Eigenvalues, absolute continuity and localizations for periodic unitary transition operators

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The localization phenomenon for periodic unitary transition operators on a Hilbert space consisting of square summable functions on an integer lattice with values in a finite-dimensional Hilbert space, which is a generalization of the discrete-time quantum walks with constant coin matrices, is discussed. It is proved that a periodic unitary transition operator has an eigenvalue if and only if the corresponding unitary matrix-valued function on a torus has an eigenvalue which does not depend on the points on the torus. It is also proved that the continuous spectrum of a periodic unitary transition operator is absolutely continuous. As a result, it is shown that the localization happens if and only if there exists an eigenvalue, and when there exists only one eigenvalue, the long-time limit of transition probabilities coincides with the point-wise norm of the projection of the initial state to the eigenspace. The results can be applied to certain unitary operators on a Hilbert space on a covering graph, called a topological crystal, over a finite graph. An analytic perturbation theory for matrices in several complex variables is employed to show the result about absolute continuity for periodic unitary transition operators.

Keywords: Quantum walks; periodic unitary transition operators; localizations; absolutely continuous spectrum.

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1. Introduction

The term *discrete-time quantum walks* has been recently used to mean probability distributions, which is called transition probabilities, defined by using unitary operators. In this context, the unitary operators are often called unitary

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transition operators or unitary time-evolutions. Originally, the specific class of unitary operators in typical models are formulated in quantum physics² and computer science.^{1,3,20} As in the theory of usual random walks, clarifying the asymptotic behavior, as time goes to infinity, of the transition probability is one of main issues for the investigation of quantum walks. It is well known that asymptotic behavior of quantum walks in typical models are quite different from that of usual random walks. The weak-limit distributions of quantum walks are usually ballistic,^{17,24} and the point-wise asymptotics are also quite different from that of the classical random walks.²³ One of the peculiar properties of quantum walks is a *localization*, which is a phenomenon that the transition probabilities, at some points, do not tend to zero as time goes to infinity. What is interesting is that, the localization phenomenon happens for quantum walks with very simple classes of unitary transition operators, even on the one-dimensional integer lattice, as discussed in Refs. 11, 12 and 13. There are numerous literatures on the localization phenomenon for quantum walks and it would be hard to mention them all, thus we just refer Ref. 18 where the localization properties of a quantum walk on certain infinite graphs called spidernets, not on the usual integer lattices, are discussed.

To be more concrete, let Z be a countable set and let W be a finite-dimensional Hilbert space with the inner product $\langle \cdot, \cdot \rangle_W$. Let U be a unitary operator on the Hilbert space $\ell^2(Z, W)$ consisting of all square summable functions on Z with values in W with the inner product defined by

$$\langle f, g \rangle = \sum_{x \in Z} \langle f(x), g(x) \rangle_W \quad (f, g \in \ell^2(Z, W)). \quad (1.1)$$

For a non-negative integer n , a nonzero vector $u \in \ell^2(Z, W)$ and a point $x \in Z$, we define the quantity $p_n(u; x)$ by

$$p_n(u; x) = \|(U^n u)(x)\|_W^2, \quad (1.2)$$

where $\|\cdot\|_W$ denotes the norm on W defined by the fixed Hermitian inner product. It is straightforward to see that the sum of $p_n(u; x)$ over all $x \in Z$ equals $\|u\|^2$, the norm square of u in $\ell^2(Z, W)$, and hence $p_n(u; x)$ defines a probability distribution on V when $\|u\| = 1$. For this reason, we call, in this note, $p_n(u; x)$ the transition probability for the unitary transition operator U with the initial state u even when u is not a unit vector.

Definition 1.1. The transition probability of the unitary transition operator U with initial state u is said to be localized at a point $x \in Z$ if $\limsup_{n \rightarrow \infty} \times p_n(u; x) > 0$.

In this paper, we mainly consider the integer lattice $\mathbb{Z}^d$ of rank $d \geq 1$ for the set Z and the *periodic unitary transition operators* on $H = \ell^2(\mathbb{Z}^d, W)$ for the unitary operator U , which is defined as follows. For each $y \in \mathbb{Z}^d$ and $\phi \in W$, we define

$\delta_y \otimes \phi \in H$ by the following formula:

$$(\delta_y \otimes \phi)(x) = \begin{cases} \phi & (\text{when } x = y), \\ 0 & (\text{otherwise}). \end{cases}$$

Definition 1.2. A unitary operator U on $H = \ell^2(\mathbb{Z}^d, W)$ is said to be a periodic unitary transition operator if the following two conditions are satisfied:

- The unitary operator U commutes with the natural action of the abelian group $\mathbb{Z}^d$ on H .
- There exists a finite set $S \subset \mathbb{Z}^d$, called the set of steps, such that for any $x \in \mathbb{Z}^d$, $y \in \mathbb{Z}^d \setminus (x + S)$ and any $\phi \in W$, we have $U(\delta_x \otimes \phi)(y) = 0$.

It is obvious that unitary transition operators in the usual model of discrete-time quantum walks with constant coin matrices and products of finite number of such operators are periodic unitary transition operators. To analyze periodic unitary transition operators, it is natural to use the Fourier transform because of their invariance under the action of $\mathbb{Z}^d$. Let T^d be the d -dimensional torus in $\mathbb{C}^d$ defined by

$$T^d = \{z = (z_1, \dots, z_d) \in \mathbb{C}^d; |z_j| = 1 \ (j = 1, \dots, d)\}.$$

Let $\mathcal{H} = L^2(T^d, W)$ be the Hilbert space consisting of all square integrable functions on T^d (with respect to the Lebesgue measure on T^d) with values in W . The normalized Lebesgue measure on T^d is denoted by ν_d . The inner product on $\mathcal{H}$ is defined in a usual manner with the Hermitian inner product on W . Let $\mathcal{F} : \mathcal{H} \rightarrow H$ be the Fourier transform defined by

$$\mathcal{F}(f)(x) = \int_{T^d} z^x f(z) d\nu_d(z) \quad (f \in \mathcal{H}), \quad (1.3)$$

where we write $z^x = z_1^{x_1} \cdots z_d^{x_d}$ for a point $z = (z_1, \dots, z_d)$ in the complex torus $T_{\mathbb{C}}^d = (\mathbb{C} \setminus \{0\})^d$ and a lattice point $x = (x_1, \dots, x_d)$ in $\mathbb{Z}^d$. The Fourier transform $\mathcal{F}$ is a unitary operator with the inverse $\mathcal{F}^* = \mathcal{F}^{-1} : H \rightarrow \mathcal{H}$ given by

$$(\mathcal{F}^* g)(z) = \sum_{x \in \mathbb{Z}^d} g(x) z^{-x} \quad (z \in T^d). \quad (1.4)$$

For a periodic unitary transition operator U , we define a unitary operator $\mathcal{U}$ on $\mathcal{H}$ by $\mathcal{U} = \mathcal{F}^* U \mathcal{F}$. Then, the unitary operator $\mathcal{U}$ can be written in the form

$$(\mathcal{U}f)(z) = \widehat{U}(z)f(z) \quad (f \in \mathcal{H}, z \in T^d) \quad (1.5)$$

with a unitary operator $\widehat{U}(z)$ on the finite-dimensional vector space W given by

$$\widehat{U}(z)\phi = \mathcal{U}(1 \otimes \phi)(z) \quad (\phi \in W), \quad (1.6)$$

where for a scalar function $f \in L^2(T^d)$ and a vector $\phi \in W$, we define $f \otimes \phi \in \mathcal{H}$ by

$$(f \otimes \phi)(z) = f(z)\phi \quad (z \in T^d).$$

Our main theorem is then described as follows.

Theorem 1.3. *For a periodic unitary transition operator U on $\ell^2(\mathbb{Z}^d, W)$, we have the following:*

- (1) *U has an eigenvalue ω if and only if the matrix-valued function $\hat{U}(z)$ on T^d has an eigenvalue ω for all points z in T^d . Hence, the number of eigenvalues of U is finite.*
- (2) *The continuous spectrum of U is absolutely continuous with respect to the Lebesgue measure on the unit circle S^1 in $\mathbb{C}$.*

Therefore, by the absolute continuity of the continuous spectrum, we have the following corollary.

Corollary 1.4. *The periodic unitary transition operator U has no eigenvalues if and only if we have $\limsup_{n \rightarrow \infty} p_n(u; x) = 0$ for any $u \in \ell^2(\mathbb{Z}^d, W)$ and $x \in \mathbb{Z}^d$. Therefore, the localization phenomenon does not happen to the quantum walks defined by such unitary operators.*

A simple observation shows the following corollary.

