 = 0. \tag{3.10}$$

By Assumption 1 and $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$, $\phi_{l,2} \ne 0$, $p_l \ne 1$, and hence $l \notin A$. This contradicts (3.10). Therefore $a_\Phi(\boldsymbol{p}) \ne -1$. The remainder can be shown similarly. □

To state our main result, we introduce the following assumption.

Assumption 2. *$a_\Omega(\boldsymbol{p}_0) \neq a_\Phi(\boldsymbol{p}_0)$ holds with some $\boldsymbol{p}_0 \in \{-1, 1\}^d$.*

Remark 3.4. *If $d = 1$, then Assumptions 1-2 are not compatible. See [12] for $d = 1$.*

Theorem 3.7 (Existence of eigenvalues)**.** *Let $d \geq 2$ and suppose that Assumptions 1-2 holds. Then, there exists $\delta > 0$ such that if $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$ satisfies $\|(\boldsymbol{p}, \boldsymbol{q}) - (\boldsymbol{p}_0, \boldsymbol{0})\|_{\mathbb{R}^d \times \mathbb{C}^d} < \delta$, then there exist eigenvalues of U. Moreover, the following hold.*

(1) If, in addition, $a_\Omega(\boldsymbol{p}_0) < a_\Phi(\boldsymbol{p}_0)$, then $g_-(\lambda_\star)$ and $g_+(\lambda_\star)$ are eigenvalues of U_{I} with some $\lambda_\star \in \mathbb{T}_-$;

(2) If, in addition, $a_\Omega(\boldsymbol{p}_0) > a_\Phi(\boldsymbol{p}_0)$, then $g_-(\lambda_\star)$ and $g_+(\lambda_\star)$ are eigenvalues of U_{I} with some $\lambda_\star \in \mathbb{T}_+$.

Proof. Observe that $\varphi_{\boldsymbol{q}} \neq 0$ and $\lambda(\boldsymbol{q}) > 0$ whenever $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$. By continuity, we have

$$\lim_{\boldsymbol{q} \to \boldsymbol{0}} \|\varphi(\boldsymbol{q})\| = \lim_{\boldsymbol{q} \to \boldsymbol{0}} \lambda(\boldsymbol{q}) = 0, \ \lim_{\boldsymbol{p} \to \boldsymbol{p}_0} a_\Omega(\boldsymbol{p}) = a_\Omega(\boldsymbol{p}_0), \text{ and } \lim_{\boldsymbol{p} \to \boldsymbol{p}_0} a_\Phi(\boldsymbol{p}) = a_\Phi(\boldsymbol{p}_0). \tag{3.11}$$

Suppose that $a_\Omega(\boldsymbol{p}_0) < a_\Phi(\boldsymbol{p}_0)$. Then, there exists $\delta_0 > 0$ such that if $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$ and $\|(\boldsymbol{p}, \boldsymbol{q}) - (\boldsymbol{p}_0, \boldsymbol{0})\|_{\mathbb{R}^d \times \mathbb{C}^d} < \delta_0$, then $\lambda(\boldsymbol{q})(\lambda(\boldsymbol{q}) + a_\Omega(\boldsymbol{p}) - a_\Phi(\boldsymbol{p})) < 0$. By Lemma 3.6 and (3.11),

$$\lim_{(\boldsymbol{p}, \boldsymbol{q}) \to (\boldsymbol{p}_0, \boldsymbol{0})} (1 + a_\Omega(\boldsymbol{p})) \frac{(1 + a_\Phi(\boldsymbol{p}))^2 - \lambda(\boldsymbol{q})^2}{1 + a_\Phi(\boldsymbol{p})} = (1 + a_\Omega(\boldsymbol{p}_0))(1 + a_\Phi(\boldsymbol{p}_0)) > 0.$$

Hence (3.8) holds if $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$ satisfies $\|(\boldsymbol{p}, \boldsymbol{q}) - (\boldsymbol{p}_0, \boldsymbol{0})\|_{\mathbb{R}^d \times \mathbb{C}^d} < \delta$ with some $\delta > 0$. Similarly, $a_\Omega(\boldsymbol{p}_0) > a_\Phi(\boldsymbol{p}_0)$ concludes that (3.9) holds. Applying Theorems 2.1 and 3.5 completes the proof. $\square$

Remark 3.5. *Theorem 3.7 has demonstrated the existence of eigenvalues of U_{I} for sufficiently small $\boldsymbol{q}$. It would be interesting to study the existence of eigenvalues of U_{I} without such a condition.*

Example 3.1. *Let $d = 2$ and set*

$$\Phi := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \Omega := \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ \sqrt{2} \\ 0 \end{pmatrix}, \quad \boldsymbol{p}_0 = (1, 1).$$

