Random Quantum Walks and Non-Unitary Band Operators

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We consider the transport properties of random quantum walks on the lattice under a constraint on the motion in a certain direction. This leads naturally to the study of random contraction operators on $l^2(\mathbb{Z})$ with a band structure, that can be considered as non-unitary deformations of unitary CMV matrices. We describe recent results on the spectral properties of the latter and their consequences on the random quantum walks they stem from.

Keywords: Band matrices, random quantum walks.

1. Introduction

Quantum walks, deterministic or random, appear at the crossroads between Physics, Computer Science and Mathematics, thanks to their versatility. They are used as effective discrete time dynamics of complex quantum systems in appropriate regimes, they appear as building blocks in the design of quantum algorithms as well as tools to assess their efficiency, and they are also considered as non-commutative extensions of classical random walks in deterministic or random environments, see *e.g.* Ref. 1–3.

We define a quantum walk on an infinite graph as a unitary operator on the Hilbert space of a particle with an internal degree of freedom or spin, which describes the way the particle hops on the vertices, depending on the state of its spin. The latter is also called "coin state". The unitary operators only couple sites that are nearest neighbors on the underlying graph. In case of the lattice $\mathbb{Z}^d$, the spin space is $\mathbb{C}^{2d}$ and a deterministic quantum walk is defined as the composition of the action of a unitary matrix C acting on the spin variable only, followed by a shift on $\mathbb{Z}^d$, depending on the spin of the particle. A random quantum walk is supplemented by site and spin dependent random phases which make the environment in which the particle moves disordered. In both cases, the deterministic matrix C is a parameter of the walk.

The spectral properties of quantum walks are closely related to the existence of transport, see e.g. Ref. 4. For random quantum walk with *i.i.d.* disorder, it is known (Ref 5–7) that dynamical localization always takes place for $d = 1$, and for $d > 1$ provided C is close enough to certain permutation matrices, a condition to be interpreted as a large disorder regime. In case the underlying graph is a tree, a spectral transition monitored by the spin matrix takes place as described in Ref. 8.

In this note, we consider random quantum walks $U_\omega(C)$ on $\mathbb{Z}^2$ characterized by a spin matrix $C \in U(4)$ that allow the quantum walker to move freely horizontally, but constraint it to move upwards only. We describe our recent results (Ref. 9) on the transport properties of such random quantum walks addressed through their spectra and their connections with random contraction operators on $l^2(\mathbb{Z})$ which are non-unitary deformations of certain random CMV matrices. In a nutshell, we consider the restriction of the random quantum walk to the horizontal subspace to get a random non-normal contraction T_ω with a band structure in the natural orthonormal basis of the problem, which depends parametrically on C. It turns out the structure and spectral properties of T_ω are instrumental in the determination of the spectrum of $U_\omega(C)$. In particular, the fact that T_ω is (generically) completely non unitary implies that $\sigma(U_\omega(C))$, the spectrum of $U_\omega(C)$, is purely absolutely continuous, an expression of delocalization, see Theorem 5.3. Beyond this result, motivated by the fact that the random contractions T_ω obtained this way are natural deformations of the well known (extended) CMV matrices of the theory of unitary operators, see Ref. 3, we further analyze the spectrum of these non-normal operators parametrized by the spin matrices C. We finally remark that the results described here also hold, *mutatis mutandis*, for random quantum walks defined on trees with coordination number 4, as explained in Ref. 9.

2. Random Quantum Walk on $\mathbb{Z}^2$

We define a random quantum walks on the regular lattice $\mathbb{Z}^2$ with spin space $\mathbb{C}^4$, *i.e.* a unitary random operator on $\mathcal{K} = l^2(\mathbb{Z}^2) \otimes \mathbb{C}^4$. The standard basis of $\mathbb{C}^4$ is denoted by $\{|\tau\rangle\}_{\tau\in I}$, where $I = \{+1, -1, +2, -2\}$ and that of $l^2(\mathbb{Z}^2)$ by $\{|x\rangle\}_{x\in\mathbb{Z}^2}$. The corresponding basis vectors of the tensor product $\mathcal{K}$ will be written as $|x \otimes \tau\rangle = |x\rangle \otimes |\tau\rangle$ and the unit vector in $\mathbb{R}^2$ by e_j, $j = 1, 2$.