Corollary 1.5. *Suppose that the periodic unitary transition operator U has only one eigenvalue ω , and let π be the orthogonal projection onto the eigenspace corresponding to the eigenvalue ω . Then, for any $u \in H$ and $x \in \mathbb{Z}^d$, the limit $\lim_{n \rightarrow \infty} p_n(u; x)$ exists and the following formula holds:*

$$\lim_{n \rightarrow \infty} p_n(u; x) = \|(\pi u)(x)\|_W^2. \quad (1.7)$$

It would be necessary here to give some remarks on these results. First, it was pointed out to the author by professor Alain Joye that the singular continuous spectrum of (general unitary operator) U does not affect the *long-time average* of the transition probabilities,

$$\bar{p}(u; x) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N p_n(u; x). \quad (1.8)$$

Indeed, let U be a general unitary operator on $\ell^2(Z, W)$ (for a general countable set Z) and let π_λ be the orthogonal projection onto the eigenspace corresponding to an eigenvalue λ of U . Then, Wiener's formula¹⁶ tells us that the limit $\bar{p}(u; x)$ exists and satisfies

$$\bar{p}(u; x) = \sum_{\lambda: \text{eigenvalue of } U} \|(\pi_\lambda u)(x)\|_W^2. \quad (1.9)$$

From this it is obvious that if U has an eigenvalue then a localization takes place at some point $x \in Z$ and an initial state $u \in \ell^2(Z, W)$. In Corollary 1.5, we take the long-time limit (but not the average) itself of the transition probability under the assumption that U has only one eigenvalue. For example, it is well known that the three-state Grover walk on $\mathbb{Z}$ and the square of the two-dimensional Grover walk satisfy this assumption.

The absolute continuity of continuous spectrum for certain class of self-adjoint operators has been obtained in the work of Gérard–Nier.⁷ The theory developed in Ref. 7 is very powerful, and it might be possible to apply this theory to the generator of the periodic unitary transition operators. However, taking a logarithm of the periodic unitary transition operators would cause singularities of the function corresponding to $\widehat{U}$ introduced above and hence it does not seem so straightforward to apply it. Since our situation is rather easier, it would be reasonable to give a direct and constructive proof of absolute continuity.

Since in the setting up described above the vector space W can be arbitrarily chosen, Theorem 1.3 is applicable to certain unitary operators on topological crystal over finite graphs. As is discussed in Sec. 2, some unitary transition operators are defined over the set of oriented edges. But, the set of vertices, as in the classical case, might be used to formulate quantum system over a topological crystal. Therefore, we use a setting described as follows. As before, let Z be a countable set and let W_0 be a finite-dimensional Hilbert space with the inner product $\langle \cdot, \cdot \rangle_{W_0}$. Suppose that a free abelian group Γ of finite rank d acts on Z freely and the quotient set $Z_0 = Z/\Gamma$ is finite. Let $p : Z \rightarrow Z_0$ be the natural projection. Identifying the finite set Z_0 with a fixed fundamental set F_0 of the action of Γ , we may regard Z_0 as a subset of Z . Let $C(Z, W_0)$ be the vector space of all function from Z to W_0 . Let U be a unitary operator on the Hilbert space $\ell^2(Z, W_0)$ satisfying the following two conditions:

- (i) U commutes with the action of Γ on $\ell^2(Z, W_0)$.
- (ii) There exists a finite set $S \subset \Gamma$ such that, for any $x_0, y_0 \in Z_0$, $\alpha \in \Gamma$, $\beta \in \Gamma \setminus \alpha S$ and $\phi \in W_0$, we have $U(\delta_{\alpha x_0} \otimes \phi)(\beta y_0) = 0$.

Here, we note that the group operation on Γ is written as a multiplication because it would be better to describe the action of Γ on Z . Condition (ii) means that if the quantum walker with the time evolution U start at a point in the fundamental set, αF_0 , the walker can arrive in one step at points in $\bigcup_{\gamma \in S} \gamma \alpha F_0$. Thus, the finite set S depends on the choice of the fundamental set F_0 . Let $\widehat{\Gamma}$ be the group of $U(1)$ -character on Γ . For each $\chi \in \widehat{\Gamma}$, we set

$$C_\chi(Z, W_0) = \{f : Z \rightarrow W_0 ; f(\alpha x) = \chi(\alpha)f(x) \ (x \in Z, \alpha \in \Gamma)\}.$$

The space $C_\chi(Z, W_0)$ is finite-dimensional and is isomorphic to $\ell^2(Z_0, W_0)$, and it is equipped with a natural Hermitian inner product inherited from $\ell^2(Z_0, W_0)$. By the assumption (i), (ii), the operator U is continuous with respect to the topology of point-wise convergence, and thus it defines a linear map on the space of all W_0 -valued function on Z . For each $\chi \in \widehat{\Gamma}$, we define a unitary operator U_χ on $C_\chi(Z, W_0)$ as the restriction of U to $C_\chi(Z, W_0)$.

Corollary 1.6. *Let U be a unitary operator on $\ell^2(Z, W_0)$ satisfying the above two conditions and, for $\chi \in \widehat{\Gamma}$, let U_χ be the unitary operator on $C_\chi(Z, W_0)$ defined as*

above. Then, we have the following:

- (1) U has an eigenvalue ω if and only if the unitary operator U_χ on $C_\chi(Z, W_0)$ has an eigenvalue ω for all points $\chi \in \hat{\Gamma}$. Hence, the number of eigenvalues of U is finite.
- (2) The continuous spectrum of U is absolutely continuous with respect to the Lebesgue measure on the unit circle S^1 in $\mathbb{C}$.

Hence, the statements in Corollaries 1.4 and 1.5 holds true for U .

Organization of this paper is as follows. First, in Sec. 2, the corollaries are proved. Main reason for applicability of Theorem 1.3 to the setting-up in Corollary 1.6 is that, under the assumption (i), (ii), the operator U becomes a periodic unitary transition operator on $\ell^2(Z, W_0) \cong \ell^2(\Gamma, W)$ with $W = \ell^2(Z_0, W_0)$. An example, the Grover walks on topological crystals will be explained in Sec. 2. In Sec. 3, some simple but important properties of periodic unitary transition operators are summarized. The item (1) in Theorem 1.3 is an easy consequence of the formula (1.5), but its proof is written, for completeness of the presentation, in Sec. 4. In Sec. 5, absolute continuity of the continuous spectrum is discussed. In this section, we employ the analytic perturbation theory developed by Baumgärtel⁴ and use a coarea formula to construct a density function of the spectral measures.

2. Proofs of Corollaries

Let Z be, as in Sec. 1, a countable set and let W be a complex vector space of dimension D with a fixed Hermitian inner product $\langle \cdot, \cdot \rangle_W$. Let U be a unitary operator on the Hilbert space $H = \ell^2(Z, W)$ with the inner product given by (1.1). Let $\text{spec}(U)$ and $\text{spec}(U)_p$ denote the spectrum and the set of eigenvalues of U , respectively. Since U is unitary, $\text{spec}(U)$ is contained in the unit circle S^1 in the complex plane, and the spectral resolution of U takes the form

$$U = \int_{S^1} \lambda dE(\lambda), \quad (2.1)$$

where E is a projection-valued measure on S^1 . If $\omega \in \text{spec}(U)_p$, then $\pi_\omega = E(\{\omega\})$ is the projection onto the eigenspace corresponding to ω . We say that $u \in H$ has absolutely continuous spectral measure if the measure $\|E(\cdot)u\|^2$ is absolutely continuous with respect to the Lebesgue measure on the circle. The following lemma can be proved by using the Riemann–Lebesgue lemma.

Lemma 2.1. *Let $u \in H$. Suppose that u has absolutely continuous spectral measure. Then, for any $x \in Z$, we have $\lim_{n \rightarrow \infty} p_n(u; x) = 0$.*

Using Lemma 2.1, it is easy to show the following lemma.

Lemma 2.2. *Suppose that a unitary operator U on H has only one eigenvalue and that the continuous spectrum of U is absolutely continuous. Let π be the orthogonal*

projection onto the eigenspace of U . Then, we have $\lim_{n \rightarrow \infty} p_n(u; x) = \|(\pi u)(x)\|_W^2$ for any $u \in H$ and $x \in Z$.

Proof. The transition probability $p_n(u; x)$ can be written as

$$\begin{aligned} p_n(u; x) &= p_n(\pi u; x) + p_n(\pi_c u; x) + r_n(u; x) \\ &= \|(\pi u)(x)\|_W^2 + p_n(\pi_c u; x) + r_n(u; x), \end{aligned} \quad (2.2)$$

where we set $\pi_c = I - \pi$ and the quantity $r_n(u; x)$ is defined by

$$r_n(u; x) = 2\operatorname{Re} \langle (U^n \pi u)(x), (U^n \pi_c u)(x) \rangle_W. \quad (2.3)$$

By the assumption on the absolute continuity and Lemma 2.1, we see $\lim_{n \rightarrow \infty} p_n(\pi_c u; x) = 0$. Cauchy-Schwarz inequality shows $r_n(u; x) \leq 2\|\pi u(x)\|_{\mathbb{C}^D} \times p_n(\pi_c u; x)^{1/2}$ which tends to zero as $n \rightarrow \infty$. $\square$

Corollaries 1.4 and 1.5 are direct consequences of the Wiener formula (1.9), Lemmas 2.1 and 2.2 and Theorem 1.3.

