Spectral and topological properties of quantum walks

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Outline

1. Quantum walks and the chiral symmetry index,
2. The ‘anisotropic algebra’, crossed products and the essential spectrum,
3. Index formulas,
4. (Appendix) Miscellaneous extra topics (おまけ).

Quantum walks – a rough introduction

"Quantum analogue of random walk"

Discrete time step – unitary operator U on $\mathcal{H} = \ell^2(\mathbb{Z}^d, \mathbb{C}^n)$ with decomposition into a *shift* and *coin*,

$$U = \widetilde{S}C, \qquad \widetilde{S},\ C \in \mathcal{U}[\ell^2(\mathbb{Z}^d, \mathbb{C}^n)],$$

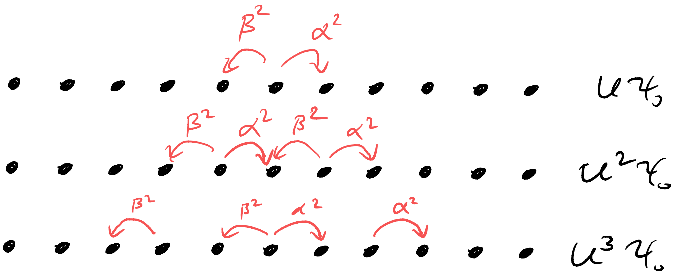
$$\widetilde{S} \sim \text{matrix of shift operators}, \qquad C : \mathbb{Z}^d \to \mathcal{U}(\mathbb{C}^n).$$

Studied from many perspectives (probability, quantum information theory, mathematical physics, ...)

Example – flip a coin and move left/right

Take $\mathcal{H} = \ell^2(\mathbb{Z}, \mathbb{C}^2)$, initial state $\psi_0 = \delta_0 \otimes \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ and consider $U^n \psi_0$, where

$$U = \widetilde{S}C = \begin{pmatrix} S & 0 \\ 0 & S^* \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix}, \qquad \alpha^2 + \beta^2 = 1.$$



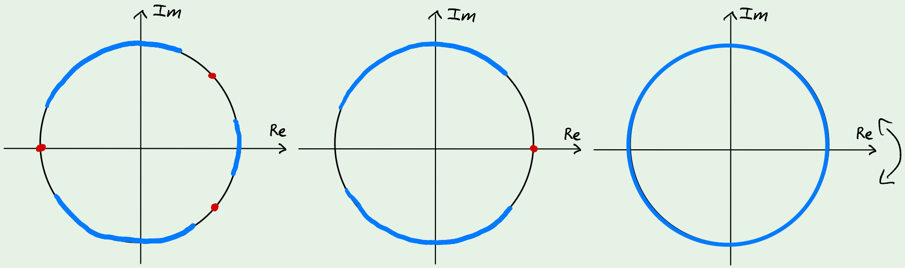
Can define random variables using quantum measurement and superposition of states.

Chiral symmetric unitaries

We say that U is chiral symmetric if there is a self-adjoint unitary Γ such that $\Gamma U \Gamma = U^*$.

The spectrum of chiral-symmetric U is symmetric about the real axis.

Examples (Chiral-symmetric $\sigma(U)$)



Symmetry index [Cedzich et al. '18]

Recall that for $T \in \mathcal{B}(\mathcal{H})$

$$\sigma_{\mathrm{ess}}(T) = \{\lambda \in \sigma(T) \mid T - \lambda\mathbf{1} \text{ not Fredholm}\}.$$

If U chiral symmetric and $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$, can define the symmetry index,

$$\mathrm{si}_{\pm}(U, \Gamma) = \mathrm{Tr}\left(\Gamma|_{\mathrm{Ker}(U \mp \mathbf{1})}\right) \in \mathbb{Z}.$$

Lemma (Basic properties, [Cedzich et al. '18] [B. '23])

1. $\left|\mathrm{si}_{\pm}(U, \Gamma)\right|$ *gives a lower-bound on the number of 'bound states' of* U *at* ± 1.
2. $\mathrm{si}_{\pm}(U, \Gamma)$ *is locally constant in the norm-topology.*
3. *If* $\{U_t\}_{t\in[0,1]}$ *is a strongly-continuous path of chiral unitaries and* $\{\phi(U_t)\}_{t\in[0,1]} \subset \mathcal{K}(\mathcal{H})$ *norm-continous for* $\mathrm{supp}(\phi)$ *in a neighbourhood of* ± 1*, then* $\mathrm{si}_{\pm}(U_t, \Gamma)$ *constant.*
4. *If* $U, \Gamma \in B$*, a* C^**-algebra, and* $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$*, there exists* $F_{\pm} \in B$ *Fredholm such that* $\mathrm{si}_{\pm}(U, \Gamma) = \mathrm{Index}(F_{\pm})$.