Let S be the spin state dependent shift operator defined on $\mathcal{K}$ by

$$S|x \otimes \tau\rangle = |x + \mathrm{sign}(\tau)e_{|\tau|} \otimes \tau\rangle,$$

and $C \in U(4)$ be a unitary spin matrix on $\mathbb{C}^4$. Then the unitary operator $U(C)$ on $\mathcal{K}$ is given by

$$U(C) = S(\mathbb{I} \otimes C) = \sum_{\substack{\tau\in I\\ x\in\mathbb{Z}^2}} |x + \mathrm{sign}(\tau)e_{|\tau|}\rangle\langle x| \otimes |\tau\rangle\langle\tau|C, \tag{1}$$

defines a deterministic quantum walk.

Consider now $\mathbb{T}^{\mathbb{Z}^2\times I}$ as a probability space with σ algebra generated by the cylinder sets and measure $\mathbb{P} = \otimes_{\substack{y\in\mathbb{Z}^2\\ \tau\in I}} d\mu$ where $d\mu$ is a probability measure on the torus $\mathbb{T}$. Introduce accordingly the set of *i.i.d.* random variables $\omega_x^\tau \in \mathbb{T}$ labeled by

$x \in \mathbb{Z}^2$ and $\tau \in I$, with common distribution $d\mu$. We construct a diagonal random unitary operator $\mathbb{D}(\omega)$ on $\mathcal{K}$ by

$$\mathbb{D}(\omega)\,|x \otimes \tau\rangle = e^{i\omega_x^\tau}|x \otimes \tau\rangle. \tag{2}$$

Eventually, we define the random evolution operator $U_\omega(C) : \mathcal{K} \to \mathcal{K}$ as

$$U_\omega(C) = \mathbb{D}(\omega)U(C). \tag{3}$$

We focus here on spin matrices C having a diagonal element of modulus one. Without loss of generality, we assume C has the following form in the ordered basis $\{|+1\rangle, |+2\rangle, |-1\rangle, |-2\rangle\}$,

$$C = \begin{pmatrix} \alpha & r & \beta & 0 \\ q & g & s & 0 \\ \gamma & t & \delta & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix} \equiv \begin{pmatrix} \tilde{C} & \mathbf{0} \\ \mathbf{0}^T & e^{i\theta} \end{pmatrix} \in U(4), \quad \text{where } \tilde{C} = \begin{pmatrix} \alpha & r & \beta \\ q & g & s \\ \gamma & t & \delta \end{pmatrix} \in U(3), \tag{4}$$

with $\theta \in \mathbb{T}$ and $0 \leq g \leq 1$. The assumption $g \geq 0$ always holds at the price of a multiplication of C, and thus of $U_\omega(C)$, by a harmless global phase.

3. Reduction to the horizontal subspace

By construction, $U_\omega(C)$ admits the subspace $\mathcal{K}_{-2}$ characterized by a spin variable equal to -2, as an invariant subspace on which it acts as the shift, up to phases. Using that the absolutely continuous subspace of a unitary operator U is given by

$$\mathcal{H}^{ac}(U) = \overline{\Big\{\phi \mid \sum_{n\in\mathbb{N}} |\langle\phi|U^n\phi\rangle|^2 < \infty\Big\}}, \tag{5}$$

we get

$$\sigma\left(U_\omega(C)|_{\mathcal{K}_{-2}}\right) = \sigma_{ac}\left(U_\omega(C)|_{\mathcal{K}_{-2}}\right) = \mathbb{S}. \tag{6}$$