Next, we give a proof of Corollary 1.6. To begin with, we prepare notation. Let Z be, as before, a countable set and let Γ be a free abelian group of finite rank d . We suppose that Γ acts on Z freely with the finite quotient $Z_0 = Z/\Gamma$. Let $F_0 \subset Z$ be a complete set of representatives of elements in the orbit space Z_0 , which is often called a fundamental set of the action of Γ on Z . The natural projection $p : Z \rightarrow Z_0$ maps F_0 bijectively onto Z_0 . We set $q = (p|_{F_0})^{-1} : Z_0 \rightarrow F_0$. Let U be a unitary operator on $\ell^2(Z, W_0)$ satisfying conditions (i), (ii) described before Corollary 1.6. Define the operator $r : \ell^2(Z, W_0) \rightarrow \ell^2(\Gamma, \ell^2(Z_0, W_0))$ by

$$r(f)(\alpha)(x_0) = f(\alpha q(x_0)) \quad (f \in \ell^2(Z, W_0), \alpha \in \Gamma, x_0 \in Z_0).$$

The operator r is unitary with the natural Hermitian inner product on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$. Since the action of Γ on $\ell^2(Z, W_0)$ is intertwined by the unitary operator $r : \ell^2(Z, W_0) \rightarrow \ell^2(\Gamma, \ell^2(Z_0, W_0))$ with the natural action of Γ on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$, the unitary operator rUr^* on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$ is still Γ -equivariant.

Lemma 2.3. *The unitary operator rUr^* on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$ is a periodic unitary transition operator in the sense of Definition 1.2.*

Proof. Condition (i) for U ensures that rUr^* commutes with the action of Γ on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$. We take a finite set $S \subset \Gamma$ as in condition (ii) imposed on U . Let $\alpha \in \Gamma$ and $\beta \in \Gamma \setminus \alpha S$, and let $f_0 \in \ell^2(Z_0, W_0)$ be arbitrary. We have to compute $rUr^*(\delta_\alpha \otimes f_0)(\beta)$. The function $\delta_\alpha \otimes f_0$ is in $\ell^2(\Gamma, \ell^2(Z_0, W_0))$, and the function in $\ell^2(Z, W_0)$ corresponding to it is given by

$$r^*(\delta_\alpha \otimes f_0) = \sum_{x_0 \in Z_0} \delta_{\alpha q(x_0)} \otimes f_0(x_0). \quad (2.4)$$

Thus, we get

$$Ur^*(\delta_\alpha \otimes f_0) = \sum_{x_0 \in Z_0} U(\delta_{\alpha q(x_0)} \otimes f_0(x_0)).$$

Condition (ii) imposed on U implies that, for $\beta \notin \alpha S$ and $y_0 \in Z_0$, the value at $\beta q(y_0)$ of each of the summand in the right-hand side vanishes. Hence $rUr^*(\delta_\alpha \otimes f_0)(\beta) = 0$ for each $\beta \notin \alpha S$, which shows that rUr^* is a periodic unitary transition operator on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$. $\square$

The map r is naturally extended to the map $r : C(Z, W_0) \rightarrow C(\Gamma, \ell^2(Z_0, W_0))$. Since r commutes with the action of Γ , we have the following isomorphism:

$$r : C_\chi(Z, W_0) \xrightarrow{\cong} \chi \otimes \ell^2(Z_0, W_0), \quad (2.5)$$

where for a function μ on Γ and $f_0 \in \ell^2(Z_0, W_0)$, the function $\mu \otimes f_0 \in C(\Gamma, \ell^2(Z_0, W_0))$ is defined by

$$(\mu \otimes f_0)(\alpha)(x_0) = \mu(\alpha)f_0(x_0) \quad (\alpha \in \Gamma, x_0 \in Z_0).$$

The map r on $C_\chi(Z, W_0)$ composed with the map

$$\chi \otimes \ell^2(Z_0, W_0) \ni \chi \otimes f_0 \mapsto f_0 = (\chi \otimes f_0)(1) \in \ell^2(Z_0, W_0)$$

gives a unitary operator

$$r_\chi : C_\chi(Z, W_0) \xrightarrow{\cong} \ell^2(Z_0, W_0), \quad r_\chi(f) = q^*f. \quad (2.6)$$

The Fourier transform $\mathcal{F} : L^2(\widehat{\Gamma}, \ell^2(Z_0, W_0)) \rightarrow \ell^2(\Gamma, \ell^2(Z_0, W_0))$ and its inverse is given by

$$(\mathcal{F}f)(\alpha)(x_0) = \int_{\widehat{\Gamma}} \rho(\alpha)f(\rho)(x_0) d\nu(\rho), \quad (\mathcal{F}^{-1}g)(\chi)(x_0) = \sum_{\gamma \in \Gamma} \chi(\gamma^{-1})g(\gamma)(x_0),$$

where $f \in L^2(\widehat{\Gamma}, \ell^2(Z_0, W_0))$, $g \in \ell^2(\Gamma, \ell^2(Z_0, W_0))$, $\chi \in \widehat{\Gamma}$, $\alpha \in \Gamma$ and $x_0 \in Z_0$.

Lemma 2.4. *For each $\chi \in \widehat{\Gamma}$, we have $\widehat{rUr^*}(\chi) = r_\chi U_\chi r_\chi^*$, where U_χ is the restriction of U on $C_\chi(Z, W_0)$.*

Proof. We take $f_0 \in \ell^2(Z_0, W_0)$. Then, we have $\mathcal{F}(\mathbf{1} \otimes f_0) = \delta_1 \otimes f_0$, where $\mathbf{1}$ is the function taking the value identically 1 on $\widehat{\Gamma}$ and δ_1 is the delta function at the identity element $1 \in \Gamma$. We see, for $\chi \in \widehat{\Gamma}$,

$$\begin{aligned} \widehat{rUr^*}(\chi)f_0 &= \mathcal{U}(\mathbf{1} \otimes f_0)(\chi) = \sum_{\gamma \in \Gamma} \chi(\gamma)rUr^*(\mathbf{1} \otimes f_0)(\gamma^{-1}) \\ &= \sum_{\gamma \in \Gamma} \chi(\gamma)rUr^*(\delta_\gamma \otimes f_0)(1). \end{aligned}$$

Now, the sum $\sum_{\gamma \in \Gamma} \chi(\gamma)\delta_\gamma \otimes f_0$ converges in the topology of point-wise convergence on $C(\Gamma, \ell^2(Z_0, W_0))$ to the function $\chi \otimes f_0$. Since, by condition (ii), rUr^* is

continuous in this topology, we have

$$\sum_{\gamma \in \Gamma} \chi(\gamma) r U r^* (\delta_\gamma \otimes f_0) = r U r^* (\chi \otimes f_0) = r_\chi U_\chi r_\chi^* f_0,$$

which completes the proof. $\square$

Now, Corollary 1.6 follows from Lemmas 2.3, 2.4 and Theorem 1.3.

We remark that, in the above proof, the space Z is regarded as a product $\Gamma \times Z_0$. This method is, for the setting-up in graph theory, not quite natural because it does not take the graph structure into account. For the setting in graph theory, it would be more transparent to use a unitary operator constructed as follows. We fix a function $s_\chi : Z \rightarrow U(1)$ satisfying $s_\chi(\alpha x) = \chi(\alpha) s_\chi(x)$ for all $\alpha \in \Gamma$, $x \in Z$. Then the operator $S_\chi : \ell^2(Z_0, W_0) \rightarrow C_\chi(Z, W_0)$ given by

$$(S_\chi f_0)(x) = s_\chi(x) f(p(x)) \quad (f_0 \in \ell^2(Z_0, W_0), x \in Z)$$

is a unitary operator. In our setting above, we formulated problems on $\ell^2(\Gamma, \ell^2(Z_0, W_0))$ rather than on $\ell^2(Z, W_0)$. Thus it would be reasonable and useful to use the operator $r_\chi : C_\chi(Z, W_0) \rightarrow \ell^2(Z_0, W_0)$. The operator $S_\chi^{-1} U_\chi S_\chi$ is unitarily equivalent to $r_\chi U_\chi r_\chi^*$ by the operator $r_\chi S_\chi$ which is just the multiplication by the function $q^* s_\chi$. Therefore, the spectral structure of U_χ or $\widehat{r U r^*}(\chi)$ is the same as that of $S_\chi^{-1} U_\chi S_\chi$.

Let us describe an example where Corollary 1.6 can be applied, Grover walks on topological crystals. In the following, the terminology, definitions and the descriptions basically follow that of Refs. 19 and 22. For a graph Y , we denote the set of vertices and the set of oriented edges by $V(Y)$, $E(Y)$, respectively. For any $e \in E(Y)$, the origin $o(e)$ and the terminus $t(e)$ are the vertices which are connected by the oriented edge e in an obvious direction. For any vertex $y \in V(Y)$, we set $E(Y)_y = \{e \in E(Y) ; o(e) = y\}$. Then the degree of $y \in V(Y)$, denoted by $\deg(y)$, is given by the number of elements in $E(Y)_y$. An orientation of the graph $Y = (V(Y), E(Y))$ is a subset $E^o(Y)$ of $E(Y)$ such that $E(Y)$ is written as the disjoint union $E(Y) = E^o(Y) \cup \overline{E^o(Y)}$.