Then, $\frac{1}{2} = a_\Omega(\boldsymbol{p}_0) > a_\Phi(\boldsymbol{p}_0) = 0$ and all assumptions in Theorem 3.7 are satisfied with $l = 1$. Hence U has two eigenvalues if $(\boldsymbol{p}, \boldsymbol{q}) \in D_1$ and $\|(\boldsymbol{p}, \boldsymbol{q}) - (\boldsymbol{p}_0, \boldsymbol{0})\|$ is sufficiently small. More precisely, $g_\pm(\lambda_\star) \in \sigma_{\mathrm{p}}(U_{\mathrm{I}})$ with some $\lambda_\star \in \mathbb{T}_+$ if $\boldsymbol{p}$ satisfies

$$p_2 < \frac{5}{2} - \frac{1}{2p_1^2}, \quad 1 < p_1^2 + \frac{4}{9} p_2^2. \tag{3.12}$$

This is because, in this case, (3.12) is equivalent to (3.9) in Theorem 3.5.

4 Feshbach map

4.1 Definition of the Feshbach map

In this subsection, we define the Feshbach map of the discriminant operator T. Recall that $\Pi = |\mathbb{1}_{\{\mathbf{0}\}}\rangle\langle\mathbb{1}_{\{\mathbf{0}\}}|$ and $\Pi^\perp = I_{\mathcal{K}} - \Pi$. Let $\lambda \in \mathbb{C}$ and $(\Pi(T-\lambda)\Pi)_{\mathrm{ran}\Pi}$ be a following operator on $\mathrm{ran}\Pi$:

$$(\Pi(T-\lambda)\Pi)_{\mathrm{ran}\Pi} : \mathrm{ran}\Pi \ni f \mapsto (\Pi(T-\lambda)\Pi)f \in \mathrm{ran}\Pi.$$

Lemma 4.1. *The following conditions are equivalent:*

(1) $\lambda \neq a_\Omega(\boldsymbol{p})$;

(2) There exists an inverse operator of $(\Pi(T-\lambda)\Pi)_{\mathrm{ran}\Pi}$.

In this case,

$$(\Pi(T-\lambda)\Pi)^{-1}_{\mathrm{ran}\Pi} = \frac{1}{a_\Omega(\boldsymbol{p})-\lambda} I_{\mathrm{ran}\Pi}, \tag{4.1}$$

where $I_{\mathrm{ran}\Pi}$ *is an identity map on* $\mathrm{ran}\Pi$.

Proof. Simple calculation show that $\langle \mathbb{1}_{\{\mathbf{0}\}}, \chi^*_{j,1} L_j \chi_{j,2} \mathbb{1}_{\{\mathbf{0}\}}\rangle = 0$ for all $j \in \{1, \cdots, d\}$ and $\Pi(T-\lambda)\Pi = (a_\Omega(\boldsymbol{p})-\lambda)\Pi$ for all $\lambda \in \mathbb{C}$. Hence,

$$(\Pi(T-\lambda)\Pi)_{\mathrm{ran}\Pi} = (a_\Omega(\boldsymbol{p})-\lambda) I_{\mathrm{ran}\Pi} \quad \text{for all } \lambda \in \mathbb{C}.$$

Therefore, (1) and (2) are equivalent and (4.1) holds for $\lambda \neq a_\Omega(\boldsymbol{p})$. □

Lemma 4.1 guarantees that the operator

$$F(\lambda) = \Pi^\perp(T-\lambda)\Pi^\perp - \Pi^\perp T \Pi (\Pi(T-\lambda)\Pi)^{-1}_{\mathrm{ran}\Pi} \Pi T \Pi^\perp$$

is well-defined whenever $\lambda \in \mathbb{C} \setminus \{a_\Omega(\boldsymbol{p})\}$. $F(\lambda)$ is called the Feshbach map of T. The following proposition reveals an isospectral property of the Feshbach map.

Proposition 4.2. *Let* $\lambda \in \mathbb{C} \setminus \{a_\Omega(\boldsymbol{p})\}$. *Then, the following are equivalent:*

(1) $\lambda \in \sigma_{\mathrm{p}}(T)$;

(2) $\ker F(\lambda)$ *is non trivial.*

In this case, $\dim\ker(T-\lambda) = \dim\ker F(\lambda)$.