Let $\mathcal{K}_{-2}^\perp$ be the complementary invariant subspace

$$\mathcal{K}_{-2}^\perp = \overline{\text{span}}\Big\{x \otimes \tau \mid x \in \mathbb{Z}^2, \tau \in \{+1, -1, +2\}\Big\}, \tag{7}$$

where the notation $\overline{\text{span}}$ means the closure of the span of vectors considered. On $\mathcal{K}_{-2}^\perp$ the action of $U_\omega(C)$ on the quantum walker makes it move horizontally back and forth, but it only makes it go up vertically. In a sense, the dynamics induces a leakage of the vectors in the direction corresponding to the spin state $|+2\rangle$. Note that by construction, for all $x \in \mathbb{Z}^2$, all $\tau \in \{+1, +2, -1\}$

$$\langle x \otimes +2|U_\omega(C)^n x \otimes \tau\rangle = \delta_{n,0}\delta_{+2,\tau}, \quad \forall\, n \in \mathbb{N}, \forall\, x \in \mathbb{Z}^2. \tag{8}$$

In particular we get that all spectral measures $d\mu_{x\otimes+2}(\theta) = \frac{d\theta}{2\pi}$ on $\mathbb{T}$ and $\sigma\left(U_\omega(C)|_{\mathcal{K}^\perp}\right) = \mathbb{S}$ as well. We thus have,

$$\mathcal{H}_2 = \overline{\text{span}}\Big\{x \otimes \tau \mid x \in \mathbb{Z}^2, \tau \in \{+2, -2\}\Big\} \subset \mathcal{H}^{ac}(U_\omega(C)). \tag{9}$$

Next we look at the horizontal subspace defined by

$$\mathcal{H}_0 = \overline{\text{span}} \Big\{ (x,0) \otimes \tau \mid x \in \mathbb{Z}, \tau \in \{+1,-1\} \Big\} \subset \mathcal{K}_{-2}^{\perp} \subset \mathcal{K}, \tag{10}$$

and $P_0 : \mathcal{K} \to \mathcal{K}$, the orthogonal projector onto $\mathcal{H}_0$. To study $P_0 U_\omega(C)^n P_0$, $n \geq 0$, we first note the following simple lemma;

Lemma 3.1. *Let $T_\omega : \mathcal{H}_0 \to \mathcal{H}_0$ be defined by $T_\omega = P_0 U_\omega(C) P_0|_{\mathcal{H}_0}$ and $T = T_\omega|_{\omega=(\cdots,0,0,0,\cdots)}$. Then, T_ω is a contraction,*

$$T_\omega = \mathbb{D}_\omega^0 T, \ \text{where} \ \ \mathbb{D}_\omega^0 = \text{diag}\,(e^{i\omega_x^\tau}), \tag{11}$$

and, for any $n \in \mathbb{N}$, $P_0 U_\omega(C)^n P_0|_{\mathcal{H}_0} = T_\omega^n$.

Identifying the subspace $\mathcal{H}_0$ with $l^2(\mathbb{Z})$, we get a representation of T_ω by a 5-diagonal doubly infinite matrix. Let $\{e_j\}_{j\in\mathbb{Z}}$, resp. $\{x \otimes \tau\}_{x\in\mathbb{Z}}^{\tau\in\{+1,-1\}}$, be the canonical orthonormal basis of $l^2(\mathbb{Z})$, resp. $\mathcal{H}_0$. We map the latter to the former according to the rule $e_{2j} = j \otimes +1$, $\ e_{2j+1} = j \otimes -1$, $\ j \in \mathbb{Z}$, and relabel the random phases ω_x^τ accordingly, so that we can identify T_ω with the matrix

$$T_\omega = \mathbb{D}_\omega^0 T = \begin{pmatrix} \ddots & e^{i\omega_{2j-1}}\gamma & e^{i\omega_{2j-1}}\delta & & & \\ & 0 & 0 & & & \\ & 0 & 0 & e^{i\omega_{2j+1}}\gamma & e^{i\omega_{2j+1}}\delta & \\ & e^{i\omega_{2j+2}}\alpha & e^{i\omega_{2j+2}}\beta & 0 & 0 & \\ & & & 0 & 0 & \\ & & & e^{i\omega_{2j+4}}\alpha & e^{i\omega_{2j+4}}\beta & \ddots \end{pmatrix}, \tag{12}$$

where the dots mark the main diagonal, the first column is the image of the vector e_{2j}, and the entries are constrained by (4). We explain in Ref. 9 how to extend the spectral results on T_ω below to random contractions of a more general five-diagonal structure.