Let X be a topological crystal²² over a connected finite graph X_0 with an abstract periodic lattice Γ , namely, X is an infinite locally finite connected graph on which a free abelian group Γ of rank d ($0 < d < +\infty$) acts freely and without inversion such that the quotient graph is X_0 . The natural projection from X onto X_0 is denoted by $p : X \rightarrow X_0$. A linear map U on the space $C(E(X))$ consisting of all complex-valued function on $E(X)$ defined by

$$(U\phi)(e) = -\phi(\bar{e}) + \frac{2}{\deg(t(e))} \sum_{e' \in E(X)_{t(e)}} \phi(e') \quad (\phi \in C(E(X)), e \in E(X)), \quad (2.7)$$

is often called a *Grover walk*.²⁵ See also Ref. 9, where a generalization, called a *twisted Szegedy walk* is formulated. The restriction of U on $\ell^2(E(X))$, which is also denoted by U , defines a unitary operator on $\ell^2(E(X))$, and U commutes with the

action of Γ . Since the value $(U\phi)(e)$ depends only on $\phi(e')$ and $\phi(\bar{e})$ with the edges e' adjacent to e , the operator U satisfies conditions (i), (ii) described before the statement of Corollary 1.6.

Let us fix $\chi \in \hat{\Gamma}$ and compute the operator $\hat{U}(\chi) \cong U_\chi$ on $\ell^2(E(X_0))$. To compute it, we need to choose a fundamental set F_0 in the set of oriented edges $E(X)$ of the action of Γ . We fix a spanning tree T_0 in X_0 and its lift T in X . For any $u \in E(X_0)$, there exists a unique edge $q(u) \in E(X)$ with the properties $p(q(u)) = u$ and $o(q(u)) \in V(T)$. Then, the finite set $F_0 = q(E(X_0))$ in $E(X)$ is a fundamental set of the action of Γ on $E(X)$. Note that in general $q(\bar{u}) \neq \overline{q(u)}$. But if $u \in E(T_0)$ then we have $q(\bar{u}) = \overline{q(u)}$. We follow the construction of a unitary operator $S_\chi : \ell^2(E(X_0)) \rightarrow C_\chi(X)$ given in Ref. 19. We fix $\omega \in \text{Hom}(\Gamma, \mathbb{R})$ such that $\chi = \exp(2\pi\sqrt{-1}\omega)$. Let $\mu : H_1(X_0, \mathbb{Z}) \rightarrow \Gamma$ be the surjective homomorphism characterized by the identity

$$t(\tilde{c}) = \mu(\langle c \rangle) o(\tilde{c}),$$

where c is a closed path in X_0 , $\tilde{c}$ is a lift of c , $\langle c \rangle$ is the homology class of c (with coefficients in $\mathbb{Z}$) and $t(\tilde{c})$, $o(\tilde{c})$ denote the terminus and origin of the path $\tilde{c}$ in X . We extend μ as a linear map $\mu_{\mathbb{R}} : H_1(X_0, \mathbb{R}) \rightarrow \Gamma \otimes \mathbb{R}$. Since the dual space of $H_1(X_0, \mathbb{R})$ is naturally identified with the cohomology group $H^1(X_0, \mathbb{R})$, the transpose $\mu_{\mathbb{R}}^* : \text{Hom}(\Gamma, \mathbb{R}) \cong (\Gamma \otimes \mathbb{R})^* \rightarrow H^1(X_0, \mathbb{R})$ is an injective linear map. We take a one-form η , which is a function on $E(X_0)$ such that $\eta(\bar{e}) = -\eta(e)$, whose cohomology class is $\mu_{\mathbb{R}}^* \omega \in H^1(X_0, \mathbb{R})$. We have $\omega(\mu(\langle c \rangle)) = \eta(c)$ for any closed path c , where for $c = (e_1, \dots, e_n)$, we write $\eta(c) = \sum_{i=1}^n \eta(e_i)$. We remark that $\eta(c)$ does not depend on the choice of η representing the cohomology class $\mu_{\mathbb{R}}^* \omega$. We fix $e_* \in E(T)$ and define a function $s_\eta : E(X) \rightarrow \mathbb{C}$ by

$$s_\eta(e) = e^{2\pi\sqrt{-1}(p^*\eta)(\gamma(e_*, e))},$$

where $\gamma(e_*, e)$ denotes any path from $o(e_*)$ to $t(e)$ in X such that the first edge of $\gamma(e_*, e)$ is e_* and the last edge is e . Since $\mu(\langle p(\tilde{c}) \rangle) = 1$ for any closed path $\tilde{c}$ on X , the right-hand side in the definition of s_η does not depend on the choice of such a path from $o(e_*)$ to $t(e)$, and we have $s_\eta \in C_\chi(E(X))$. We note that s_η depends on the choice of 1-form η representing $\mu_{\mathbb{R}}^* \omega$ and even the choice of ω . Now, the linear map $S_\chi : \ell^2(E(X_0)) \rightarrow C_\chi(E(X))$ defined by

$$(S_\chi f_0)(e) = s_\eta(e) f_0(p(e)) \quad (f_0 \in \ell^2(E(X_0)), e \in E(X))$$

is a unitary isomorphism. It is straightforward to see

$$\begin{aligned} (S_\chi^{-1} U_\chi S_\chi f_0)(e_0) &= -(e^{2\pi\sqrt{-1}\eta} f_0)(\bar{e}_0) \\ &\quad + \frac{2}{\deg t(e_0)} \sum_{u \in E(X_0)_{t(e_0)}} (e^{2\pi\sqrt{-1}\eta} f_0)(u) \quad (e_0 \in E(X_0)), \end{aligned}$$

which is (unitarily equivalent to) the twisted Szegedy walk whose spectral structure is discussed in Ref. 9.

3. Simple Properties of Periodic Unitary Transition Operators

For $i = 1, \dots, d$, let τ_i be the shift operator on $H = \ell^2(\mathbb{Z}^d, \mathbb{C}^D)$ defined by

$$(\tau_i g)(x) = g(x - e_i) \quad (g \in H, x \in \mathbb{Z}^d),$$

where $\{e_1, \dots, e_d\}$ denotes the standard basis of $\mathbb{Z}^d$ over $\mathbb{Z}$. Then, τ_i 's are unitary operators on H . We note that τ_i and τ_j commutes for any i, j , and hence, for $\alpha = \sum_{i=1}^d \alpha_i e_i$, we may write $\tau^\alpha = \tau_1^{\alpha_1} \dots \tau_d^{\alpha_d}$. The action of $\mathbb{Z}^d$ on H is given by the operators τ^α .

Lemma 3.1. *Let U be a periodic unitary transition operator on H with the set of steps $S \subset \mathbb{Z}^d$. For each $\alpha \in S$, define a linear map $C(\alpha)$ on $\mathbb{C}^D$ by*

$$C(\alpha)\phi = U(\delta_0 \otimes \phi)(\alpha) \quad (\phi \in \mathbb{C}^D).$$

Then, U can be written in the following form:

$$U = \sum_{\alpha \in S} \tau^\alpha C(\alpha).$$

Proof. It is straightforward to see that, for any $\phi \in \mathbb{C}^D$ and $x \in \mathbb{Z}^d$,

$$U(\delta_x \otimes \phi) = \sum_{\alpha \in S} \tau^\alpha \delta_x \otimes C(\alpha)\phi = \left(\sum_{\alpha \in S} \tau^\alpha C(\alpha) \right) (\delta_x \otimes \phi).$$

Since the set $\{\delta_x \otimes \phi\}_{x \in \mathbb{Z}^d, \phi \in \mathbb{C}^D}$ spans H , we conclude the assertion. $\square$

The operator $\mathcal{F}^* \tau_i \mathcal{F}$, where $\mathcal{F} : \mathcal{H} \rightarrow H$ is the Fourier transform defined in (1.3) and $\mathcal{F}^*$ is its inverse, is the multiplication operator defined by the coordinate function z_i , where $z = (z_1, \dots, z_d) \in T^d$. Hence, the operator $\mathcal{U} = \mathcal{F}^* U \mathcal{F}$ is written in the form (1.5) with the matrix $\widehat{U}(z)$ given by the formula

$$\widehat{U}(z)\phi = \sum_{\alpha \in S} z^\alpha C(\alpha)\phi = \mathcal{U}(1 \otimes \phi)(z) \quad (\phi \in \mathbb{C}^D). \quad (3.1)$$

Therefore, by Lemma 3.1 and the assumption that U is a unitary operator, we see

$$\sum_{\alpha, \beta \in S, \alpha - \beta = \gamma} C(\beta)^* C(\alpha) = \delta_{\gamma, 0} I$$

for any $\gamma \in \mathbb{Z}^d$. From this and (3.1), it follows that the matrix $\widehat{U}(z)$ is unitary for any $z \in T^d$. We note that $\widehat{U}(z)$ is a Laurent polynomial in $z \in T^d$ and hence it is naturally extended to the complex torus $T_{\mathbb{C}}^d = (\mathbb{C} \setminus \{0\})^d$. However, in general, $\widehat{U}(z)$ is not normal when z is not in the real torus T^d . We remark that, for a bounded operator A on $H = \ell^2(\mathbb{Z}^d, \mathbb{C}^D)$ commuting with the action of $\mathbb{Z}^d$, the bounded operator $\mathcal{F}^* A \mathcal{F}$ on $\mathcal{H} = L^2(T^d, \mathbb{C}^D)$ commutes with multiplication operators by continuous functions on T^d . The characteristic polynomial

$$\chi(\zeta, z) = \det(\zeta - \widehat{U}(z)) \quad (z \in T_{\mathbb{C}}^d, \zeta \in \mathbb{C}) \quad (3.2)$$

of $\widehat{U}(z)$ is a polynomial in ζ of degree D with coefficients in the ring of Laurent polynomials in $z \in T_{\mathbb{C}}^d$.

