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Quantum walks with an anisotropic coin I: spectral theory

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Abstract We perform the spectral analysis of the evolution operator U of quantum walks with an anisotropic coin, which include one-defect models, two-phase quantum walks, and topological phase quantum walks as special cases. In particular, we determine the essential spectrum of U, we show the existence of locally U-smooth operators, we prove the discreteness of the eigenvalues of U outside the thresholds, and we prove the absence of singular continuous spectrum for U. Our analysis is based on new commutator methods for unitary operators in a two-Hilbert spaces setting, which are of independent interest.

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1 Introduction

Discrete-time quantum walks appear in numerous contexts [1,2,20,21,33,46]. Among them, Gudder [21], Meyer [33], and Ambainis et al. [2] introduced one-dimensional quantum walks as a quantum mechanical counterpart of classical random walks. Nowadays, these quantum walks and their generalisations have been physically implemented in various ways [31]. Versatile applications of quantum walks can be found in [12,22,35,45] and references therein.

Recently, because of the controllability of their parameters, discrete-time quantum walks have attracted attention as promising candidates to realise topological insulators. In [25,26], Kitagawa et al. have shown that one- and two-dimensional quantum walks possess topological phases, and they experimentally observed a topologically protected bound state between two distinct phases. We refer for example to [24] for an introductory review on topological phenomena in quantum walks, see also [11,19,23]. Motivated by these studies, Endo et al. [15] (see also [13,14]) have performed a thorough analysis of the asymptotic behaviour of two-phase quantum walks, whose evolution is given by unitary operators $U_{\mathrm{TP}} = SC$ with S a shift operator and C a coin operator defined as a multiplication by unitary matrices $C(x) \in \mathrm{U}(2)$, $x \in \mathbb{Z}$. When $C(x)$ is given by

$$C(x) = \begin{cases} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{e}^{i\sigma_+} \\ \mathrm{e}^{-i\sigma_+} & -1 \end{pmatrix} & \text{if } x \geq 0 \\ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{e}^{i\sigma_-} \\ \mathrm{e}^{-i\sigma_-} & -1 \end{pmatrix} & \text{if } x \leq -1 \end{cases} \tag{1.1}$$

with $\sigma_\pm \in [0, 2\pi)$, the two-phase quantum walk with evolution operator U_{TP} is called complete two-phase quantum walk, and when $C(x)$ satisfies the alternative condition at 0

$$C(0) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.2}$$

the quantum walk is called two-phase quantum walk with one defect. In [14,15], Endo et al. have proved a weak limit theorem [27,28] similar to the de Moivre–Laplace theorem (or the central limit theorem) for random walks, which describes the asymptotic behaviour of the two-phase quantum walk.

In the present paper and the companion paper [37], we consider one-dimensional quantum walks $U = SC$ with a coin operator C exhibiting an anisotropic behaviour at infinity, with short-range convergence to the asymptotics. Namely, we assume that there exist matrices $C_\ell, C_{\mathrm{r}} \in \mathrm{U}(2)$ and constants $\varepsilon_\ell, \varepsilon_{\mathrm{r}} > 0$ such that

$$C(x)=\begin{cases}C_\ell+O\big(|x|^{-1-\varepsilon_\ell}\big) & \text{as } x\to-\infty\\ C_{\rm r}+O\big(|x|^{-1-\varepsilon_r}\big) & \text{as } x\to\infty.\end{cases} \tag{1.3}$$

We call this type of quantum walks quantum walks with an anisotropic coin or simply anisotropic quantum walks. They include two-phase quantum walks with coins defined by (1.1) and (1.2) and one-defect models [10,29,30,48] as special cases. In the case $C_0:=C_\ell=C_{\rm r}$ and $\varepsilon_0:=\varepsilon_\ell=\varepsilon_{\rm r}$, quantum walks with an anisotropic coin reduce to one-dimensional quantum walks with a position dependent coin

$$C(x)=C_0+O\big(|x|^{-1-\varepsilon_0}\big),\quad |x|\to\infty,$$

for which the absence of the singular continuous spectrum was proved in [4] and for which a weak limit theorem was derived in [43].

Quantum walks with an anisotropic coin are also related to Kitagawa's topological quantum walk model called split-step quantum walk [24–26]. Indeed, if $R(\theta)\in{\rm U}(2)$ is a rotation matrix with rotation angle $\theta/2$, $R(\Theta_j)$ the multiplication operator by $R\big(\theta_j(\,\cdot\,)\big)\in{\rm U}(2)$ with $\theta_j:\mathbb{Z}\to[0,2\pi)$, $j=1,2$, and $T_\downarrow, T_\uparrow$ shift operators satisfying $S=T_\downarrow T_\uparrow=T_\uparrow T_\downarrow$, then the evolution operator of the split-step quantum walk is defined as

$$U_{\rm SS}(\theta_1,\theta_2):=T_\downarrow\,R(\Theta_2)\,T_\uparrow\,R(\Theta_1).$$

Now, as mentioned in [24], $U_{\rm SS}(\theta_1,\theta_2)$ is unitarily equivalent to $T_\uparrow R(\Theta_1)T_\downarrow R(\Theta_2)$. Thus, our evolution operator U describes a quantum walk unitarily equivalent to the one described by $U_{\rm SS}(\theta_1,\theta_2)$ if $\theta_1\equiv 0$ and $C(\,\cdot\,)=R\big(\theta_2(\,\cdot\,)\big)$ (see [34,42] for the definition of unitary equivalence between two quantum walks). In [24], Kitagawa dealt with the case

$$\theta_2(x):=\tfrac{1}{2}(\theta_{2-}+\theta_{2+})+\tfrac{1}{2}(\theta_{2+}-\theta_{2-})\tanh(x/3),\quad \theta_{2-},\theta_{2+}\in[0,2\pi),\ x\in\mathbb{Z},$$

which corresponds to taking the anisotropic coin (1.3) with $C_\ell=R(\theta_{2-})$ and $C_{\rm r}=R(\theta_{2+})$, and which cannot be covered by two-phase models.

The main goal of the present paper and [37] is to establish a weak limit theorem for the evolution operator U of the quantum walk with an anisotropic coin satisfying (1.3). As put into evidence in [43], in order to establish a weak limit theorem one has to prove along the way the following two important results: (i) absence of singular continuous spectrum and (ii) existence of the asymptotic velocity.