4. Polar decomposition of T_ω

To tackle the non-normal random contraction T_ω, we look at the properties of its polar decomposition. First note that when $g = 1$, the original random quantum walk characterized by (4) decouples into one-dimensional problems the solutions of which are known, see Ref. 5. Thus, we assume $0 \leq g < 1$.

Let us consider the unique decomposition $T_\omega = V_\omega K_\omega$, where K_ω is a non negative operator on $l^2(\mathbb{Z})$ and V_ω is an isometry on $l^2(\mathbb{Z})$. We note that due to (11), K_ω is deterministic since $T_\omega^* T_\omega = T^* T = K^2$. A straightforward computation shows that

Proposition 4.1. *The contraction T_ω defined on $l^2(\mathbb{Z})$ by (12) admits the polar decomposition $T_\omega = V_\omega K$, where $0 \leq K \leq \mathbb{I}$ is given by*

$$K = P_1 + g P_2, \quad \text{with} \ \ \sigma(K) = \sigma_{ess}(K) = \{1, g\} \ \ \text{and} \ \ \|K\| = 1. \tag{13}$$

The isometry V_ω is unitary on $l^2(\mathbb{Z})$ and takes the form $V_\omega = \mathbb{D}^0_\omega V$, with

$$V = \frac{1}{1+g}\begin{pmatrix} \ddots & \gamma(1+g)-qt & \delta(1+g)-st & & & \\ & 0 & 0 & & & \\ & 0 & 0 & \gamma(1+g)-qt & \delta(1+g)-st & \\ & \alpha(1+g)-qr & \beta(1+g)-sr & 0 & 0 & \\ & & & 0 & 0 & \\ & & & \alpha(1+g)-qr & \beta(1+g)-sr & \ddots \end{pmatrix}, \tag{14}$$

the dots mark the main diagonal and the first column is the image of the vector e_{2j}.

Remark 4.1. Actually, K is tri-diagonal in the canonical basis as the infinite dimensional spectral projectors P_j, $j = 1, 2$ are given by

$P_j = \bigoplus_{k\in\mathbb{Z}} Q_j^{(k)}$, $j = 1, 2$,

with $Q_1^{(k)} = \frac{1}{|q|^2+|s|^2}\begin{pmatrix} |s|^2 & -\bar{q}s \\ -q\bar{s} & |q|^2 \end{pmatrix} = \mathbb{I}_2 - Q_2^{(k)}$ acting on $\text{span}\{e_{2k}, e_{2k+1}\}$.

The unitary operator V_ω defines a one dimensional random quantum walk studied in Ref. 5

5. Analysis of the contraction T_ω

5.1. *Structure of T_ω and Spectrum of $U_\omega(C)$*

A contraction is said to be completely non-unitary, cnu for short, if it possesses no non-trivial closed invariant subspace on which it is unitary, see *e.g.* Ref. 10.

Lemma 5.1. *Let $0 \le g < 1$. Then, for all $\omega \in \Omega$, the operator T_ω is either cnu or it is unitarily equivalent to the direct sum of a shift and of g times a shift;*

$$\sigma_p(T_\omega) \cap \mathbb{S} = \emptyset, \quad \textit{and for } 0 < g < 1, \quad \sigma_p(T_\omega) \cap g\mathbb{S} = \emptyset. \tag{15}$$

Proof: Assume there is a closed subspace $\mathfrak{h}_0$ such that $T_\omega|_{\mathfrak{h}_0}$ is unitary. For $\psi \in \mathfrak{h}_0$, we have $\|T_\omega\psi\| = \|\psi\|$. This implies with $T_\omega = V_\omega(P_1 + gP_2)$, that

$$(\mathbb{I} - T_\omega^* T_\omega)^{1/2}\psi = \sqrt{1-g^2}P_2\psi = 0. \tag{16}$$