Our aims

Given a quantum walk unitary $U \in \mathcal{U}(\ell^2(\mathbb{Z}^d, \mathbb{C}^n))$ would like to:

1. Compute $\sigma_{\mathrm{ess}}(U)$,
2. If $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$, find 'index formulas' for $\mathrm{si}_{\pm}(U, \Gamma)$.

The anisotropic algebra

Understand $\sigma_{\mathrm{ess}}(U)$ by understanding the asymptotics of $C : \mathbb{Z}^d \to \mathcal{U}(\mathbb{C}^n)$.

Definition

The anisotropic algebra A is a separable and unital subalgebra of $L^\infty(\mathbb{Z}^d, M_n(\mathbb{C}))$ such that

1. If $a \in A$, then $\alpha_m(a)(x) = a(x+m) \in A$ for all $m \in \mathbb{Z}^d$,
2. $C_0(\mathbb{Z}^d, M_n(\mathbb{C})) \subset A$,
3. $A \simeq Z(A) \otimes M_n(\mathbb{C})$.

By Gelfand–Naimark, $A \simeq C(\Omega, M_n(\mathbb{C}))$ with Ω a compactification of $\mathbb{Z}^d$.

Example – asymptotically periodic, $d = 1$

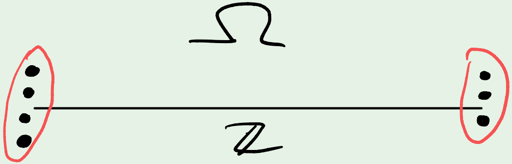
Example

Say $b : \mathbb{Z} \to M_n(\mathbb{C})$ is l-periodic, $l \in \mathbb{N}$, if $b(x + l) = b(x)$ for all $x \in \mathbb{Z}$.

Fixing $l^+, l^- \in \mathbb{N}$, we consider functions $a : \mathbb{Z} \to M_n(\mathbb{C})$ such that there are $l^\pm$-periodic functions $b^\pm$ with

$$\lim_{x \to \pm\infty} \|a(x) - b^\pm(x)\| = 0.$$

In this case $\Omega = \mathbb{Z} \cup \{0, \ldots, l^+ - 1\} \cup \{0, \ldots, l^- - 1\}$.



Example – Cartesian anisotropy, $d = 2$

Example

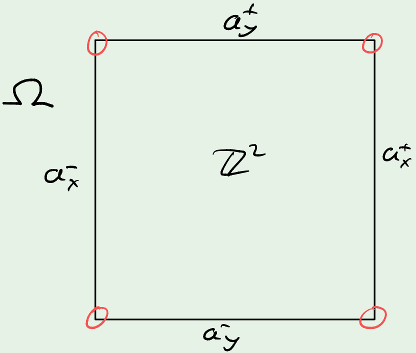
Let $\mathbb{Z}^{\pm} = \mathbb{Z} \cup \{+\infty, -\infty\}$ and consider $a : \mathbb{Z}^2 \to M_n(\mathbb{C})$ that extend to $\widetilde{a} : (\mathbb{Z}^{\pm})^{\oplus 2} \to M_n(\mathbb{C})$.

That is, we have

$$a_x^{\pm},\ a_y^{\pm} : \mathbb{Z}^{\pm} \to M_n(\mathbb{C}),$$

$$a_x^{\pm}(y) = \widetilde{a}(\pm\infty, y), \quad a_y^{\pm}(x) = \widetilde{a}(x, \pm\infty),$$

and $\Omega \simeq (\mathbb{Z}^{\pm})^{\oplus 2}$.