Proof. See [6]. □

Proposition 4.3. *Let* $\lambda \in \mathbb{C} \setminus \{a_\Omega(\boldsymbol{p})\}$. *Then,* $F(\lambda)$ *is written as*

$$F(\lambda) = \Pi^\perp \left(T_0 - \lambda - \frac{1}{a_\Omega(\boldsymbol{p})-\lambda} |\varphi_{\boldsymbol{q}}\rangle\langle\varphi_{\boldsymbol{q}}| \right) \Pi^\perp.$$

Proof. A simple calculation yields $\Pi T \Pi^\perp = |\mathbb{1}_{\{\mathbf{0}\}}\rangle\langle\varphi_{\boldsymbol{q}}|$. By definition,

$$\begin{aligned} F(\lambda) &= \Pi^\perp \left\{ T - \lambda - \frac{1}{a_\Omega(\boldsymbol{p}) - \lambda} (\Pi T \Pi^\perp)^* (\Pi T \Pi^\perp) \right\} \Pi^\perp \\ &= \Pi^\perp \left(T - \lambda - \frac{1}{a_\Omega(\boldsymbol{p}) - \lambda} |\varphi_{\boldsymbol{q}}\rangle\langle\varphi_{\boldsymbol{q}}| \right) \Pi^\perp. \end{aligned}$$

It suffices to show $\Pi^\perp T \Pi^\perp = \Pi^\perp T_0 \Pi^\perp$. By Lemma 3.2,

$$\Pi^\perp T \Pi^\perp = \Pi^\perp a(\boldsymbol{p}, \cdot) \Pi^\perp + \sum_{j=1}^{d} \left\{ q_j \Pi^\perp \chi_{j,1}^* L_j \chi_{j,2} \Pi^\perp + (q_j \Pi^\perp \chi_{j,1}^* L_j \chi_{j,2} \Pi^\perp)^* \right\}. \tag{4.2}$$

The first term of the right-hand side of (4.2) is calculated as

$$\begin{aligned} \Pi^\perp a(\boldsymbol{p}, \cdot) \Pi^\perp &= \sum_{j=1}^{d} p_j \Pi^\perp (|\chi_{j,1}|^2 - |\chi_{j,2}|^2) \Pi^\perp \\ &= \sum_{j=1}^{d} p_j \sum_{\boldsymbol{x} \neq \mathbf{0}} \sum_{\boldsymbol{y} \neq \mathbf{0}} |\mathbb{1}_{\{\boldsymbol{x}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{x}\}}, (|\chi_{j,1}(\boldsymbol{x})|^2 - |\chi_{j,2}(\boldsymbol{x})|^2) \mathbb{1}_{\{\boldsymbol{y}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{y}\}}| \\ &= \sum_{j=1}^{d} p_j \sum_{\boldsymbol{x} \neq \mathbf{0}} \sum_{\boldsymbol{y} \neq \mathbf{0}} |\mathbb{1}_{\{\boldsymbol{x}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{x}\}}, (|\phi_{j,1}|^2 - |\phi_{j,2}|^2) \mathbb{1}_{\{\boldsymbol{y}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{y}\}}| \\ &= \Pi^\perp a_\Phi(\boldsymbol{p}) \Pi^\perp. \end{aligned}$$

On the other hand,

$$\begin{aligned} \Pi^\perp \chi_{j,1}^* L_j \chi_{j,2} \Pi^\perp &= \sum_{\boldsymbol{x} \neq \mathbf{0}} \sum_{\boldsymbol{y} \neq \mathbf{0}} |\mathbb{1}_{\{\boldsymbol{x}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{x}\}}, \chi_{j,1}^* L_j \chi_{j,2} \mathbb{1}_{\{\boldsymbol{y}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{y}\}}| \\ &= \sum_{\boldsymbol{x} \neq \mathbf{0}} \sum_{\boldsymbol{y} \neq \mathbf{0}} (\chi_{j,1}^* L_j \chi_{j,2} \mathbb{1}_{\{\boldsymbol{y}\}})(\boldsymbol{x}) |\mathbb{1}_{\{\boldsymbol{x}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{y}\}}| \\ &= \sum_{\boldsymbol{x} \neq \mathbf{0}} \sum_{\boldsymbol{y} \neq \mathbf{0}} \chi_{j,1}^*(\boldsymbol{x}) \chi_{j,2}(\boldsymbol{x} + \boldsymbol{e}_j) \mathbb{1}_{\{\boldsymbol{y}\}}(\boldsymbol{x} + \boldsymbol{e}_j) |\mathbb{1}_{\{\boldsymbol{x}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{y}\}}| \\ &= \sum_{\boldsymbol{x} \neq \mathbf{0}} \phi_{j,1}^* \phi_{j,2} |\mathbb{1}_{\{\boldsymbol{x}\}}\rangle\langle\mathbb{1}_{\{\boldsymbol{x} + \boldsymbol{e}_j\}}| \\ &= \Pi^\perp \phi_{j,1}^* \phi_{j,2} L_j \Pi^\perp. \end{aligned}$$

Hence, $\Pi^\perp T \Pi^\perp = \Pi^\perp T_0 \Pi^\perp$. This completes the proof. ☐

Remark 4.1. *In the proof of Proposition 4.3, one defect condition plays an essential role. If the coin has two or more defect, then we can not conclude* $\Pi^\perp \chi_{j,1}^* L_j \chi_{j,2} \Pi^\perp = \Pi^\perp \phi_{j,1}^* \phi_{j,2} L_j \Pi^\perp$.