Hence, $\mathfrak{h}_0 \subset P_1\mathcal{H}_0$, and, $\mathfrak{h}_0$ being invariant under T_ω, $\mathfrak{h}_0 \subset \text{Ker}P_2V_\omega P_1$. A more detailed study [9] of the operator $P_2V_\omega P_1$ shows that $\text{Ker}P_2V_\omega P_1 \neq \{0\} \Leftrightarrow P_2V_\omega P_1 = 0$ and that this is equivalent to

$$\tilde{C} \in \left\{ \begin{pmatrix} \alpha & r & 0 \\ q & g & 0 \\ 0 & 0 & \delta \end{pmatrix}, \begin{pmatrix} \alpha & 0 & 0 \\ 0 & g & s \\ 0 & t & \delta \end{pmatrix} \right\} \subset U(3). \tag{17}$$

Hence if (17) doesn't hold, T_ω is cnu. In case (17) holds, a straightforward calculation shows that the subspaces $\mathcal{H}_+ = \overline{\text{span}}\{e_{2j}\}_{j\in\mathbb{Z}}$ and $\mathcal{H}_- = \overline{\text{span}}\{e_{2j+1}\}_{j\in\mathbb{Z}}$

reduce T_ω. We have, $T_\omega = T_\omega^{(+)} \oplus T_\omega^{(-)}$, where, $T_\omega^{(+)} = T_\omega|_{\mathcal{H}_+}$ is unitarily equivalent to $|\alpha|S_+$, similarly $T_\omega^{(+)} = T_\omega|_{\mathcal{H}_+}$ is unitarily equivalent to $|\delta|S_-$, with $S_\pm$ the standard shifts on $\mathcal{H}_\pm$. Since $g = \min(|\alpha|, |\delta|)$, then $\sigma(T_\omega) = \mathbb{S} \cup g\mathbb{S}$. This finishes the proof of the first statement. The fact that eigenvalues cannot sit on the unit circle is thus immediate, whereas, for $g > 0$, a similar argument applied to the contraction $(gT_\omega^{-1})^* = V_\omega(gP_1 + P_2)$ yields the last statement. ∎

Remark 5.2. The operator T_ω is cnu if and only if $0 \le g < 1$, $|\alpha| < 1$ and $|\delta| < 1$. Moreover, in case (17) holds, the corresponding random quantum walk operator $U_\omega(C)$ is purely ac by a general argument, see Ref. 9.

The fact that T_ω is completely non-unitary has immediate consequences on the spectrum of $U_\omega(C)$. In particular,

Theorem 5.3. *If $0 \le g < 1$, then $\sigma(U_\omega(C)) = \sigma_{ac}(U_\omega(C))$, for all $\omega \in \Omega$.*

Proof: We drop the dependence on ω and C in the notation for this proof, for simplicity. By Lemma 5.1, we can assume T is completely non-unitary. Let P_{sing} be the spectral projection onto the singular subspace $\mathcal{H}^{sing} = \mathcal{H}^{pp}(U) \cap \mathcal{H}^{sc}(U)$ and recall that P_0 is the orthogonal projection onto $\mathcal{H}_0$. We first show that the subspace $\mathcal{H}_0 \cap \mathcal{H}^{sing}$ reduces the operator U. Let $\psi \in \mathcal{H}_0 \cap \mathcal{H}^{sing}$,

$$U\psi = UP_{sing}\psi = P_{sing}U\psi = P_{sing}\big(P_0U\psi + (\mathbb{I} - P_0)U\psi\big), \tag{18}$$

where $(\mathbb{I} - P_0)U\psi \in \mathcal{H}_b$, see (9). Using $P_{sing}\mathcal{H}_b = 0$, we get that $U\psi = P_{sing}P_0U\psi$. But then $\|U\psi\| \le \|P_0U\psi\| \le \|U\psi\|$ implies $U\psi = P_0U\psi = P_0P_{sing}U\psi$ as well. Hence $\mathcal{H}_0 \cap \mathcal{H}^{sing}$ is invariant under U. By a similar argument, this subspace is invariant under U^* as well. Consequently, $\mathcal{H}^{sing}$ reduces $T = P_0U|_{\mathcal{H}_0}$, which shows that $\mathcal{H}^{sing} \cap \mathcal{H}_0 = \{0\}$ since T is cnu and $g < 1$. Repeating the argument with $\mathcal{H}_0$ replaced by arbitrary horizontal subspace yields $\mathcal{H}^{sing} = \{0\}$. ∎