Crossed product algebras

Coin $C \in A \subset L^\infty(\mathbb{Z}^d, M_n(\mathbb{C}))$, but $U = \widetilde{S}C$ also involves the shift operators,

$$U \in C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d = \overline{\left\{ \sum_{m\in\mathbb{Z}^d \text{ finite}} S^m a_m \,\middle|\, a_m \in A \right\}}^{\mathcal{B}[\ell^2(\mathbb{Z}^d, \mathbb{C}^n)]},$$

Because $C_0(\mathbb{Z}^d, M_n(\mathbb{C})) \subset A \simeq C(\Omega, M_n(\mathbb{C}))$, it is an ideal:

$$0 \to C_0(\mathbb{Z}^d, M_n(\mathbb{C})) \to C(\Omega, M_n(\mathbb{C})) \to C(\Omega \setminus \mathbb{Z}^d, M_n(\mathbb{C})) \to 0.$$

Using properties of crossed product algebras cf. [Williams, '07],

$$0 \to C_0(\mathbb{Z}^d, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \to C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \xrightarrow{q} C(\Omega \setminus \mathbb{Z}^d, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \to 0$$

also exact.

Crossed products and $\sigma_{\mathrm{ess}}(U)$

Using more properties of crossed product algebras,

$$C_0(\mathbb{Z}^d, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \cong \mathcal{K}[\ell^2(\mathbb{Z}^d, \mathbb{C}^n)],$$

so

$$0 \to \mathcal{K}(\mathcal{H}) \to C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \xrightarrow{q} C(\Omega \setminus \mathbb{Z}^d, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \to 0.$$

Because q is 'quotient by compacts', $\sigma_{\mathrm{ess}}(U) = \sigma(q(U))$.

However, $C(\Omega \setminus \mathbb{Z}^d, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$ can not be faithfully represented on $\ell^2(\mathbb{Z}^d, \mathbb{C}^n)$.

Boundary orbits and the essential spectrum

Let us further decompose

$$\Omega \setminus \mathbb{Z}^d \cong \bigcup_{j \in J} \Omega_j, \qquad \Omega_j = \overline{\mathrm{orbit}(\omega_j)}, \quad \omega_j \in \Omega \setminus \mathbb{Z}^d.$$

Then for each j, $C(\Omega_j, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$ *can* be faithfully represented on $\ell^2(\mathbb{Z}^d, \mathbb{C}^n)$.

Theorem (cf. [Măntoiu, '02])

Let $q_j : C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d \to C(\Omega_j, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$. Then for any $T \in C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$,

$$\sigma_{\mathrm{ess}}(T) = \overline{\bigcup_{j \in J} \sigma(q_j(T))}$$

Example – asymptotically periodic

Example

We had $\Omega \simeq \mathbb{Z} \cup \{0, \ldots, l^+ - 1\} \cup \{0, \ldots, l^- - 1\}$ and

$$\Omega \setminus \mathbb{Z} = \{0, \ldots, l^+ - 1\} \cup \{0, \ldots, l^- - 1\} =: \Omega_+ \cup \Omega_-.$$

As $|\Omega_\pm| = l^\pm < \infty$, $C(\Omega_\pm, M_n(\mathbb{C})) \rtimes \mathbb{Z} \cong C(\mathbb{T}, M_{l^\pm n}(\mathbb{C}))$ and

$$\sigma_{\mathrm{ess}}(T) = \overline{\bigcup_{k \in \mathbb{T}} \underbrace{\sigma(T_+(k)) \cup \sigma(T_-(k))}_{\text{eigenvalues}}}.$$

Symmetry index I

Suppose $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ and $\Gamma U \Gamma = U^*$ so

$$\mathrm{si}_\pm(U,\Gamma) = \mathrm{Tr}\left(\Gamma|_{\mathrm{Ker}(U\mp\mathbf{1})}\right) = \mathrm{Index}(F_\pm), \qquad F_\pm \in C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d.$$

If $F \in C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$ is Fredholm, $q_j(F) \in C(\Omega_j) \rtimes \mathbb{Z}^d$ invertible for all $j \in J$.

We further assume

$$\Omega \setminus \mathbb{Z}^d \cong \bigsqcup_{j=1}^{N} \Omega_j.$$

Lemma

There is a function $\mathrm{sgn} : \{1, \ldots, N\} \to \{\pm 1\}$ *such that*

$$\mathrm{Index}(F) = \sum_{j=1}^{N} \mathrm{sgn}(j)\, \mathrm{Index}(\widetilde{F}_j).$$

Symmetry index II – odd dimension

Given a component Ω_j of $\Omega \setminus \mathbb{Z}^d$ in odd dimensions, we can also consider the 'Chern number' of the invertible element $q_j(F) \in C(\Omega_j, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$.