In the present paper, we perform the spectral analysis of the evolution operator U of quantum walks with an anisotropic coin. We determine the essential spectrum of U, we show the existence of locally U-smooth operators, we prove the discreteness of the eigenvalues of U outside the thresholds, and we prove the absence of singular continuous spectrum for U. In the companion paper [37], we will develop the scattering theory for the evolution operator U. We will prove the existence and the completeness of wave operators for U and a free evolution operator U_0, we will show the existence of the asymptotic velocity for U, and we will finally establish a weak limit theorem for

U. Other interesting related topics such as the existence and the robustness of a bound state localised around the phase boundary or a weak limit theorem for the split-step quantum walk with $\theta_1 \neq 0$ are considered in [18] and [17], respectively.

The rest of this paper is structured as follows. In Sect. 2, we give the precise definition of the evolution operator U for the quantum walk with an anisotropic coin and we state our main results on the essential spectrum of U (Theorem 2.2), the locally U-smooth operators (Theorem 2.3), and the eigenvalues and singular continuous spectrum of U (Theorem 2.4). Section 3 is devoted to mathematical preliminaries. Here, we develop new commutator methods for unitary operators in a two-Hilbert spaces setting, which are a key ingredient for our analysis and are of independent interest. In Sect. 4, we prove our main theorems as an application of the commutator methods developed in Sect. 3. In Sect. 4.2, we prove Theorem 2.2 and we define in Lemma 4.9 a conjugate operator A for the evolution operator U built from conjugate operators for the asymptotic evolution operators $U_\ell := SC_\ell$ and $U_{\rm r} := SC_{\rm r}$, where C_ℓ and $C_{\rm r}$ are the constant coin matrices given in (1.3). Finally, in Sect. 4.3 we prove Theorems 2.3 and 2.4.

2 Model and main results

In this section, we give the definition of the model of anisotropic quantum walks that we consider, we state our main results on quantum walks, and we present the main tools we use for the proofs. These tools are results of independent interest on commutator methods for unitary operators in a two-Hilbert spaces setting. The proofs of our results on commutator methods are given in Sect. 3, and the proofs of our results on quantum walks are given in Sect. 4.

Let $\mathcal{H}$ be the Hilbert space of square-summable $\mathbb{C}^2$-valued sequences

$$\mathcal{H} := \ell^2(\mathbb{Z}, \mathbb{C}^2) = \big\{\Psi : \mathbb{Z} \to \mathbb{C}^2 \mid \textstyle\sum_{x\in\mathbb{Z}} \|\Psi(x)\|_2^2 < \infty\big\},$$

where $\|\cdot\|_2$ is the usual norm on $\mathbb{C}^2$. The evolution operator of the one-dimensional quantum walk in $\mathcal{H}$ that we consider is given by $U := SC$, with S a shift operator and C a coin operator defined by

$$(S\Psi)(x) := \begin{pmatrix} \Psi^{(0)}(x+1) \\ \Psi^{(1)}(x-1) \end{pmatrix}, \quad \Psi = \begin{pmatrix} \Psi^{(0)} \\ \Psi^{(1)} \end{pmatrix} \in \mathcal{H},\ x \in \mathbb{Z},$$
$$(C\Psi)(x) := C(x)\Psi(x), \quad \Psi \in \mathcal{H},\ x \in \mathbb{Z},\ C(x) \in \mathrm{U}(2).$$

In particular, the evolution operator U is unitary in $\mathcal{H}$ since both S and C are unitary in $\mathcal{H}$.

Throughout the paper, we assume that the coin operator C exhibits an anisotropic behaviour at infinity. More precisely, we assume that C converges with short-range rate to two asymptotic coin operators, one on the left and one on the right in the following way:

Assumption 2.1 (*Short-range*) There exist $C_\ell, C_\mathrm{r} \in \mathrm{U}(2)$, $\kappa_\ell, \kappa_\mathrm{r} > 0$, and $\varepsilon_\ell, \varepsilon_\mathrm{r} > 0$ such that

$$\begin{aligned} \big\| C(x) - C_\ell \big\|_{\mathscr{B}(\mathbb{C}^2)} &\le \kappa_\ell \, |x|^{-1-\varepsilon_\ell} \quad \text{if } x < 0 \\ \big\| C(x) - C_\mathrm{r} \big\|_{\mathscr{B}(\mathbb{C}^2)} &\le \kappa_\mathrm{r} \, |x|^{-1-\varepsilon_\mathrm{r}} \quad \text{if } x > 0, \end{aligned}$$

where the indexes ℓ and r stand for "left" and "right".

This assumption provides us two new unitary operators

$$U_\ell := SC_\ell \quad \text{and} \quad U_\mathrm{r} := SC_\mathrm{r} \tag{2.1}$$

describing the asymptotic behaviour of U on the left and on the right. The precise sense (from the scattering point of view) in which the operators U_ℓ, U_r describe the asymptotic behaviour of U on the left and on the right will be given in [37], and the spectral properties of U_ℓ, U_r are determined in Sect. 4.1. Here, we just introduce the set

$$\tau(U) := \partial\sigma(U_\ell) \cup \partial\sigma(U_\mathrm{r}),$$

where $\partial\sigma(U_\ell)$, $\partial\sigma(U_\mathrm{r})$ denote the boundaries in the unit circle $\mathbb{T} := \{z \in \mathbb{C} \mid |z| = 1\}$ of the spectra $\sigma(U_\ell), \sigma(U_\mathrm{r})$ of U_ℓ, U_r. In Sect. 4.1, we show that $\tau(U)$ is finite and can be interpreted as the set of thresholds in the spectrum of U.

Our main results on U, proved in Sects. 4.2 and 4.3, are the following three theorems on locally U-smooth operators and on the structure of the spectrum of U. The symbols $\sigma_\mathrm{ess}(U)$, $\sigma_\mathrm{p}(U)$ and Q stand for the essential spectrum of U, the pure point spectrum of U, and the position operator in $\mathcal{H}$, respectively (see (4.9) for precise definition of Q).

Theorem 2.2 (Essential spectrum of U) *One has* $\sigma_\mathrm{ess}(U) = \sigma(U_\ell) \cup \sigma(U_\mathrm{r})$.