4.2 Non-triviality of the kernel of $F(\lambda)$

The following proposition ensures the non-triviality of $\ker F(\lambda)$ in the proof of Theorem 3.4. Recall that $\psi_\lambda = (T_0 - \lambda)^{-1}\varphi_{\boldsymbol{q}} \in \mathcal{K}$.

Proposition 4.4. *Suppose that Assumption 1 holds and $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$. Then, $\psi_\lambda \in \mathrm{ran}\Pi^\perp \setminus \{0\}$ for all $\lambda \in [-1, 1] \setminus \sigma(T_0)$.*

To prove Proposition 4.4, we need the following lemma.

Lemma 4.5. *The following are equivalent:*

(1) $\psi_\lambda \in \mathrm{ran}\Pi^\perp$;

(2) $\displaystyle\int_{[0,2\pi]^d} \hat{\psi}_\lambda(\boldsymbol{k}) \frac{d\boldsymbol{k}}{(2\pi)^d} = 0.$

Proof. Since $\Pi^\perp\psi_\lambda = \psi_\lambda$ is equivalent that $\mathcal{F}\Pi^\perp\mathcal{F}^*\hat{\psi}_\lambda = \hat{\psi}_\lambda$, then (1) is equivalent the following:

$$\hat{\psi}_\lambda \in \mathrm{ran}\mathcal{F}\Pi^\perp\mathcal{F}^*. \tag{4.3}$$

Because by direct calculation, $\mathcal{F}\mathbb{1}_{\{\boldsymbol{0}\}} = \mathbb{1}_{[0,2\pi]^d}$, the following holds:

$$\begin{aligned} \mathcal{F}\Pi^\perp\mathcal{F}^*\hat{\psi}_\lambda &= \mathcal{F}(I_\mathcal{K} - \Pi)\mathcal{F}^*\hat{\psi}_\lambda \\ &= (I_{\mathcal{F}\mathcal{K}} - |\mathbb{1}_{[0,2\pi]^d}\rangle\langle\mathbb{1}_{[0,2\pi]^d}|)\hat{\psi}_\lambda \\ &= \hat{\psi}_\lambda - \left(\int_{[0,2\pi]^d} \hat{\psi}_\lambda(\boldsymbol{k}) \frac{d\boldsymbol{k}}{(2\pi)^d}\right) \mathbb{1}_{[0,2\pi]^d}. \end{aligned} \tag{4.4}$$

By (4.3) and (4.4), (1) holds if and only if $\left(\int_{[0,2\pi]^d} \hat{\psi}_\lambda(\boldsymbol{k}) \frac{d\boldsymbol{k}}{(2\pi)^d}\right) \mathbb{1}_{[0,2\pi]^d} = 0$. This proves the lemma. □

Proof of Proposition 4.4. Fix $\lambda \in [-1, 1] \setminus \sigma(T_0)$. Because $\lambda \notin \sigma(T_0)$ and $\varphi_{\boldsymbol{q}} \neq 0$, we observe that $\psi_\lambda \neq 0$. By using (3.5) and changing variables, we have

$$\begin{aligned} &\int_{[0,2\pi]^d} \hat{\psi}_\lambda(\boldsymbol{k}) \frac{d\boldsymbol{k}}{(2\pi)^d} = \int_{[0,2\pi]^d} \frac{\hat{\varphi}_{\boldsymbol{q}}(\boldsymbol{k})}{\hat{T}_0(\boldsymbol{k}) - \lambda} \frac{d\boldsymbol{k}}{(2\pi)^d} \\ &= \int_{[0,2\pi]^d} \frac{\sum_{j=1}^d \left(\varphi_{\boldsymbol{q}}(\boldsymbol{e}_j)e^{-ik_j} + \varphi_{\boldsymbol{q}}(-\boldsymbol{e}_j)e^{ik_j}\right)}{a_\Phi(\boldsymbol{p}) + 2\sum_{j=1}^d |\alpha_j| \cos(k_j + \theta_j) - \lambda} \frac{d\boldsymbol{k}}{(2\pi)^d} \\ &= \int_{\prod_{j=1}^d [\theta_j, 2\pi+\theta_j]} \frac{\sum_{j=1}^d \left(\varphi_{\boldsymbol{q}}(\boldsymbol{e}_j)e^{-i(t_j-\theta_j)} + \varphi_{\boldsymbol{q}}(-\boldsymbol{e}_j)e^{i(t_j-\theta_j)}\right)}{a_\Phi(\boldsymbol{p}) + 2\sum_{j=1}^d |\alpha_j| \cos t_j - \lambda} \frac{d\boldsymbol{t}}{(2\pi)^d} \\ &= \int_{[0,2\pi]^d} \frac{\sum_{j=1}^d \left(\varphi_{\boldsymbol{q}}(\boldsymbol{e}_j)e^{i\theta_j} + \varphi_{\boldsymbol{q}}(-\boldsymbol{e}_j)e^{-i\theta_j}\right) \cos t_j}{a_\Phi(\boldsymbol{p}) + 2\sum_{j=1}^d |\alpha_j| \cos t_j - \lambda} \frac{d\boldsymbol{t}}{(2\pi)^d}. \end{aligned} \tag{4.5}$$