Lemma 3.2. *We have the following:*

$$\text{spec}(U) = \{\lambda \in S^1; \text{ There exists a point } z \in T^d \text{ such that } \lambda \text{ is an eigenvalue of } \widehat{U}(z)\}.$$

Proof. It is easy to show that the spectrum $\text{spec}(U)$ is contained in the set in the right-hand side above. Thus, we prove that $\text{spec}(U)$ contains the set in the right-hand side. Suppose that λ is in the resolvent set of U and set $V = \{z \in T^d; \chi(\lambda, z) \neq 0\}$. Then, $\mathcal{R} = (\lambda - U)^{-1}$ is a bounded operator on $\mathcal{H}$. Let $W \subset T^d$ be a Borel set such that $\nu_d(W) = 1$ and $\widehat{R}(z)\phi := (\lambda - U)^{-1}(1 \otimes \phi)(z)$ is defined for any $z \in W$ and any $\phi \in \mathbb{C}^D$. Then, we have $\phi = (\lambda - \widehat{U}(z))\widehat{R}(z)\phi$ for any $z \in W$ and $\phi \in \mathbb{C}^D$. Thus, $W \subset V$. This shows that $\nu_d(V) = 1$ and that V is an open dense set such that $T^d \setminus V$ does not contain any non-empty open set. Therefore we write $\widehat{R}(z) = (\lambda - \widehat{U}(z))^{-1}$ for $z \in V$. We claim that $V = T^d$. To show this, suppose contrary that $T^d \setminus V \neq \emptyset$ and we take $z_o \in T^d \setminus V$. We take $\phi_o \in \mathbb{C}^D$ such that $\|\phi_o\|_{\mathbb{C}^D} = 1$ and $(\lambda - \widehat{U}(z_o))\phi_o = 0$. For any positive integer n , there exists a neighborhood U_n of z_o in T^d such that $\|(\lambda - \widehat{U}(z))\phi_o\|_{\mathbb{C}^D} < 1/(n+1)$ for any $z \in U_n$. Then, for any $z \in U_n \cap V$, we have

$$1 = \|\widehat{R}(z)(\lambda - \widehat{U}(z))\phi_o\|_{\mathbb{C}^D} \leq \|\widehat{R}(z)\|_{\text{op}}\|(\lambda - \widehat{U}(z))\phi_o\|_{\mathbb{C}^D} \leq \|\widehat{R}(z)\|_{\text{op}}/(n+1),$$

where $\|\cdot\|_{\text{op}}$ denotes the operator norm. For each n , we fix $z_n \in U_n \cap V$. One can find $\phi_n \in \mathbb{C}^D$ with $\|\phi_n\|_{\mathbb{C}^D} = 1$ such that $n < \|\widehat{R}(z_n)\phi_n\|_{\mathbb{C}^D}$. There exists a neighborhood V_n of z_n such that $V_n \subset U_n \cap V$ and $n < \|\widehat{R}(z)\phi_n\|_{\mathbb{C}^D}$ for any $z \in V_n$. We take a continuous function f_n on T^d such that the support of f_n is contained in V_n and $\|f_n\|_{L^2(T^d)} = 1$. We set $v_n = f_n \otimes \phi_n = f_n(1 \otimes \phi_n) \in \mathcal{H}$ which satisfies $\|v_n\| = 1$. We see $(\mathcal{R}v_n)(z) = f_n(z)\widehat{R}(z)\phi_n$ for any $z \in W$. Then,

$$\|\mathcal{R}\|_{\text{op}}^2 \geq \|\mathcal{R}v_n\|^2 = \int_{V_n} |f_n(z)|^2 \|\widehat{R}(z)\phi_n\|_{\mathbb{C}^D}^2 d\nu_d(z) \geq n^2,$$

which contradicts the fact that $\mathcal{R}$ is a bounded operator. This shows that $V = T^d$, and hence λ is not an eigenvalue of $\widehat{U}(z)$ for all $z \in T^d$. $\square$

4. Eigenvalues of Periodic Unitary Transition Operators

In this section and the next section, we frequently use the following lemma. This lemma is essentially the same as Lemma 4.4 in Ref. 10. However, we give its proof for convenience.

Lemma 4.1. *Let $\Delta \subset \mathbb{C}^d$ be a domain. Let f be a holomorphic function on Δ . Suppose that $f^{-1}(0) \cap T^d$ has positive Lebesgue measure on T^d . Then f is identically zero on Δ .*

Proof. First, let us assume that Δ is a polydisk in $\mathbb{C}^d$, that is, Δ is a product of d disks in $\mathbb{C}$. We use an induction on the dimension d . When $d = 1$, the assertion is

trivial since $f^{-1}(0) \cap S^1$ is finite if f is not identically zero. Suppose that, for $d \geq 2$, the assertion is true in the dimension $d-1$. Let $\Delta \subset \mathbb{C}^d$ be a polydisk and let f be a holomorphic function on Δ . Suppose that f is not identically zero. We would like to show that $\nu_d(f^{-1}(0) \cap T^d) = 0$. We may assume that $\Delta \cap T^d \neq \emptyset$. In the following, a point in $\mathbb{C}^d$ is written as (z, w) with $z \in \mathbb{C}^{d-1}$ and $w \in \mathbb{C}$. We set $\Delta = V_{d-1} \times V_1$ where $V_{d-1} \subset \mathbb{C}^{d-1}$ is a polydisk and $V_1 \subset \mathbb{C}$ is a disk. For any $(z, w) \in \Delta$, we set $g_w(z) = h_z(w) = f(z, w)$. The functions g_w and h_z are holomorphic on V_{d-1} and V_1 , respectively. Fubini's theorem shows

$$\nu_d(f^{-1}(0) \cap T^d) = \int_{S^1} \nu_{d-1}(g_w^{-1}(0) \cap T^{d-1}) d\nu_1(w).$$

We set $M = \{w \in S^1; \nu_{d-1}(g_w^{-1}(0) \cap T^{d-1}) > 0\}$. We show that $\nu_1(M) = 0$. By induction hypothesis, $w \in M$ if and only if g_w is identically zero on V_{d-1} . Suppose that $M \neq \emptyset$ and we take $w_o \in M$. Since $g_{w_o} = 0$ on V_{d-1} , $h_{z_o}(w_o) = 0$ for any $z \in V_{d-1}$. Since f is not identically zero, one can take a point $z_o \in V_{d-1}$ such that h_{z_o} is not identically zero on V_1 . For such a point, one can take z_o in $V_{d-1} \cap T^{d-1}$ by the induction hypothesis and the assumption that f is not identically zero. Since h_{z_o} is holomorphic on the disk V_1 in $\mathbb{C}$, $h_{z_o}^{-1}(0)$ is a discrete set containing w_o . There exists an open neighborhood I of w_o in V_1 such that $h_{z_o}^{-1}(0) \cap I = \{w_o\}$. We clearly have $M \cap I = \{w_o\}$. This means that M is a discrete set in $S^1 \cap V_1$ and hence M is at most countable and its Lebesgue measure is zero. Now, let $\Delta \subset \mathbb{C}^d$ be a general domain and let f be a holomorphic function on Δ . Since Δ is second countable, one can find a countable open covering $\{\Delta_n\}_{n=1}^\infty$ of Δ such that each Δ_n is a polydisk. Suppose that $\nu_d(f^{-1}(0) \cap T^d) > 0$. Then, we have

$$0 < \nu_d(f^{-1}(0) \cap T^d) \leq \sum_n \nu_d(\Delta_n \cap f^{-1}(0) \cap T^d),$$

and hence there exists an integer n such that $\nu_d(\Delta_n \cap f^{-1}(0) \cap T^d) > 0$. Thus, from what we have just proved above, f is identically zero on Δ_n . Now, the identity theorem for holomorphic functions shows that f is identically zero on Δ . $\square$

Lemma 4.2. *Suppose that U has an eigenvalue λ . Then λ is an eigenvalue of $\widehat{U}(z)$ for any $z \in T_{\mathbb{C}}^d$.*

Proof. Let $0 \neq w \in \mathcal{H}$ be an eigenvector of $\mathcal{U}$ with the eigenvalue λ . Then, there exists a Borel set $W \subset T^d$ such that $\nu_d(W) = 1$ and $\widehat{U}(z)w(z) = \lambda w(z)$ for all $z \in W$. We may set $w(z) = 0$ for $z \in T^d \setminus W$. We have $\chi_\lambda(z) = 0$ for any $z \in T^d \setminus w^{-1}(0)$, where $\chi_\lambda(z) := \chi(\lambda, z)$ is a Laurent polynomial in $z \in T_{\mathbb{C}}^d$. Since $w \neq 0$, we have $\nu_d(T^d \setminus w^{-1}(0)) > 0$. Therefore, Lemma 4.1 shows that the function χ_λ is identically zero on $T_{\mathbb{C}}^d$. Thus, λ is an eigenvalue of $\widehat{U}(z)$ for any $z \in T_{\mathbb{C}}^d$. $\square$

We have to show the converse to Lemma 4.2. Suppose that $\lambda \in S^1$ is an eigenvalue of the unitary matrix $\widehat{U}(z)$ for any $z \in T^d$. By Lemma 4.1, we have $\chi(\lambda, z) = 0$ for any $z \in T_{\mathbb{C}}^d$. Therefore, for each fixed $z \in T_{\mathbb{C}}^d$, the polynomial $\chi(\zeta, z)$ in $\zeta \in \mathbb{C}$

is divisible by $\zeta - \lambda$. However, the multiplicity of $\zeta - \lambda$ in $\chi(\zeta, z)$ depends on $z \in T_{\mathbb{C}}^d$. To handle this situation, let R_d denote the ring of Laurent polynomials in $z = (z_1, \dots, z_d)$ with complex coefficients. The quotient field of R_d , denoted by k_d , is the field of rational functions on $\mathbb{C}^d$. Let $R_d[\zeta]$, respectively $k_d[\zeta]$, be the ring of polynomials in one variable ζ with coefficients in R_d , respectively, in k_d . We have $\chi \in R_d[\zeta] \subset k_d[\zeta]$. Since $\chi(\lambda, z) = 0$ for any $z \in T_{\mathbb{C}}^d$, the polynomial $\zeta - \lambda \in k_d[\zeta]$ divides χ in $k_d[\zeta]$.