Theorem 2.3 (U-smooth operators) *Let $\mathcal{G}$ be an auxiliary Hilbert space, and let $\Theta \subset \mathbb{T}$ be an open set with closure $\overline{\Theta} \subset \mathbb{T}\setminus\tau(U)$. Then, each operator $T \in \mathscr{B}(\mathcal{H}, \mathcal{G})$ which extends continuously to an element of $\mathscr{B}\big(\mathcal{D}(\langle Q\rangle^{-s}), \mathcal{G}\big)$ for some $s > 1/2$ is locally U-smooth on $\Theta\setminus\sigma_\mathrm{p}(U)$.*

Theorem 2.4 (Spectrum of U) *For any closed set $\Theta \subset \mathbb{T}\setminus\tau(U)$, the operator U has at most finitely many eigenvalues in Θ, each one of finite multiplicity, and U has no singular continuous spectrum in Θ.*

The content of Theorem 2.2 could be inferred from [9, Thm. 3.1], but we provide an alternative proof. To prove these theorems, we develop in Sect. 3 commutator methods for unitary operators in a two-Hilbert spaces setting: Given a triple $(\mathcal{H}, U, A)$ consisting in a Hilbert space $\mathcal{H}$, a unitary operator U, and a self-adjoint operator A, we determine how to obtain commutator results for $(\mathcal{H}, U, A)$ in terms of commutator results for a second triple $(\mathcal{H}_0, U_0, A_0)$ also consisting in a Hilbert space, a unitary operator, and a self-adjoint operator. In the process, an identification operator

$J : \mathcal{H}_0 \to \mathcal{H}$ must also be chosen. The intuition behind this approach comes from scattering theory which tells us that given a unitary operator U describing some quantum system in a Hilbert space $\mathcal{H}$ there often exists a simpler unitary operator U_0 in a second Hilbert space $\mathcal{H}_0$ describing the same quantum system in some asymptotic regime.

Our main results in this context are the following. First, we present in Theorem 3.6 conditions guaranteeing that U and A satisfy a Mourre estimate on a Borel set $\Theta \subset \mathbb{T}$ as soon as U_0 and A_0 satisfy a Mourre estimate on Θ (equivalently, we present conditions guaranteeing that A is a conjugate operator for U on Θ as soon as A_0 is a conjugate operator for U_0 on Θ). Next, we present in Proposition 3.7 conditions guaranteeing that U is regular with respect to A (that is, $U \in C^1(A)$) as soon as U_0 is regular with respect to A_0 (that is, $U_0 \in C^1(A_0)$). Finally, we give in Assumption 3.9 and Corollaries 3.10–3.11 conditions guaranteeing that the most natural choice for the operator A, namely $A = JA_0J^*$, is indeed a conjugate operator for U as soon as A_0 is a conjugate operator for U_0.

3 Unitary operators in a two-Hilbert spaces setting

In this section, we start by recalling some facts on the spectral family of unitary operators, on locally smooth operators for unitary operators, and on commutator methods for unitary operators in one Hilbert space. In particular, we introduce in (3.2)–(3.3) the functions ϱ and $\widetilde{\varrho}$ which will play an essential role in the two-Hilbert space setting and which have never been used before for unitary operators. Then, we develop the abstract theory of commutator methods for unitary operators in a two-Hilbert spaces setting. Note that the theory in one Hilbert space has also been introduced in [5,6], but without the ϱ-functions mentioned above.

3.1 Commutator methods in one Hilbert space

Let $\mathcal{H}$ be a Hilbert space with norm $\|\cdot\|_{\mathcal{H}}$ and scalar product $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ linear in the second argument, $\mathscr{B}(\mathcal{H})$ the set of bounded linear operators in $\mathcal{H}$ with norm $\|\cdot\|_{\mathscr{B}(\mathcal{H})}$, and $\mathscr{K}(\mathcal{H})$ the set of compact linear operators in $\mathcal{H}$. A unitary operator U in $\mathcal{H}$ is an element $U \in \mathscr{B}(\mathcal{H})$ satisfying $U^*U = UU^* = 1$. Since $U^*U = UU^*$, the spectral theorem for normal operators implies that U admits exactly one complex spectral family E^U, with support $\operatorname{supp}(E^U) \subset \mathbb{T}$, such that $U = \int_{\mathbb{C}} z\, E^U(\mathrm{d}z)$. The support $\operatorname{supp}(E^U)$ is the set of points of non-constancy of E^U, which coincides with the spectrum $\sigma(U)$ of U [47, Thm. 7.34(a)]. In addition, the measure E^U admits a decomposition into a pure point, a singular continuous and an absolutely continuous components, and the corresponding orthogonal decomposition

$$\mathcal{H} = \mathcal{H}_{\rm p}(U) \oplus \mathcal{H}_{\rm sc}(U) \oplus \mathcal{H}_{\rm ac}(U)$$

reduces the operator U. The sets $\sigma_{\rm p}(U) := \sigma\big(U|_{\mathcal{H}_{\rm p}(U)}\big)$, $\sigma_{\rm sc}(U) := \sigma\big(U|_{\mathcal{H}_{\rm sc}(U)}\big)$, and $\sigma_{\rm ac}(U) := \sigma\big(U|_{\mathcal{H}_{\rm ac}(U)}\big)$ are called pure point spectrum, singular continuous spectrum, and absolutely continuous spectrum of U, respectively, and the set $\sigma_{\rm c}(U) := \sigma_{\rm sc}(U) \cup \sigma_{\rm ac}(U)$ is called the continuous spectrum of U. Finally, if $\mathcal{G}$ is an auxiliary Hilbert space, then an operator $T \in \mathscr{B}(\mathcal{H}, \mathcal{G})$ is locally U-smooth on an open set $\Theta \subset \mathbb{T}$ if for each closed set $\Theta' \subset \Theta$ there exists $c_{\Theta'} \geq 0$ such that

$$\sum_{n\in\mathbb{Z}} \big\| T\, U^n E^U(\Theta')\varphi \big\|_{\mathcal{G}}^2 \leq c_{\Theta'} \, \|\varphi\|_{\mathcal{H}}^2 \quad \text{for each } \varphi \in \mathcal{H}, \tag{3.1}$$

and T is (globally) U-smooth if (3.1) is satisfied with $\Theta' = \mathbb{T}$. The condition (3.1) is invariant under rotation by $\omega \in \mathbb{T}$ in the sense that if T is U-smooth on Θ, then T is (ωU)-smooth on $\omega\Theta$ since

$$\big\| T(\omega U)^n E^{\omega U}(\omega\Theta')\varphi \big\|_{\mathcal{G}} = \big\| T\, U^n E^U(\Theta')\varphi \big\|_{\mathcal{G}}$$

for each closed set $\Theta' \subset \Theta$ and each $\varphi \in \mathcal{H}$. An important consequence of the existence of a locally U-smooth operator T on Θ is the inclusion $\overline{E^U(\Theta)T^*\mathcal{G}^*} \subset \mathcal{H}_{\rm ac}(U)$, with $\mathcal{G}^*$ the adjoint space of $\mathcal{G}$ (see [7, Thm. 2.1] for a proof).