By (3.7), we observe that

$$\varphi_{\boldsymbol{q}}(\boldsymbol{e}_j)e^{i\theta_j} + \varphi_{\boldsymbol{q}}(-\boldsymbol{e}_j)e^{-i\theta_j} = q_j^* e^{i\theta_j}\langle \Phi_j, \sigma_- \Omega_j\rangle, + q_j e^{-i\theta_j}\langle \Phi_j, \sigma_+ \Omega_j\rangle. \tag{4.6}$$

Let $B = \{j \mid q_j \neq 0,\ \langle \Phi_j, \sigma_+\Omega_j\rangle \neq 0\}$. Assumption 1 (b) and $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$ imply $B \neq \emptyset$. If $j \notin B$, then the right-hand side (RHS) of (4.6) is zero, because by $\sigma_1 = \sigma_+ + \sigma_-$, Assumption 1 (a) implies that

$$|\langle \Phi_j, \sigma_+\Omega_j\rangle| = |\Phi_j \cdot (\sigma_+\Omega_j)| = |\Phi_j \cdot (\sigma_-\Omega_j)| = |\langle \Phi_j, \sigma_-\Omega_j\rangle|. \tag{4.7}$$

Let $j \in B$. By (4.7), we have $\phi_{j,1} \neq 0$, $\phi_{j,2} \neq 0$, and hence $\alpha_j = q_j \phi_{j,1}^* \phi_{j,2} \neq 0$. Using $e^{i\theta_j} = q_j\phi_{j,1}^*\phi_{j,2}/|\alpha_j|$, we observe that

$$\begin{aligned}
\text{RHS of (4.6)} &= \left\langle \Phi_j, \begin{pmatrix} 0 & q_j e^{-i\theta_j} \\ q_j^* e^{i\theta_j} & 0 \end{pmatrix} \Omega_j \right\rangle = \frac{|q_j|^2}{|\alpha_j|} \left\langle \begin{pmatrix} 0 & \phi_{j,1}\phi_{j,2}^* \\ \phi_{j,1}^*\phi_{j,2} & 0 \end{pmatrix} \Phi_j, \Omega_j \right\rangle \\
&= \frac{|q_j|^2 \phi_{j,1}^* \phi_{j,2}^*}{|\alpha_j|} \Phi_j \cdot (\sigma_1 \Omega_j) = 0.
\end{aligned}$$

Therefore,

$$\varphi_{\boldsymbol{q}}(\boldsymbol{e}_j)e^{i\theta_j} + \varphi_{\boldsymbol{q}}(-\boldsymbol{e}_j)e^{-i\theta_j} = 0, \quad j = 1, \ldots, d,$$

which, in conjunction with (4.5), gives $\displaystyle\int_{[0,2\pi]^d} \hat{\psi}_\lambda(\boldsymbol{k}) \frac{d\boldsymbol{k}}{(2\pi)^d} = 0$. Lemma 4.5 concludes the proof. ∎

5 Zeros of $\mathfrak{f}$

In this section we prove Theorem 3.5. We henceforth suppose that Assumption 1 holds and fix $(\boldsymbol{p}, \boldsymbol{q}) \in D_l$. Recall that $\mathfrak{f} : [-1, 1] \setminus \sigma(T_0) \to \mathbb{R}$ is defined as

$$\mathfrak{f}(\lambda) = \lambda - a_\Omega(\boldsymbol{p}) + \langle \varphi_{\boldsymbol{q}}, \psi_\lambda \rangle_{\mathcal{K}}$$

and that we set $\mathbb{T}_- = [-1, -\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}))$ and $\mathbb{T}_+ = (\lambda(\boldsymbol{q}) + a_\Phi(\boldsymbol{p}), 1]$. We need the following lemmas.