Lemma 4.3. *Let $p, q \in k_d[\zeta]$ be monic polynomials and let $r \in R_d[\zeta]$. If $r = pq$, then $p, q \in R_d[\zeta]$.*

Proof. It follows from Lemma 2 in Supplement of Ref. 4 that each coefficient of p and q is holomorphic on $T_{\mathbb{C}}^d$. Thus, what we need is to prove that a rational function $m(z)$ in $z \in \mathbb{C}^d$ which is holomorphic on $T_{\mathbb{C}}^d$ is actually a Laurent polynomial in z . We use an induction on d . Let us consider the case where $d = 1$. Let g/f ($f, g \in \mathbb{C}[z]$) be a rational function holomorphic on $T_{\mathbb{C}}^1$. We may suppose that f and g have no common roots. Since g/f is holomorphic on $T_{\mathbb{C}}^1$, it is possible for f to have a root only at the origin. Thus, f is a monomial and hence g/f is a Laurent polynomial.

Suppose that the assertion holds in the dimension $d - 1$. For $z \in \mathbb{C}^d$, we write, as before, $z = (\xi, w)$ with $\xi \in \mathbb{C}$ and $w = (w_1, \dots, w_{d-1}) \in \mathbb{C}^{d-1}$. Let $m(\xi, w)$ be a rational function in $(\xi, w) \in \mathbb{C}^d$ holomorphic in $T_{\mathbb{C}}^d$. We write $m(\xi, w) = g(\xi, w)/f(\xi, w)$ with polynomials f and g having no common irreducible factors in $\mathbb{C}[\xi, w]$. The assertion is trivial if f is constant. Thus, suppose that f is non-constant. First, suppose that g is a nonzero constant. Since $m = g/f$ is holomorphic on $T_{\mathbb{C}}^d$, f can not be zero on $T_{\mathbb{C}}^d$. Let $s = \xi w_1 \cdots w_{d-1}$. By Hilbert's Nullstellensatz (see, for instance, Chap. 4 of Ref. 6), each irreducible factor of f divides s , and hence f is a monomial. Next, suppose that g is not constant. We may suppose that g has a positive degree in ξ , and we write $g = b_0 \xi^m + \cdots + b_m$ with $m > 0$, $b_j \in \mathbb{C}[w]$ and $b_0 \neq 0$. If f is constant in ξ , then $f \in \mathbb{C}[w]$, and $m = (b_0/f)\xi^m + \cdots + (b_m/f)$. Since b_j/f 's are rational functions on $\mathbb{C}^{d-1}$ holomorphic in $T_{\mathbb{C}}^{d-1}$, the inductive hypothesis shows that these are Laurent polynomials in w . Thus, we may suppose that f and g have positive degrees in ξ . Let f be a polynomial in ξ of degree $l > 0$, and we write $f = a_0 \xi^l + \cdots + a_l$ with $a_j \in \mathbb{C}[w]$ and $a_0 \neq 0$. Let $r \in \mathbb{C}[w]$ be the resultant of the polynomials f, g with respect to ξ . (See, for instance, Chap. 3 of Ref. 6 for the properties of resultants.) Since f and g have no common factors, r is not the zero polynomial. Suppose that $a_l \neq 0$. We set $a = a_l r \in \mathbb{C}[w]$. Then, the polynomial a is not the zero polynomial and $U = \{w \in \mathbb{C}^{d-1}; a(w) \neq 0\}$ is an open dense subset in $\mathbb{C}^{d-1}$. Fix $w_o \in U \cap T_{\mathbb{C}}^{d-1}$. Since $r(w_o) \neq 0$, $f(\xi, w_o)$ and $g(\xi, w_o)$ have no common zeros as polynomials in $\xi \in \mathbb{C}$. Since $m = g/f$ is holomorphic on $T_{\mathbb{C}}^d$, $f(\xi, w_o) = 0$ only at $\xi = 0$. However, since $a_l(w_o) \neq 0$, we have $f(\xi, w_o) \neq 0$ for any $\xi \in \mathbb{C}$, which is a contradiction to the assumption that f has a positive degree in ξ . Thus, a_l is zero. This shows that f is divisible by ξ . We write $f = \xi^k h$ where $k > 0$ and h is a polynomial in $\mathbb{C}[\xi, w]$ which is not divisible by ξ . Then $\xi^k m = g/h$ is again a

rational function holomorphic on $T_{\mathbb{C}}^d$. Applying the above discussion shows that h must be a constant in ξ . Thus, $h \in \mathbb{C}[w]$. Therefore, the previous discussion shows that $\xi^k m = g(\xi, w)/h(w)$ is a Laurent polynomial in (ξ, w) . $\square$

Proof of Theorem 1.3. (1) Suppose, as above, that $\lambda \in S^1$ is an eigenvalue of $\widehat{U}(z)$ for any $z \in T^d$ and hence for any $z \in T_{\mathbb{C}}^d$. We divide χ by $\zeta - \lambda$ in $k_d[\zeta]$ and write $\chi(\zeta, z) = (\zeta - \lambda)^m q(\zeta, z)$, where q is not divisible by $\zeta - \lambda$ in $k_d[\zeta]$. By Lemma 4.3, q is in $R_d[\zeta]$. By the Hamilton–Cayley theorem, we have

$$0 = \chi(\widehat{U}(z), z) = (\widehat{U}(z) - \lambda)^m q(\widehat{U}(z), z) \quad (4.1)$$

as a matrix for any $z \in T_{\mathbb{C}}^d$. We note that $q(\widehat{U}(z), z)$ is not identically zero on T^d . Indeed, suppose contrary that $q(\widehat{U}(z), z) = 0$ for any $z \in T^d$. Then, for any fixed $z \in T^d$, $q(\zeta, z)$ is divisible by the minimal polynomial of the matrix $\widehat{U}(z)$. Since $\widehat{U}(z)$ has λ as an eigenvalue, $q(\zeta, z)$ is divisible by $\zeta - \lambda$ for any $z \in T^d$. Hence $q(\lambda, z) = 0$ for any $z \in T_{\mathbb{C}}^d$ by Lemma 4.1. Thus, q is divisible by $\zeta - \lambda$ in $k_d[\zeta]$ which is a contradiction. Therefore, $q(\widehat{U}(z), z)$ is not identically zero. By the Fourier transform, the bounded operator $q(U, \tau)$ on H is not identically zero. From (4.1), it follows that $0 = \chi(U, \tau) = (U - \lambda)^m q(U, \tau)$. We take $w \in H$ such that $h := q(U, \tau)w$ is not zero. Since $(U - \lambda)^m h = 0$, there exists a number j ($1 \leq j < m$) such that $(U - \lambda)^j h \neq 0$ and $(U - \lambda)^{j+1} h = 0$. Then $v = (U - \lambda)^j h$ is an eigenvector of U with the eigenvalue λ . $\square$

To close this section, it would be worth mentioning that the proof given above also shows the following proposition.