Now, we present some results on commutator methods for unitary operators in one Hilbert space, starting with definitions and results borrowed from [3,16,41]. Let $S \in \mathscr{B}(\mathcal{H})$ and let A be a self-adjoint operator in $\mathcal{H}$ with domain $\mathcal{D}(A)$. For $k \in \mathbb{N}$, we say that S belongs to $C^k(A)$, with notation $S \in C^k(A)$, if the map $\mathbb{R} \ni t \mapsto \mathrm{e}^{-itA}\, S\, \mathrm{e}^{itA} \in \mathscr{B}(\mathcal{H})$ is strongly of class C^k. In the case $k = 1$, one has $S \in C^1(A)$ if and only if the quadratic form

$$\mathcal{D}(A) \ni \varphi \mapsto \big\langle A\varphi, S\varphi \big\rangle_{\mathcal{H}} - \big\langle \varphi, SA\varphi \big\rangle_{\mathcal{H}} \in \mathbb{C}$$

is continuous for the topology induced by $\mathcal{H}$ on $\mathcal{D}(A)$. The operator associated to the continuous extension of the form is denoted by $[A, S] \in \mathscr{B}(\mathcal{H})$, and it verifies

$$[A, S] = \operatorname*{s-lim}_{\tau\to 0} [A_\tau, S] \quad \text{with} \quad A_\tau := (i\tau)^{-1}\big(\mathrm{e}^{i\tau A} - 1\big) \in \mathscr{B}(\mathcal{H}), \quad \tau \in \mathbb{R}\setminus\{0\}.$$

Three regularity conditions slightly stronger than $S \in C^1(A)$ are defined as follows: S belongs to $C^{1,1}(A)$, with notation $S \in C^{1,1}(A)$, if

$$\int_0^1 \big\| \mathrm{e}^{-itA}\, S\, \mathrm{e}^{itA} + \mathrm{e}^{itA}\, S\, \mathrm{e}^{-itA} - 2S \big\|_{\mathscr{B}(\mathcal{H})} \frac{\mathrm{d}t}{t^2} < \infty.$$

S belongs to $C^{1+0}(A)$, with notation $S \in C^{1+0}(A)$, if $S \in C^1(A)$ and

$$\int_0^1 \big\| \mathrm{e}^{-itA}[A, S]\, \mathrm{e}^{itA} - [A, S] \big\|_{\mathscr{B}(\mathcal{H})} \frac{\mathrm{d}t}{t} < \infty.$$

S belongs to $C^{1+\varepsilon}(A)$ for some $\varepsilon \in (0, 1)$, with notation $S \in C^{1+\varepsilon}(A)$, if $S \in C^1(A)$ and

$$\big\| \mathrm{e}^{-itA}[A, S]\, \mathrm{e}^{itA} - [A, S] \big\|_{\mathscr{B}(\mathcal{H})} \leq \text{Const.}\, t^{\varepsilon} \quad \text{for all } t \in (0, 1).$$

As banachisable topological vector spaces, the sets $C^2(A)$, $C^{1+\varepsilon}(A)$, $C^{1+0}(A)$, $C^{1,1}(A)$, $C^1(A)$, and $C^0(A)=\mathscr{B}(\mathcal{H})$, satisfy the continuous inclusions [3, Sec. 5.2.4]

$$C^2(A)\subset C^{1+\varepsilon}(A)\subset C^{1+0}(A)\subset C^{1,1}(A)\subset C^1(A)\subset C^0(A).$$

Now, we adapt to the unitary framework the definition of two functions introduced in [3, Sec. 7.2] in the self-adjoint set-up. For that purpose, we let U be a unitary operator with $U\in C^1(A)$, for $S,T\in\mathscr{B}(\mathcal{H})$ we write $T\gtrsim S$ if there exists an operator $K\in\mathscr{K}(\mathcal{H})$ such that $T+K\geq S$, and for $\theta\in\mathbb{T}$ and $\varepsilon>0$ we set

$$\Theta(\theta;\varepsilon):=\big\{\theta'\in\mathbb{T}\mid|\arg(\theta-\theta')|<\varepsilon\big\}\quad\text{and}\quad E^U(\theta;\varepsilon):=E^U\big(\Theta(\theta;\varepsilon)\big).$$

With these notations at hand, we define the functions $\varrho_U^A:\mathbb{T}\to(-\infty,\infty]$ and $\widetilde{\varrho}_U^A:\mathbb{T}\to(-\infty,\infty]$ by

$$\varrho_U^A(\theta):=\sup\big\{a\in\mathbb{R}\mid\exists\,\varepsilon>0\text{ such that }E^U(\theta;\varepsilon)U^{-1}[A,U]E^U(\theta;\varepsilon)\geq a\,E^U(\theta;\varepsilon)\big\}\tag{3.2}$$

and

$$\widetilde{\varrho}_U^A(\theta):=\sup\big\{a\in\mathbb{R}\mid\exists\,\varepsilon>0\text{ such that }E^U(\theta;\varepsilon)U^{-1}[A,U]E^U(\theta;\varepsilon)\gtrsim a\,E^U(\theta;\varepsilon)\big\}.\tag{3.3}$$

In applications, the function $\widetilde{\varrho}_U^A$ is more convenient than the function ϱ_U^A since it is defined in terms of a weaker positivity condition (positivity up to compact terms). A simple argument shows that $\widetilde{\varrho}_U^A(\theta)$ can be defined in an equivalent way by

$$\begin{aligned}\widetilde{\varrho}_U^A(\theta)=\sup\big\{&a\in\mathbb{R}\mid\exists\,\eta\in C^\infty(\mathbb{T},\mathbb{R})\text{ such that }\eta(\theta)\neq0\\&\text{and }\eta(U)U^{-1}[A,U]\eta(U)\gtrsim a\,\eta(U)^2\big\}.\end{aligned}\tag{3.4}$$

Further properties of the functions $\widetilde{\varrho}_U^A$ and ϱ_U^A are collected in the following lemmas, with first lemma corresponding to [16, Prop. 2.3].