5.2. *Spectral Analysis of T_ω*

We simply state a few of the results on the spectrum of T_ω provided in Ref. 9. We denote the spectral radius of T_ω by spr (T_ω) and its resolvent set by $\rho(T_\omega)$.

The polar decomposition of the operator T_ω in Proposition 4.1 strongly suggests a block decomposition with respect to the orthogonal projection P_j, $j = 1, 2$, and the use of the Feschbach-Schur method. This allows us to localize the spectrum of T_ω in an annulus. Consider $P_jVP_k = V_{jk}$, $j, k \in \{1, 2\}$, as operators on $P_k\mathcal{H}$ and g as a control parameter.

Proposition 5.1. *Let $T_\omega = V_\omega(P_1 + gP_2)$, where P_j are defined in (13) and $0 \le g < 1$. If $\|V_{11}\| < 1$, and $g < (1 - \|V_{11}\|)/(\|V_{21}\|\|V_{12}\| + \|V_{22}\|(1 - \|V_{11}\|))$ then, the set $\{|z| < g\} \cup \{r(V) < |z| \le 1\} \subset \rho(T_\omega)$ for all realizations $\omega \in \Omega$, where*

$$r(V) = \frac{1}{2}\left(\|V_{11}\| + g\|V_{22}\| + \sqrt{(\|V_{11}\| - g\|V_{22}\|)^2 + 4g\|V_{21}\|\|V_{12}\|\|}\right) < 1. \tag{19}$$

Note that $\|V_{11}\|$ depends on g, so that the condition on the size of g is implicit. Moreover, it is worth noting that the bound spr $(T_\omega) < 1$ is not satisfied in general, even for small g, as illustrated by the following special case;

Proposition 5.2. *Assume $g = 0$ and $d\nu(\theta) = d\theta/2\pi$. Then, $T_\omega = V_\omega P_1$ satisfies*

$$\sigma(T_\omega) = \{0\} \cup \Big\{ \big||\alpha| - |\delta|\big| \leq |z| \leq |\alpha| + |\delta| \Big\}, \ \ a.s. \tag{20}$$

For $|\alpha| + |\delta| = 1$, the peripheral spectra of the relevant operators coincide with $\mathbb{S}$,

$$\sigma(T_\omega) \cap \mathbb{S} = \sigma(P_1 V_\omega P_1|_{\mathcal{H}_1}) \cap \mathbb{S} = \sigma(V_\omega) = \mathbb{S}, \ \ a.s. \tag{21}$$

We can get informations on the angular localization of the spectrum by means of the following general result about the spectrum of products of normal operators.

Proposition 5.3. *Let $T = AB$, where A, B are bounded normal operators on $\mathcal{H}_0$ and let $B_c(r)$ denote the open disc of radius $r > 0$ and center $c \in \mathbb{C}$. Then,*

$$B^{-1} \in \mathcal{B}(\mathcal{H}_0) \Rightarrow \bigcup_{\tau \in \rho(A)} \bigcap_{b \in \sigma(B)} B_{\tau b}(|b| \ \ dist(\tau, \sigma(A))) \subset \rho(AB),$$
$$A^{-1} \in \mathcal{B}(\mathcal{H}_0) \Rightarrow \bigcup_{\tau \in \rho(B)} \bigcap_{a \in \sigma(A)} B_{\tau a}(|a| \ \ dist(\tau, \sigma(B))) \subset \rho(AB). \tag{22}$$

Since $T_\omega = V_\omega K$, we show in Ref. 9 that the above result provides non trivial explicit subsets of the resolvent set of T_ω, if $\rho(V_\omega)$ contains an arc of positive opening. We also provide explicit examples displaying the stated hypotheses.

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