Proposition 4.4. *Let λ be an eigenvalue of the periodic unitary transition operator U on $H = \ell^2(\mathbb{Z}^d, W)$. We decompose the characteristic polynomial $\chi(\zeta, z)$ in $k_d[\zeta]$ in the form $\chi(\zeta, z) = (\zeta - \lambda)^m q(\zeta, z)$, where $q(\zeta, z) \in R_d[\zeta]$ is an irreducible polynomial in $R_d[\zeta]$. Then, for any $w \in \ell^2(\mathbb{Z}^d, W)$, we have $q(U, \tau)w = 0$ or $(U - \lambda)^j q(U, \tau)w$ is an eigenfunction of U for some j with $1 \leq j < m$.*

5. Absolute Continuity of the Continuous Spectrum

Finally, we discuss the absolute continuity of the continuous spectrum of a periodic unitary transition operator U . As before, let $\text{spec}(U)_p = \{\omega_1, \dots, \omega_K\}$ be the set of eigenvalues of U and let π_j be the orthogonal projection onto the eigenspace of U corresponding to ω_j . We set $\pi_p = \pi_1 + \dots + \pi_K$ and $\pi_c = I - \pi_p$. If $\text{spec}(U)_p = \emptyset$, then we set $\pi_p = 0$. The characteristic polynomial χ defined in (3.2) is divisible by $\zeta - \omega_j$ in the ring of polynomials $k_d[\zeta]$ with coefficients in the field k_d of rational functions in $z = (z_1, \dots, z_d)$. The characteristic polynomial χ is monic in the sense that the coefficient of the leading term of χ is the identity in k_d . The ring $k_d[\zeta]$ is a unique factorization domain (UFD for short), and hence $\chi \in k_d[\zeta]$ can be decomposed into powers of monic irreducible elements in $k_d[\zeta]$. It should be remarked that the ring R_d of Laurent polynomials in $z = (z_1, \dots, z_d)$ is a UFD because it

is a localization of the ring $\mathbb{C}[z_1, \dots, z_d]$ of polynomials in z . Thus, $R_d[\zeta]$ is also a UFD, and hence χ can be decomposed into irreducibles in $R_d[\zeta]$. However, we need to use some properties of the notion of discriminants which are valid for polynomials with coefficients in a field. Since the polynomials $\zeta - \omega_j$ are irreducible, the decomposition of χ into monic irreducible elements in $k_d[\zeta]$ can be written as

$$\chi(\zeta, z) = \prod_{j=1}^K (\zeta - \omega_j)^{m_j} \times \prod_{\rho=1}^r \pi_\rho(\zeta, z)^{n_\rho}, \quad (5.1)$$

where $\pi_\rho \in k_d[\zeta]$ are monic irreducible polynomials in $k_d[\zeta]$, and $\zeta - \omega_j$ ($j = 1, \dots, K$) and π_ρ ($\rho = 1, \dots, r$) are mutually different. We set

$$\pi(\zeta, z) = \prod_{j=1}^K (\zeta - \omega_j) \times \prod_{\rho=1}^r \pi_\rho(\zeta, z) \quad (5.2)$$

so that $\chi^{-1}(0) = \pi^{-1}(0) \subset T_{\mathbb{C}}^{d+1}$. If π_ρ ($1 \leq \rho \leq r$) is of the form $\zeta - \lambda$ with a constant $\lambda \in \mathbb{C}$, then $\chi(\lambda, z) = 0$ for any $z \in T_{\mathbb{C}}^d$ and hence by Theorem 1.3, (1), λ is an eigenvalue of the operator U . Thus, $\lambda = \omega_j$ for some $j = 1, \dots, K$. However, π_ρ is different from $\zeta - \omega_j$, and hence it is a contradiction. Thus, π_ρ is not of the form $\zeta - \lambda$ with a constant λ . By Lemma 4.3, each polynomial π_ρ in (5.2) is in $R_d[\zeta]$. Let d_π denote the discriminant of π , namely, $d_\pi = \pm$ resultant of π and $\partial_\zeta \pi$. d_π is a Laurent polynomial in $z \in T_{\mathbb{C}}^d$. Note that d_π is identically zero if and only if π and $\partial_\zeta \pi$ has a common irreducible factor in $k_d[\zeta]$. Since π is a product of mutually different irreducible elements in $k_d[\zeta]$, d_π is not identically zero. Hence the discriminant set $D = d_\pi^{-1}(0) \subset T_{\mathbb{C}}^d$ is an algebraic variety such that $T_{\mathbb{C}}^d \setminus D$ is a connected open dense set (Ref. 8, Chap. 1). By Lemma 4.1, $T^d \cap D$ is a closed set in T^d having Lebesgue measure zero. For any $z \in T_{\mathbb{C}}^d \setminus D$, the equation $\pi(\zeta, z) = 0$ has $K + L = \deg \pi$ distinct roots in $\mathbb{C}$ because $d_\pi = d_\pi(z)$ is the discriminant of $\pi(\zeta, z)$ in $\mathbb{C}[\zeta]$ when z is fixed and hence $\pi(\zeta, z)$ does not have multiple roots for fixed $z \notin D$. (see Ref. 6 for the properties of discriminants.)

Lemma 5.1. *Let $z_o \in T_{\mathbb{C}}^d \setminus D$. Then, there exists a neighborhood $V \subset T_{\mathbb{C}}^d \setminus D$ of z_o and holomorphic functions $\lambda_1(z), \dots, \lambda_L(z)$ on V such that, for each $z \in V$, the roots of the equation $\pi(\zeta, z) = 0$ is given by $\omega_1, \dots, \omega_K, \lambda_1(z), \dots, \lambda_L(z)$.*

Proof. Let $\omega_1, \dots, \omega_K, \lambda_1, \dots, \lambda_L$ be the roots of the equation $\pi(\zeta, z_o) = 0$, each of which is different from others. Let λ_o denote one of λ_j 's. Since $z_o \notin D$ and since $\pi(\lambda_o, z_o) = 0$, we have $\partial_\zeta \pi(\lambda_o, z_o) \neq 0$. Applying the implicit function theorem (Ref. 8, Chap. 1), there exists a neighborhood V of z_o and a holomorphic function $\lambda(z)$ on V such that $\pi(\lambda(z), z) = 0$ for any $z \in V$ and $\lambda(z_o) = \lambda_o$. This shows the lemma. $\square$

The projections onto algebraic (generalized) eigenspaces (called the eigenprojection in Ref. 15) are also holomorphic near $z_o \in T^d \setminus D$. Namely, we have the following lemma.

Lemma 5.2. *Let $z_o \in T_{\mathbb{C}}^d \setminus D$. Let V_o be an open neighborhood of z_o in $T_{\mathbb{C}}^d \setminus D$ as in Lemma 5.1. Then there is an open neighborhood V_1 of z_o in V_o and holomorphic projection-valued functions $R_j(z)$ ($1 \leq j \leq K$), $P_k(z)$ ($1 \leq k \leq L$) such that $R_j(z)$, $P_k(z)$ are the projections onto the algebraic eigenspaces corresponding to ω_j , $\lambda_k(z)$, respectively, for each $z \in V_1$.*

Proof. As before, let $\omega_1, \dots, \omega_K$, $\lambda_1, \dots, \lambda_L$ be mutually different eigenvalues of the matrix $\widehat{U}(z_o)$. Let λ_o be one of them. We take a small circle Γ around λ_o such that Γ and the disk bounded by Γ do not contain any other eigenvalues. Let $\lambda_o(z)$ denote the eigenvalue of $\widehat{U}(z)$ in V_o such that $\lambda_o(z_o) = \lambda_o$ which is holomorphic on V_o , and let $\lambda(z)$ be any other holomorphic function which is an eigenvalue of $\widehat{U}(z)$ in V_o . Since $\lambda_o(z)$ and $\lambda(z)$ are continuous, there exists a neighborhood V_1 of z_o in V_o such that, for each $z \in V_1$, $\lambda(z)$ is not contained in Γ and the disk bounded by Γ and $\lambda_o(z)$ is inside Γ . Then, the eigenprojection $P(z)$ onto the algebraic eigenspace corresponding to $\lambda_o(z)$ along other algebraic eigenspaces is given by the contour integral (Ref. 15, Chap. 1)

$$P(z) = \frac{1}{2\pi i} \int_{\Gamma} (\zeta - \widehat{U}(z))^{-1} d\zeta. \quad (5.3)$$

From this expression, $P(z)$ is holomorphic in $z \in V_1$. $\square$

We remark that, when $z_o \in T^d \setminus D$, $R_j(z)$ and $P_k(z)$ in Lemma 5.2 are smooth functions on $T^d \cap V_1$ which are the orthogonal projections onto the geometric eigenspaces because $\widehat{U}(z)$ is a unitary matrix for $z \in T^d$. For $R_j(z)$, we have the following lemma.

Lemma 5.3. *In the above, $R_j(z)$ ($1 \leq j \leq K$) is extended to $T^d \setminus D$ as a smooth orthogonal projection-valued bounded function, and it is the orthogonal projection onto the eigenspace corresponding to the eigenvalue ω_j of $\widehat{U}(z)$ for each $z \in T^d \setminus D$.*

Proof. For each fixed $z \in T_{\mathbb{C}}^d$, let $R_j(z)$ be the eigenprojection onto the algebraic eigenspace corresponding to the eigenvalue ω_j of $\widehat{U}(z)$ defined by a contour integral as in (5.3). $R_j(z)$ is well-defined as a single-valued function on $T_{\mathbb{C}}^d$. By Lemma 5.2, it is holomorphic on $T_{\mathbb{C}}^d \setminus D$, and hence its restriction to $T^d \setminus D$ is smooth. For $z \in T^d$, $\widehat{U}(z)$ is a unitary matrix and hence $R_j(z)$ is the orthogonal projection onto the (geometric) eigenspaces corresponding to ω_j . Thus, the operator norm of $R_j(z)$ for $z \in T^d$ is bounded. $\square$

Lemma 5.4. *Let $R_j(z)$ be the orthogonal projection-valued functions on $T^d \setminus D$ in Lemma 5.3. Then, the orthogonal projection π_j onto the eigenspace of $\mathcal{U}$ corresponding to the eigenvalue ω_j is given by the following formula:*

$$(\pi_j w)(z) = R_j(z)w(z) \quad (w \in L^2(T^d, \mathbb{C}^D), z \in T^d \setminus D).$$