Lemma 3.1 (Virial Theorem for U) *Let U be a unitary operator in $\mathcal{H}$, and let A be a self-adjoint operator in $\mathcal{H}$ with $U\in C^1(A)$. Then, $E^U(\{\theta\})U^{-1}[A,U]E^U(\{\theta\})=0$ for each $\theta\in\mathbb{T}$. In particular, one has $\langle\varphi,U^{-1}[A,U]\varphi\rangle_{\mathcal{H}}=0$ for each eigenvector $\varphi\in\mathcal{H}$ of U.*

Lemma 3.2 *Let U be a unitary operator in $\mathcal{H}$, and let A be a self-adjoint operator in $\mathcal{H}$ with $U\in C^1(A)$. Assume there exist an open set $\Theta\subset\mathbb{T}$ and $a\in\mathbb{R}$ such that $E^U(\Theta)U^{-1}[A,U]E^U(\Theta)\gtrsim a\,E^U(\Theta)$. Then, for each $\theta\in\Theta$ and $\eta>0$ there exist $\varepsilon>0$ and a finite rank orthogonal projection F with $E^U(\{\theta\})\geq F$ such that*

$$E^U(\theta;\varepsilon)U^{-1}[A,U]E^U(\theta;\varepsilon)\geq(a-\eta)\big(E^U(\theta;\varepsilon)-F\big)-\eta F.$$

In particular, if θ is not an eigenvalue of U, then

$$E^U(\theta;\varepsilon)U^{-1}[A,U]E^U(\theta;\varepsilon)\geq(a-\eta)E^U(\theta;\varepsilon),$$

while if θ is an eigenvalue of U, one has only

$$E^U(\theta;\varepsilon)U^{-1}[A,U]E^U(\theta;\varepsilon) \geq \min\{a-\eta,-\eta\}E^U(\theta;\varepsilon).$$

Proof The proof relies on the Virial Theorem for U and is analogous to the proof of [3, Lemma 7.2.12] in the self-adjoint case. One just needs to replace in that proof $[iH, A]$ by $U^{-1}[A, U]$, $E(J)$ by $E^U(\Theta)$, $E(\{\lambda\})$ by $E^U(\{\theta\})$, and $E(\lambda; 1/k)$ by $E^U(\theta; 1/k)$. □

Lemma 3.3 *Let U be a unitary operator in $\mathcal{H}$, and let A be a self-adjoint operator in $\mathcal{H}$ with $U \in C^1(A)$.*

(a) *The function $\varrho_U^A : \mathbb{T} \to (-\infty, \infty]$ is lower semicontinuous, and $\varrho_U^A(\theta) < \infty$ if and only if $\theta \in \sigma(U)$.*
(b) *The function $\widetilde{\varrho}_U^A : \mathbb{T} \to (-\infty, \infty]$ is lower semicontinuous, and $\widetilde{\varrho}_U^A(\theta) < \infty$ if and only if $\theta \in \sigma_{\rm ess}(U)$.*
(c) $\widetilde{\varrho}_U^A \geq \varrho_U^A$.
(d) *If $\theta \in \mathbb{T}$ is an eigenvalue of U and $\widetilde{\varrho}_U^A(\theta) > 0$, then $\varrho_U^A(\theta) = 0$. Otherwise, $\varrho_U^A(\theta) = \widetilde{\varrho}_U^A(\theta)$.*

Proof The claims are shown as in the proofs of Lemma 7.2.1, Proposition 7.2.3(a), Proposition 7.2.6, and Theorem 7.2.13 of [3] in the self-adjoint case. □

By analogy with the self-adjoint case, we say that A is conjugate to U at a point $\theta \in \mathbb{T}$ if $\widetilde{\varrho}_U^A(\theta) > 0$, and that A is strictly conjugate to U at θ if $\varrho_U^A(\theta) > 0$. Since $\widetilde{\varrho}_U^A(\theta) \geq \varrho_U^A(\theta)$ for each $\theta \in \mathbb{T}$ by Lemma 3.3(c), strict conjugation is a property stronger than conjugation.

Theorem 3.4 (U-smooth operators) *Let U be a unitary operator in $\mathcal{H}$, let A be a self-adjoint operator in $\mathcal{H}$, and let $\mathcal{G}$ be an auxiliary Hilbert space. Assume either that U has a spectral gap and $U \in C^{1,1}(A)$, or that $U \in C^{1+0}(A)$. Suppose also there exist an open set $\Theta \subset \mathbb{T}$, a number $a > 0$ and an operator $K \in \mathscr{K}(\mathcal{H})$ such that*

$$E^U(\Theta)\,U^{-1}[A,U]\,E^U(\Theta) \geq a E^U(\Theta) + K.$$

Then, each operator $T \in \mathscr{B}(\mathcal{H},\mathcal{G})$ which extends continuously to an element of $\mathscr{B}\big(\mathcal{D}(\langle A\rangle^s)^*,\mathcal{G}\big)$ for some $s > 1/2$ is locally U-smooth on $\Theta\setminus\sigma_{\rm p}(U)$.

Proof The claim follows by adapting the proof of [16, Prop. 2.9] to locally U-smooth operators T with values in the auxiliary Hilbert space $\mathcal{G}$. □

The last theorem of this section corresponds to [16, Thm. 2.7]:

Theorem 3.5 (Spectrum of U) *Let U be a unitary operator in $\mathcal{H}$, and let A be a self-adjoint operator in $\mathcal{H}$. Assume either that U has a spectral gap and $U \in C^{1,1}(A)$, or that $U \in C^{1+0}(A)$. Suppose also there exist an open set $\Theta \subset \mathbb{T}$, a number $a > 0$ and an operator $K \in \mathscr{K}(\mathcal{H})$ such that*

$$E^U(\Theta)\,U^{-1}[A,U]\,E^U(\Theta) \geq a E^U(\Theta) + K.$$

Then, U has at most finitely many eigenvalues in Θ, each one of finite multiplicity, and U has no singular continuous spectrum in Θ.

3.2 Commutator methods in a two-Hilbert spaces setting

From now on, in addition to the triple $(\mathcal{H}, U, A)$, we consider a second triple $(\mathcal{H}_0, U_0, A_0)$ with $\mathcal{H}_0$ a Hilbert space, U_0 a unitary operator in $\mathcal{H}_0$, and A_0 a self-adjoint operator in $\mathcal{H}_0$. We also consider an identification operator $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$. The existence of two such triples with an identification operator is quite standard in scattering theory of unitary operators, at least for the pairs $(\mathcal{H}, U)$ and $(\mathcal{H}_0, U_0)$ (see for instance [8,49]). Part of our goal in this section is to show that the existence of the conjugate operators A and A_0 is also natural, in the same way it is in the self-adjoint case [38].