Lemma 5.1. *The function $\mathfrak{f}$ is continuously differentiable and monotonically increasing.*

Proof. The lemma is evident from

$$\mathfrak{f}'(\lambda) = 1 + \int_{[0,2\pi]^d} \frac{|\hat{\varphi}_{\boldsymbol{q}}(\boldsymbol{k})|^2}{(\hat{T}_0(\boldsymbol{k}) - \lambda)^2} \frac{d\boldsymbol{k}}{(2\pi)^d} > 0.$$

∎

Lemma 5.2. *The following hold:*

(1) If $\lambda \in \mathbb{T}_-$, then

$$\lambda - a_\Omega(\boldsymbol{p}) + \frac{\|\varphi_{\boldsymbol{q}}\|^2}{a_\Phi(\boldsymbol{p}) - \lambda} < \mathfrak{f}(\lambda) < \lambda - a_\Omega(\boldsymbol{p}) + \frac{a_\Phi(\boldsymbol{p}) - \lambda}{(a_\Phi(\boldsymbol{p}) - \lambda)^2 - \lambda(\boldsymbol{q})^2}\|\varphi_{\boldsymbol{q}}\|^2. \quad (5.1)$$

(2) If $\lambda \in \mathbb{T}_+$, then

$$\lambda - a_\Omega(\boldsymbol{p}) + \frac{\|\varphi_{\boldsymbol{q}}\|^2}{a_\Phi(\boldsymbol{p}) - \lambda} > \mathfrak{f}(\lambda) > \lambda - a_\Omega(\boldsymbol{p}) + \frac{a_\Phi(\boldsymbol{p}) - \lambda}{(a_\Phi(\boldsymbol{p}) - \lambda)^2 - \lambda(\boldsymbol{q})^2}\|\varphi_{\boldsymbol{q}}\|^2. \quad (5.2)$$

(3) If $a_\Omega(\boldsymbol{p}) \in [-1, 1] \setminus \sigma(T_0)$, then $\mathfrak{f}(a_\Omega(\boldsymbol{p})) \neq 0$.

Proof. Let $\lambda \in \mathbb{T}_-$. Since $\varphi_{\boldsymbol{q}} \neq 0$, $\mathfrak{f}(\lambda)$ can be written as

$$\mathfrak{f}(\lambda) = \lambda - a_\Omega(\boldsymbol{p}) + \|\varphi_{\boldsymbol{q}}\|^2 \int_{\sigma(T_0)} g_\lambda(x) d\langle \varphi_{\boldsymbol{q}}, E_{T_0}(x)\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2,$$

where $E_{T_0}(\cdot)$ is the spectral measure of T_0 and $g_\lambda(x) = \frac{1}{x-\lambda}$. Note that $\langle \varphi_{\boldsymbol{q}}, E_{T_0}(\cdot)\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2$ is a probability measure on $\sigma(T_0) = [a_\Phi(\boldsymbol{p}) - \lambda_{\boldsymbol{q}}, a_\Phi(\boldsymbol{p}) + \lambda_{\boldsymbol{q}}]$. By Jensen's inequality, we have

$$\begin{aligned}\int_{\sigma(T_0)} g_\lambda(x) d\langle \varphi_{\boldsymbol{q}}, E_{T_0}(x)\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2 &> g_\lambda\left(\int_{\sigma(T_0)} x d\langle \varphi_{\boldsymbol{q}}, E_{T_0}(x)\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2\right) \\ &= g_\lambda\left(\langle \varphi_{\boldsymbol{q}}, T_0\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2\right).\end{aligned}$$

Because $\langle \varphi_{\boldsymbol{q}}, T_0\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2 = a_\Phi(\boldsymbol{p})$, we have,

$$\mathfrak{f}(\lambda) > \lambda - a_\Omega(\boldsymbol{p}) + \|\varphi_{\boldsymbol{q}}\|^2 g_\lambda(a_\Phi(\boldsymbol{p})) = \lambda - a_\Omega(\boldsymbol{p}) + \frac{\|\varphi_{\boldsymbol{q}}\|^2}{a_\Phi(\boldsymbol{p}) - \lambda}. \quad (5.3)$$

Let $u : [a_\Phi(\boldsymbol{p}) - \lambda(\boldsymbol{q}), a_\Phi(\boldsymbol{p}) + \lambda(\boldsymbol{q})] \to \mathbb{R}$ be a linear function such that $u(a_\Phi(\boldsymbol{p}) - \lambda(\boldsymbol{q})) = g_\lambda(a_\Phi(\boldsymbol{p}) - \lambda(\boldsymbol{q}))$ and $u(a_\Phi(\boldsymbol{p}) + \lambda(\boldsymbol{q})) = g_\lambda(a_\Phi(\boldsymbol{p}) + \lambda(\boldsymbol{q}))$, i.e.,

$$u(x) = \frac{-x + 2a_\Phi(\boldsymbol{p}) - \lambda}{(a_\Phi(\boldsymbol{p}) - \lambda)^2 - \lambda(\boldsymbol{q})^2}.$$