Proof. Since $T^d \cap D$ has Lebesgue measure zero and since $R_j(z)$ is bounded on $T^d \setminus D$, the right-hand side of the above expression defines a bounded operator R_j on

$L^2(T^d, \mathbb{C}^D)$ which commutes with $\mathcal{U}$. By Lemma 5.3, the image of R_j is contained in that of π_j . But, it is obvious that, for $w \in \text{Im}(\pi_j)$, $w(z)$ is an eigenvector of $\widehat{U}(z)$ with eigenvalue ω_j when $w(z) \neq 0$. Thus, we have $R_j w = w$, which completes the proof. $\square$

For each $z_o \in T^d \setminus D$, we take a small neighborhood V_{z_o} such that $\overline{V_{z_o}}$ is a compact subset contained in a neighborhood of z_o as in Lemmas 5.1 and 5.2. We set $W_{z_o} = V_{z_o} \cap T^d$. We may assume that W_{z_o} is connected. Let $\mathcal{H}(W_{z_o})$ be the closed subspace in $\mathcal{H}$ consisting of all $w \in L^2(T^d, \mathbb{C}^D)$ whose essential support is contained in W_{z_o} . It is obvious that the orthogonal projection onto $\mathcal{H}(W_{z_o})$ is given by the multiplication of the characteristic function of W_{z_o} , and hence it commutes with $\mathcal{U}$. Thus, the spectral projection of $\mathcal{U}$ also commutes with the orthogonal projection onto $\mathcal{H}(W_{z_o})$. Let $R_j(z)$, $P_i(z)$ ($1 \leq j \leq K$, $1 \leq i \leq L$) denote the projection-valued holomorphic function on V_{z_o} given in Lemma 5.2. As in Ref. 15, we have

$$\sum_{j=1}^K R_j(z) + \sum_{i=1}^L P_i(z) = I \quad (z \in V_{z_o}).$$

By Lemma 5.4, for each $w \in \mathcal{H}(W_{z_o})$, we see

$$w(z) = (\pi_p w)(z) + \sum_{i=1}^L P_i(z) w(z)$$

for almost all $z \in W_{z_o}$. Since $w = \pi_p w + \pi_c w$, we have

$$(\pi_c w)(z) = \sum_{i=1}^L P_i(z) w(z) \quad (w \in \mathcal{H}(W_{z_o})). \quad (5.4)$$

From (5.4), we obtain

$$\mathcal{U}^n \pi_c w(z) = \sum_{i=1}^L \lambda_i(z)^n P_i(z) w(z) \quad (w \in \mathcal{H}(W_{z_o})) \quad (5.5)$$

for any integer n . Since the ring of Laurent polynomials on S^1 is dense in the space $C(S^1)$ of continuous functions on S^1 with respect to the supremum norm, we see

$$f(\mathcal{U}) \pi_c w(z) = \sum_{i=1}^L f(\lambda_i(z)) P_i(z) w(z) \quad (w \in \mathcal{H}(W_{z_o})) \quad (5.6)$$

for any $f \in C(S^1)$.

Proposition 5.5. *Let $V_{z_o} \subset T_{\mathbb{C}^D}^d \setminus D$ and $W_{z_o} \subset T^d \setminus D$ be as above. Let $w \in \mathcal{H}(W_{z_o})$. Then, the spectral measure $\|E(\cdot) \pi_c w\|^2$ of $\pi_c w$ is absolutely continuous with respect to the Lebesgue measure.*

Proof. We first show that the gradient $\nabla \lambda_k$ of the eigenvalues $\lambda_k(z)$ ($1 \leq k \leq L$), considered as a function on W_{z_o} , does not vanish almost everywhere on W_{z_o} . To

show this, let $(\theta_1, \dots, \theta_d) \in \mathbb{R}^d$ be a coordinates on W_{z_o} defined so that $z = (e^{i\theta_1}, \dots, e^{i\theta_d}) \in W_{z_o}$. We denote ∂_{θ_j} the partial derivative with respect to θ_j . Then $\partial_{\theta_j} \lambda_k = iz_j \partial_j \lambda_k$ on W_{z_o} , where $\partial_j \lambda_k$ denotes the derivative in z_j of the holomorphic function λ_k . Let $N_k \subset W_{z_o}$ be the set of points $z \in W_{z_o}$ where $\nabla \lambda_k(z) = 0$. Thus, N_k is the intersection of the sets $(\partial_j \lambda_k)^{-1}(0) \cap T^d$ for $j = 1, \dots, d$. If N_k has positive Lebesgue measure on T^d , then by Lemma 4.1, $\partial_j \lambda_k$ vanishes identically on V_{z_o} for any $j = 1, \dots, d$. Therefore, λ_k is constant on V_{z_o} . Now, we have $\pi(\lambda_k, z) = 0$ in $z \in V_{z_o}$. By the identity theorem for holomorphic functions, $\pi(\lambda_k, z) = 0$ for any $z \in T_{\mathbb{C}}^d$. This means that the irreducible monic polynomial $\zeta - \lambda_k \in k_d[\zeta]$ divides π , which is a contradiction to the fact that each π_ρ in (5.2) is not of the form $\zeta - \lambda$. Therefore, $\nabla \lambda_k$ does not vanish almost everywhere on W_{z_o} .

Now, let f be a continuous function on S^1 . Since $P_i(z)$ and $P_j(z)$ ($i \neq j$) are orthogonal to each other for $z \in W_{z_o}$, (5.6) shows

$$\|f(\mathcal{U})\pi_c w\|^2 = \sum_{i=1}^L \int_{W_{z_o}} |f(\lambda_i(z))|^2 \|P_i(z)w(z)\|_{\mathbb{C}^D}^2 d\nu_d(z).$$

As is shown in the above, we have $\nu_d(W_{z_o}) = \nu_d(W_{z_o} \cap N_i^c)$ where N_i^c is the complement of N_i . The function λ_i restricted to $W_{z_o} \cap N_i^c$ has no critical points, and hence for each $t \in S^1$, the set $\lambda_i^{-1}(t) \cap W_{z_o} \cap N_i^c$ is a smooth hyper-surface. For each $t \in S^1$ and $i = 1, \dots, K$, we set

$$\Gamma_i(t) = \int_{\lambda_i^{-1}(t) \cap W_{z_o} \cap N_i^c} \|P_i(z)w(z)\|_{\mathbb{C}^D}^2 \frac{dS_t(z)}{|\nabla \lambda_i(z)|}$$

if $\lambda_i^{-1}(t) \cap W_{z_o} \cap N_i^c \neq \emptyset$, where dS_t denotes the volume element of the hyper-surface $\lambda_i^{-1}(t) \cap W_{z_o} \cap N_i^c$. Then the coarea formula (see Ref. 5 or Ref. 14, Appendix A) shows that $\Gamma_i(t)$ is an L^1 -function on S^1 and

$$\int_{S^1} |f(t)|^2 d\|E(t)\pi_c w\|^2 = \|f(\mathcal{U})\pi_c w\|^2 = \int_{S^1} |f(t)|^2 \Gamma(t) d\nu_1(t), \quad \Gamma(t) = \sum_{i=1}^L \Gamma_i(t),$$

which proves that the measure $d\|E(t)\pi_c w\|^2$ is absolutely continuous with respect to $d\nu_1(t)$. $\square$

Proof of Theorem 1.3(2). For each $z_o \in T^d \setminus D$, we take a small neighborhood V_{z_o} such that $\overline{V_{z_o}}$ is a compact set contained in a neighborhood of z_o as in Lemmas 5.1 and 5.2. We set, as before, $W_{z_o} = T^d \cap V_{z_o}$. Then $\{W_{z_o}\}_{z_o \in T^d \setminus D}$ is an open covering of $T^d \setminus D$. We can choose a locally finite countable open covering $\{W_i\}_{i=1}^\infty$ which is a refinement of a countable sub-covering of the covering $\{W_{z_o}\}_{z_o \in T^d \setminus D}$. We take a partition of unity $\{\rho_i\}_{i=1}^\infty$ subordinated to the covering $\{W_i\}_{i=1}^\infty$. Then, the sum $\sum_{i=1}^\infty M_i$ converges in the strong operator topology and equals the identity operator on $\mathcal{H}$. Let $w \in \mathcal{H}$. Let $\Lambda \subset S^1$ be a Borel subset having Lebesgue measure zero. Since $\mathcal{U}$ commutes with the operator M_i defined by the multiplication by ρ_i ,

the spectral measure $E(\Lambda)$ and the projection π_c also commute with M_i . Therefore, we obtain

$$\langle E(\Lambda)\pi_c w, \pi_c w \rangle = \sum_{i=1}^{\infty} \int_{T^d \setminus D} \|E(\Lambda)\pi_c(\rho_i^{1/2} w)(z)\|_{\mathbb{C}^D}^2 d\nu_d(z).$$

Now Proposition 5.5 shows that $E(\Lambda)\pi_c(\rho_i^{1/2} w) = 0$ in $\mathcal{H}$. Therefore, we have $E(\Lambda)\pi_c w = 0$, which completes the proof of Theorem 1.3(2). $\square$

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