In the one-Hilbert space setting, the unitary operator U is usually a multiplicative perturbation of the unitary operator U_0. In this case, if $U - U_0$ is compact, the stability of the function $\widetilde{\varrho}_{U_0}^{A_0}$ under compact perturbations allows one to infer information on U from similar information on U_0 (see [16, Cor. 2.10]). In the two-Hilbert spaces setting, we are not aware of any general result relating the functions $\widetilde{\varrho}_U^A$ and $\widetilde{\varrho}_{U_0}^{A_0}$. The obvious reason for this being the impossibility to consider U as a direct perturbation of U_0 since these operators do not act in the same Hilbert space. Nonetheless, the next theorem provides a result in that direction. For Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ and operators $S, T \in \mathscr{B}(\mathcal{H}_1, \mathcal{H}_2)$, we use the notation $T \approx S$ if $(T - S) \in \mathscr{K}(\mathcal{H}_1, \mathcal{H}_2)$.

Theorem 3.6 *Let $(\mathcal{H}_0, U_0, A_0)$ and $(\mathcal{H}, U, A)$ be as above, let $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$, and assume that*

(i) $U_0 \in C^1(A_0)$ *and* $U \in C^1(A)$,
(ii) $JU_0^{-1}[A_0, U_0]J^* - U^{-1}[A, U] \in \mathscr{K}(\mathcal{H})$,
(iii) $JU_0 - UJ \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$,
(iv) *For each* $\eta \in C(\mathbb{C}, \mathbb{R})$, $\eta(U)(JJ^* - 1)\eta(U) \in \mathscr{K}(\mathcal{H})$.

Then, one has $\widetilde{\varrho}_U^A \geq \widetilde{\varrho}_{U_0}^{A_0}$.

An induction argument together with a Stone–Weierstrass density argument shows that (iii) is equivalent to the apparently stronger condition

(iii') For each $\eta \in C(\mathbb{C}, \mathbb{R})$, $J\eta(U_0) - \eta(U)J \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$.

Therefore, in the sequel, we will sometimes use the condition (iii') instead of (iii).

Proof For each $\eta \in C(\mathbb{C}, \mathbb{R})$, we have

$$\begin{aligned} \eta(U)U^{-1}[A, U]\eta(U) &\approx \eta(U)JU_0^{-1}[A_0, U_0]J^*\eta(U) \\ &\approx J\eta(U_0)U_0^{-1}[A_0, U_0]\eta(U_0)J^* \end{aligned} \tag{3.5}$$

due to Assumption (i)–(iii). Furthermore, if there exists $a \in \mathbb{R}$ such that

$$\eta(U_0)U_0^{-1}[A_0, U_0]\eta(U_0) \gtrsim a\,\eta(U_0)^2,$$

then Assumptions (iii)–(iv) imply that

$$J\eta(U_0)U_0^{-1}[A_0,U_0]\eta(U_0)J^* \gtrsim a\,J\eta(U_0)^2J^* \approx a\,\eta(U)JJ^*\eta(U) \approx a\,\eta(U)^2. \tag{3.6}$$

Thus, we obtain $\eta(U)U^{-1}[A,U]\eta(U) \gtrsim a\,\eta(U)^2$ by combining (3.5) and (3.6). This last estimate, together with the definition (3.4) of the functions $\widetilde{\varrho}_{U_0}^{A_0}$ and $\widetilde{\varrho}_U^A$, implies the claim. □

The regularity of U_0 with respect to A_0 is usually easy to check, while the regularity of U with respect to A is in general difficult to establish. For that purpose, various perturbative criteria have been developed for self-adjoint operators in one Hilbert space, and often a distinction is made between short-range and long-range perturbations. Roughly speaking, the two terms of the formal commutator $[A,U]=AU-UA$ are treated separately in the short-range case, while $[A,U]$ is really computed in the long-range case. In the sequel, we discuss short-range type perturbations for unitary operators in a two-Hilbert spaces setting. The results we obtain are analogous to the ones obtained in [38, Sec. 3.1] for self-adjoint operators in a two-Hilbert spaces setting.

We start by showing how the condition $U\in C^1(A)$ and the assumptions (ii)-(iii) of Theorem 3.6 can be verified for a class of short-range type perturbations. Our approach is to infer the desired information on U from equivalent information on U_0, which are usually easier to obtain. Accordingly, our results exhibit some perturbative flavour. The price one has to pay is to impose some compatibility conditions between A_0 and A. For brevity, we set

$$B:=JU_0-UJ\in\mathscr{B}(\mathcal{H}_0,\mathcal{H}) \quad\text{and}\quad B_*:=JU_0^*-U^*J\in\mathscr{B}(\mathcal{H}_0,\mathcal{H}).$$

Proposition 3.7 *Let $U_0\in C^1(A_0)$, assume that $\mathscr{D}\subset\mathcal{H}$ is a core for A such that $J^*\mathscr{D}\subset\mathcal{D}(A_0)$, and suppose that*

$$\overline{BA_0\restriction\mathcal{D}(A_0)}\in\mathscr{B}(\mathcal{H}_0,\mathcal{H}),\quad \overline{B_*A_0\restriction\mathcal{D}(A_0)}\in\mathscr{B}(\mathcal{H}_0,\mathcal{H})$$
$$\text{and}\quad \overline{(JA_0J^*-A)\restriction\mathscr{D}}\in\mathscr{B}(\mathcal{H}). \tag{3.7}$$

Then, $U\in C^1(A)$.

Proof For $\varphi\in\mathscr{D}$, a direct calculation gives

$$\begin{aligned}\langle A\varphi,U\varphi\rangle_{\mathcal{H}}-\langle\varphi,UA\varphi\rangle_{\mathcal{H}} &= \langle A\varphi,U\varphi\rangle_{\mathcal{H}}-\langle\varphi,UA\varphi\rangle_{\mathcal{H}}-\langle\varphi,J[A_0,U_0]J^*\varphi\rangle_{\mathcal{H}}\\ &\quad+\langle\varphi,J[A_0,U_0]J^*\varphi\rangle_{\mathcal{H}}\\ &=\langle\varphi,BA_0J^*\varphi\rangle_{\mathcal{H}}-\langle B_*A_0J^*\varphi,\varphi\rangle_{\mathcal{H}}\\ &\quad+\langle U^*\varphi,(JA_0J^*-A)\varphi\rangle_{\mathcal{H}}\\ &\quad-\langle(JA_0J^*-A)\varphi,U\varphi\rangle_{\mathcal{H}}+\langle\varphi,J[A_0,U_0]J^*\varphi\rangle_{\mathcal{H}}.\end{aligned}$$