By the convexity of g_λ, we have

$$\begin{aligned}\int_{\sigma(T_0)} g_\lambda(x) d\langle \varphi_{\boldsymbol{q}}, E_{T_0}(x)\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2 &< \int_{\sigma(T_0)} u(x) d\langle \varphi_{\boldsymbol{q}}, E_{T_0}(x)\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2 \\ &= \frac{-\langle \varphi_{\boldsymbol{q}}, T_0\varphi_{\boldsymbol{q}}\rangle / \|\varphi_{\boldsymbol{q}}\|^2 + 2a_\Phi(\boldsymbol{p}) - \lambda}{(a_\Phi(\boldsymbol{p}) - \lambda)^2 - \lambda(\boldsymbol{q})^2} \\ &= \frac{a_\Phi(\boldsymbol{p}) - \lambda}{(a_\Phi(\boldsymbol{p}) - \lambda)^2 - \lambda(\boldsymbol{q})^2}.\end{aligned}$$

Hence,

$$\mathfrak{f}(\lambda) < \lambda - a_\Omega(\boldsymbol{p}) + \frac{a_\Phi(\boldsymbol{p}) - \lambda}{(a_\Phi(\boldsymbol{p}) - \lambda)^2 - \lambda_{\boldsymbol{q}}^2} \|\varphi_{\boldsymbol{q}}\|^2. \tag{5.4}$$

(5.3) and (5.4) imply (5.1). Hence (1) is proved. The same proof works for (2).

We prove (3). If $a_\Omega(\boldsymbol{p}) \in \mathbb{T}_-$, then, $a_\Omega(\boldsymbol{p}) < a_\Phi(\boldsymbol{p})$. By (5.3), we have $\mathfrak{f}(a_\Omega(\boldsymbol{p})) > 0$. Similarly, if $a_\Omega(\boldsymbol{p}) \in \mathbb{T}_+$, then $\mathfrak{f}(a_\Omega(\boldsymbol{p})) < 0$. □

Because by Lemma 5.1 $\mathfrak{f}$ is monotonically increasing , $\mathfrak{f}(\lambda)$ has a zero in $\mathbb{T}_-$ if and only if

$$f(-1) \le 0 \quad \text{and} \quad \lim_{\lambda \uparrow a_\Phi(\boldsymbol{p}) - \lambda(\boldsymbol{q})} \mathfrak{f}(\lambda) > 0. \tag{L}$$

Similarly, $\mathfrak{f}(\lambda)$ has a zero in $\mathbb{T}_+$ if and only if

$$f(1) \ge 0 \quad \text{and} \quad \lim_{\lambda \downarrow a_\Phi(\boldsymbol{p}) + \lambda(\boldsymbol{q})} \mathfrak{f}(\lambda) < 0. \tag{R}$$

Proof of Theorem 3.5. Let $\lambda \in \mathbb{T}_-$. By Lemma 5.2, (L) holds if

$$\begin{cases} -1 - a_\Omega(\boldsymbol{p}) + \dfrac{a_\Phi(\boldsymbol{p}) + 1}{(a_\Phi(\boldsymbol{p}) + 1)^2 - \lambda(\boldsymbol{q})^2} \|\varphi_{\boldsymbol{q}}\|^2 \le 0, \\ 0 < a_\Phi(\boldsymbol{p}) - \lambda(\boldsymbol{q}) - a_\Omega(\boldsymbol{p}) + \dfrac{\|\varphi_{\boldsymbol{q}}\|^2}{\lambda(\boldsymbol{q})}, \end{cases} \tag{5.5}$$

which is equivalent to (3.8). Thus, (3.8) concludes (L). This proves (1) of Theorem 3.5. The same proof works for (2). □

Acknowledgments

This work was supported by JSPS Grant in Aid for Young Scientists (B) 26800054.

References

[1] Aharonov, Y., Davidovich, L., Zagury, N.: Quantum random walks, Phy. Rev. A **48**, 1687–1690 (1993)

[2] Ambainis, A., Bach, E., Nayak, A., Vishwanath, A., Watrous, J.: One-dimensional quantum walks, ACM Symp. Theor. Comupt., 37–49 (2001)

[3] Aharonov, D., Ambainis, A., Kempe, J., and Vazirani, U.: Quantum walks on graphs, Proceedings of STOC01, pp. 50–59. quant-ph/0012090.

[4] Ambainis, A.: Quantum walks and their algorithmic applications, *Int. J. Quantum Inf.* **1**, 507–518, (2003)

[5] Ambainis, A., Kempe, J., Rivosh, A.: Coins make quantum walks faster, ACM-SIAM Symp. Discrete Algorithm, 1099–1108 (2005)

[6] Bach, V., Fröhlich, J., Sigal, I. M.: Renormalization group analysis of spectral problems in quantum field theory, *Adv. in Math.*, **137**, 205, (1998).

[7] Cantero, M. J., Grünbaum, F. A., Moral, L. , Velázquez, L.: One dimensional quantum walks with one defect, *Rev. Math. Phys.* **24**, 1250002 (2012).

[8] Childs, A. M., Farhi, E., Gutmann, S.: An example of the difference between quantum and classical random walks, Quantum Inf. Process. **1**, 35–43 (2002).