Proposition

Suppose $d = 2l+1$, $F \in C(\Omega, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$ is Fredholm and $q_j(F)$ in a 'smooth' subalgebra of $C(\Omega_j, M_n(\mathbb{C})) \rtimes \mathbb{Z}^d$. Let $\mathbf{P}$ be an invariant and ergodic measure of Ω_j. Then $\mathbf{P}$-almost surely,

$$\mathrm{Index}(\widetilde{F}_j) = \mathrm{Ch}_{2l+1}(u) = C_d \sum_{\rho \in S_d} (-1)^\rho (\mathrm{Tr}_{\mathbb{C}^n} \otimes \mathrm{Tr}_{\mathrm{vol}}) \Big(\prod_{j=1}^{d} q_j(F)^{-1} [X_{\rho(j)}, q_j(F)] \Big).$$

When $|\Omega_j| < \infty$, $\mathrm{Ch}_{2l+1}(u)$ is an integral of a differential form on $\mathbb{T}^{2l+1}$.

Example – asymptotically periodic, $d = 1$

Example

When $d = 1$ and $\Omega \setminus \mathbb{Z}$ is finite, we recover a Nöther–Toeplitz index formula:

$\Omega_\pm = \{0, \ldots, l^\pm - 1\}$, $q(F_\pm) \in C(\mathbb{T}, M_{nl^\pm}(\mathbb{C}))$ invertible and

$$\mathrm{Index}(\widetilde{F}_\pm) = \frac{-1}{2\pi i}\mathrm{Wind}\big(\det(q_\pm(F))\big).$$

Supposing that $-1 \neq \sigma_{\mathrm{ess}}(U)$,

$$\mathrm{si}_-(U, \Gamma) = \frac{1}{2\pi i}\Big(\mathrm{Wind}\big(\det(q_+(F))\big) - \mathrm{Wind}\big(\det(q_-(F))\big)\Big).$$

References

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2. C. Cedzich, T. Geib, F. A. Grünbaum, C. Stahl, L. Velázquez, A. H. Werner, and R. F. Werner. *The topological classification of one-dimensional symmetric quantum walks*. Ann. Henri Poincaré, **19** (2018), no. 2, 325–383.

3. M. Măntoiu. *C^*-algebras, dynamical systems at infinity and the essential spectrum of generalized Schrödinger operators*. J. Reine Angew. Math., **550** (2002), 211–229.

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Case $U = e^{i\pi H}$

Suppose $H = H^*$ and $\Gamma H \Gamma = -H$. If H is Fredholm, we can also define

$$\mathrm{Ind}(H,\Gamma) = \mathrm{Tr}\left(\Gamma|_{\mathrm{Ker}(H)}\right) = \mathrm{Index}\left(\tfrac{1}{2}(\mathbf{1}-\Gamma)H\tfrac{1}{2}(\mathbf{1}+\Gamma)\right)$$

Proposition

If H is Fredholm and $\|H\| \leq 1$, then

$$\mathrm{Ind}(H,\Gamma) = \mathrm{si}_+(e^{i\pi H},\Gamma).$$

Proof. First note $\mathrm{Ker}(H) = \mathrm{Ker}(e^{i\pi H} - \mathbf{1})$. Then

$$\mathrm{si}_+(e^{i\pi H},\Gamma) = \mathrm{Tr}\left(\Gamma|_{\mathrm{Ker}(e^{i\pi H}-\mathbf{1})}\right) = \mathrm{Tr}\left(\Gamma|_{\mathrm{Ker}(H)}\right) = \mathrm{Ind}(H,\Gamma).$$

□

Non-Fredholm indices and K-theory

Would also like 'topological indices' in the case $\pm 1 \in \sigma_{\mathrm{ess}}(U)$.

We assume $U \in B$, a unital C^*-algebra with a closed ideal $B_0 \subset B$ (cf. $\mathcal{K}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$).

Lemma (B., '23)

If $\Gamma \in B$, $\Gamma U \Gamma = U^*$ and

$$\|q(U) \mp \mathbf{1}\|_{B/B_0} < 2.$$

Then there is a well-defined index $\mathrm{si}_{\pm}(U, \Gamma) \in K_0(B_0)$.

- Non-trivial indices also possible for non-chiral symmetric U ($K_1(B_0)$-index).
- Many of the previous results also extend to the abstract K-theoretic setting.[1]
- See also T. Natsume's talk and [Natsume–Nest, arXiv:2310.13094].

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[1] Conditions apply.