Furthermore, we have

$$\left|\langle\varphi,BA_0J^*\varphi\rangle_{\mathcal{H}}-\langle B_*A_0J^*\varphi,\varphi\rangle_{\mathcal{H}}\right|\le\text{Const.}\,\|\varphi\|_{\mathcal{H}}^2$$

due to the first two conditions in (3.7), and we have

$$\left|\langle U^*\varphi, (JA_0J^* - A)\varphi\rangle_{\mathcal{H}} - \langle (JA_0J^* - A)\varphi, U\varphi\rangle_{\mathcal{H}}\right| \le \text{Const.}\, \|\varphi\|^2_{\mathcal{H}}$$

due to the third condition in (3.7). Finally, since $U_0 \in C^1(A_0)$ and $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ we also have

$$\left|\langle \varphi, J[A_0, U_0]J^*\varphi\rangle_{\mathcal{H}}\right| \le \text{Const.}\, \|\varphi\|^2_{\mathcal{H}}.$$

Since $\mathscr{D}$ is a core for A, this implies that $U \in C^1(A)$. □

In the next proposition, we show how the assumption (ii) of Theorem 3.6 is verified for short-range type perturbations. Since the hypotheses are slightly stronger than the ones of Proposition 3.7, U automatically belongs to $C^1(A)$.

Proposition 3.8 *Let $U_0 \in C^1(A_0)$, assume that $\mathscr{D} \subset \mathcal{H}$ is a core for A such that $J^*\mathscr{D} \subset \mathcal{D}(A_0)$, and suppose that*

$$\begin{aligned} &\overline{BA_0 \restriction \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H}), \quad \overline{B_*A_0 \restriction \mathcal{D}(A_0)} \in \mathscr{K}(\mathcal{H}_0, \mathcal{H}) \\ &\quad \text{and} \quad \overline{(JA_0J^* - A) \restriction \mathscr{D}} \in \mathscr{K}(\mathcal{H}). \end{aligned} \tag{3.8}$$

Then, the difference of bounded operators $JU_0^{-1}[A_0, U_0]J^* - U^{-1}[A, U]$ belongs to $\mathscr{K}(\mathcal{H})$.

Proof The facts that $U_0 \in C^1(A_0)$ and $J^*\mathscr{D} \subset \mathcal{D}(A_0)$ imply the inclusions

$$U_0J^*\mathscr{D} \subset U_0\mathcal{D}(A_0) \subset \mathcal{D}(A_0).$$

Using this and the last two conditions of (3.8), we obtain for $\varphi \in \mathscr{D}$ and $\psi \in U^{-1}\mathscr{D}$ that

$$\begin{aligned} &\langle \psi, \big(JU_0^{-1}[A_0, U_0]J^* - U^{-1}[A, U]\big)\varphi\rangle_{\mathcal{H}} \\ &\quad = \langle \psi, B_*A_0U_0J^*\varphi\rangle_{\mathcal{H}} + \langle B_*A_0J^*U\psi, \varphi\rangle_{\mathcal{H}} + \langle (JA_0J^* - A)U\psi, U\varphi\rangle_{\mathcal{H}} \\ &\quad\quad - \langle \psi, (JA_0J^* - A)\varphi\rangle_{\mathcal{H}} \\ &\quad = \langle \psi, K_1U_0J^*\varphi\rangle_{\mathcal{H}} + \langle K_1J^*U\psi, \varphi\rangle_{\mathcal{H}} + \langle K_2U\psi, U\varphi\rangle_{\mathcal{H}} - \langle \psi, K_2\varphi\rangle_{\mathcal{H}} \end{aligned}$$

with $K_1 \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$ and $K_2 \in \mathscr{K}(\mathcal{H})$. Since $\mathscr{D}$ and $U^{-1}\mathscr{D}$ are dense in $\mathcal{H}$, it follows that the operator $JU_0^{-1}[A_0, U_0]J^* - U^{-1}[A, U]$ belongs to $\mathscr{K}(\mathcal{H})$. □

In the rest of the section, we particularise the previous results to the case $A = JA_0J^*$. This case deserves a special attention since it represents the most natural choice of conjugate operator A for U when a conjugate operator A_0 for U_0 is given. However, one needs in this case the following assumption to guarantee the self-adjointness of the operator A:

Assumption 3.9 There exists a set $\mathscr{D} \subset \mathcal{D}(A_0 J^*) \subset \mathcal{H}$ such that $J A_0 J^* \upharpoonright \mathscr{D}$ is essentially self-adjoint, with corresponding self-adjoint extension denoted by A.

Assumption 3.9 might be difficult to check in general, but in concrete situations the choice of the set $\mathscr{D}$ can be quite natural (see for example Lemma 4.9 for the case of quantum walks or [39, Rem. 4.3] for the case of manifolds with asymptotically cylindrical ends). The following two corollaries follow directly from Propositions 3.7-3.8 in the case Assumption 3.9 is satisfied.

Corollary 3.10 *Let $U_0 \in C^1(A_0)$, suppose that Assumption 3.9 holds for some set $\mathscr{D} \subset \mathcal{H}$, and assume that $\overline{B A_0 \upharpoonright \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ and $\overline{B_* A_0 \upharpoonright \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$. Then, U belongs to $C^1(A)$.*

Corollary 3.11 *Let $U_0 \in C^1(A_0)$, suppose that Assumption 3.9 holds for some set $\mathscr{D} \subset \mathcal{H}$, and assume that $\overline{B A_0 \upharpoonright \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ and $\overline{B_* A_0 \upharpoonright \mathcal{D}(A_0)} \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$. Then, the difference of bounded operators $J U_0^{-1}[A_0, U_0] J^* - U^{-1}[A, U]$ belongs to $\mathscr{K}(\mathcal{H})$.*

4 Quantum walks with an anisotropic coin

In this section, we apply the abstract theory of Sect. 3 to prove our results on the spectrum of the evolution operator U of the quantum walk with an anisotropic coin defined in Sect. 2. For this, we first determine in Sect. 4.1 the spectral properties and prove a Mourre estimate for the asymptotic operators U_ℓ and U_{r}. Then, in Sect. 4.2, we use the Mourre estimate for U_ℓ and U_{r} to derive a Mourre estimate for U. Finally, in Sect. 4.3, we use the Mourre estimate for U to prove our results on U. We recall that the behaviour of the coin operator C at infinity is determined by Assumption 2.1.