[9] Feshbach, H.: Unified theory of nuclear reactions, *Ann. Phys.* **5**, 357–390 (1958).

[10] Di Franco, C., Mc Gettrick, M., Busch, Th.: Mimicking the probability distribution of a two-dimensional Grover walk with a single-qubit coin. *Phys. Rev. Lett.* **106**, 080502 (2011).

[11] Fuda, T., Funakawa, D., Suzuki, A.: Weak limit theorem for a one-dimensional split-step quantum walk, in preparation.

[12] Fuda, T., Funakawa, D., Suzuki, A.: Localization of a one-dimensional split-step quantum walk with a position-dependent coin, in preparation.

[13] Gudder, S.: Quantum Probability, Academic Press Inc., Boston (1988).

[14] Grover, L.: A fast quantum mechanical algorithm for database search, ACM Symp. Theor. Comp., 212–219 (1996).

[15] Grössing, G., Zelilinger, A.: Quantum cellular automata, *Complex Systems* **2**, 197 – 208 (1988).

[16] Higuchi, Yu., Konno, N., Sato, I., Segawa, E. : Spectral and asymptotic properties of Grover walks on crystal lattices, *J. Funct. Anal.* **267**, 4197–4235 (2014)

[17] Higuchi, Yu., Segawa, E.: The spreading behavior of quantum walks induced by drifted random walks on some magnifier graph, arXiv:1506.00381 .

[18] Y. Higuchi, E. Segawa, A. Suzuki, Spectral mapping theorem of an abstract quantum walk, arXiv:1506.06457

[19] Hiroshima, F., Sasaki, I., Shirai, T., Suzuki, A.: Note on the spectrum of discrete Schroedinger operators, *J. Math-for-Ind.* **4**, 105–108 (2012).

[20] Inui, K., Konishi, Y., Konno, N.: Localization of two-dimensional quantum walks, *Phys. Rev.* **A69**, 052323 (2004).

[21] Kempe, J.: Quantum random walks: An introductory overview, *Contemp. Phys.* **44**, 307–327 (2003).

[22] Kendon, V.: Quantum walks on general graphs, *Int. J Quantum Inf.* **4**, 791-805 (2006).

[23] Kitagawa, T., Rudner, M. S., Berg, E., Demler, E. : Exploring topological phases with quantum walks, *Phys. Rev. A*, **82**, 033429, (2010).

[24] Konno, N.: Quantum walks, in Quantum Potential Theory (U. Franz and M. Schurmann, Eds.), pp. 309–452, Lecture Notes in Math. 1954, Springer, 2008.

[25] Mackay, T. D., Bartlett, S. D., Stephanson, L. T., Sanders, B. C.: Quantum walks in higher dimensions, *J. Phys. A: Math. Gen.* **35**, 2745 (2002).

[26] Matsue, K., Ogurisu, O., Segawa, E.: A note on the spectral mapping theorem of quantum walk models, arXiv:1604.00581

[27] Machida, T., Segawa, E.: Trapping and spreading properties of quantum walk in homological structure, *Quantum Inf. Process.* 14 (2015) 1539–1558.

[28] Meyer, D: From quantum cellular automata to quantum lattice gases, J. Stat. Phys., **85**, 551–574 (1996).

[29] Magniez, F., Nayak, A., Roland, J., Santha, M.: Search via quantum walk, ACM Symp. Theor. Comput., 575–584 (2007)

[30] Magniez, F., Nayak, A., Richter, P., Santha, M.: On the hitting times of quantum versus random walks, Algorithmica, Springer (2009).

[31] H. Ohno, Unitary equivalent classes of one-dimensional quantum walks, *Quantum Inf. Process.*, **15**, 3599, (2016).

[32] Szegedy, M.: Quantum speed-up of Markov chain based algorithms, Ann. IEEE. Symp. Found., 32–41 (2004)

[33] Segawa, E.: Localization of quantum walks induced by recurrence properties of random walks, J. Comput. Theor. Nanos. **10**, 1583–1590 (2013).

[34] E. Segawa, A. Suzuki, Generator of an abstract quantum walk, *Quantum Stud.: Math. Found.*, **3**, 11, (2016).

[35] Shenvi, N., Kempe, J., Whaley, K.: Quantum random-walk search algorithm, Phys. Rev. A **67**, 052307 (2003)

[36] Tregenna, B., Flanagan, W., Maile, W., Kendon, V.: *New J. Phys.* **5**, 83 (2003).

[37] Venegas-Andraca, S. E.: Quantum walks: a comprehensive review, Quantum Inf. Process. **11**, 1015–1106 (2012).

[38] Watrous, J.: Quantum simulations of classical random walks and undirected graph connectivity, J. Comput. Syst. Sci. **62**, 376–391 (2001)