4.1 Asymptotic operators U_ℓ and U_{r}

For the study of the asymptotic operators U_ℓ and U_{r}, we use the symbol $\star$ to denote either the index ℓ or the index r. Also, we introduce the subspace $\mathcal{H}_{\mathrm{fin}} \subset \mathcal{H}$ of elements with finite support

$$\mathcal{H}_{\mathrm{fin}} := \bigcup_{n \in \mathbb{N}} \left\{ \Psi \in \mathcal{H} \mid \Psi(x) = 0 \text{ if } |x| \geq n \right\},$$

the Hilbert space $\mathcal{K} := \mathrm{L}^2\left([0, 2\pi), \frac{\mathrm{d}k}{2\pi}, \mathbb{C}^2\right)$, and the discrete Fourier transform $\mathscr{F} : \mathcal{H} \to \mathcal{K}$, which is the unitary operator defined as the unique continuous extension of the operator

$$(\mathscr{F}\Psi)(k) := \sum_{x \in \mathbb{Z}} \mathrm{e}^{-ikx}\, \Psi(x), \quad \Psi \in \mathcal{H}_{\mathrm{fin}},\ k \in [0, 2\pi).$$

A direct computation shows that the operator $U_\star$ is decomposable in the Fourier representation, namely for all $f \in \mathcal{K}$ and almost every $k \in [0, 2\pi)$ we have

$$(\mathscr{F} U_\star \mathscr{F}^* f)(k) = \widehat{U_\star}(k) f(k) \quad \text{with} \quad \widehat{U_\star}(k) := \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} C_\star \in \mathrm{U}(2).$$

Moreover, since $\widehat{U_\star}(k) \in \mathrm{U}(2)$ the spectral theorem implies that $\widehat{U_\star}(k)$ can be written as

$$\widehat{U_\star}(k) = \sum_{j=1}^{2} \lambda_{\star,j}(k)\, \Pi_{\star,j}(k),$$

with $\lambda_{\star,j}(k)$ the eigenvalues of $\widehat{U_\star}(k)$ and $\Pi_{\star,j}(k)$ the corresponding orthogonal projections.

The next lemma furnishes some information on the spectrum of $U_\star$. To state it, we use the following parametrisation for the matrices $C_\star$:

$$C_\star = e^{i\delta_\star/2} \begin{pmatrix} a_\star\, e^{i(\alpha_\star - \delta_\star/2)} & b_\star\, e^{i(\beta_\star - \delta_\star/2)} \\ -b_\star\, e^{-i(\beta_\star - \delta_\star/2)} & a_\star\, e^{-i(\alpha_\star - \delta_\star/2)} \end{pmatrix} \tag{4.1}$$

with $a_\star, b_\star \in [0, 1]$ satisfying $a_\star^2 + b_\star^2 = 1$, and $\alpha_\star, \beta_\star, \delta_\star \in (-\pi, \pi]$. The determinant $\det(C_\star)$ of $C_\star$ is equal to $e^{i\delta_\star}$. For brevity, we also set

$$\begin{aligned} \tau_\star(k) &:= a_\star \cos(k + \alpha_\star - \delta_\star/2), \\ \eta_\star(k) &:= \sqrt{1 - \tau_\star(k)^2}, \\ \varsigma_\star(k) &:= a_\star \sin(k + \alpha_\star - \delta_\star/2), \\ \theta_\star &:= \arccos(a_\star). \end{aligned}$$

Lemma 4.1 (Spectrum of $U_\star$)

(a) *If $a_\star = 0$, then $U_\star$ has pure point spectrum*

$$\sigma(U_\star) = \sigma_{\mathrm{p}}(U_\star) = \left\{ i\, e^{i\delta_\star/2}, -i\, e^{i\delta_\star/2} \right\}$$

with each point an eigenvalue of $U_\star$ of infinite multiplicity.

(b) *If $a_\star \in (0, 1)$, then $\sigma_{\mathrm{p}}(U_\star) = \varnothing$ and*

$$\begin{aligned} \sigma(U_\star) = \sigma_{\mathrm{c}}(U_\star) = \big\{ e^{i\gamma} \mid \gamma \in {} & [\delta_\star/2 + \theta_\star, \pi + \delta_\star/2 - \theta_\star] \\ & \cup [\pi + \delta_\star/2 + \theta_\star, 2\pi + \delta_\star/2 - \theta_\star] \big\}. \end{aligned}$$

(c) *If $a_\star = 1$, then $\sigma_{\mathrm{p}}(U_\star) = \varnothing$ and $\sigma(U_\star) = \sigma_{\mathrm{c}}(U_\star) = \mathbb{T}$.*

Proof Using the parametrisation (4.1), one gets $\widehat{U_\star}(k) = \mathrm{e}^{i\delta_\star/2}\begin{pmatrix} a_\star(k) & b_\star(k) \\ -\overline{b_\star(k)} & \overline{a_\star(k)} \end{pmatrix}$ with the coefficients $a_\star(k) := a_\star\,\mathrm{e}^{i(k+\alpha_\star-\delta_\star/2)}$ and $b_\star(k) := b_\star\,\mathrm{e}^{i(k+\beta_\star-\delta_\star/2)}$. Therefore, the spectrum of $U_\star$ is given by

$$\sigma(U_\star) = \big\{\lambda_{\star,j}(k) \mid j = 1, 2,\ k \in [0, 2\pi)\big\},$$

with $\lambda_{\star,j}(k)$ the solution of the characteristic equation $\det\big(\widehat{U_\star}(k) - \lambda_{\star,j}(k)\big) = 0$, $j = 1, 2$ and $k \in [0, 2\pi)$. □

We now exhibit normalised eigenvectors $u_{\star,j}(k)$ of $\widehat{U_\star}(k)$ for the eigenvalues $\lambda_{\star,j}(k)$ which are C^∞ in the variable k :

$$\begin{cases} u_{\star,j}(k) := \frac{\sqrt{\eta_\star(k)+(-1)^{j-1}\varsigma_\star(k)}}{b_\star\sqrt{2\eta_\star(k)}}\begin{pmatrix} i b_\star(k) \\ \varsigma_\star(k) + (-1)^j\eta_\star(k)\end{pmatrix} & \text{if } a_\star \in [0,1) \\ u_{\star,1}(k) := \binom{1}{0} \quad \text{and} \quad u_{\star,2}(k) := \binom{0}{1} & \text{if } a_\star = 1. \end{cases}$$

We leave the reader check that $u_{\star,j}(k)$ are indeed normalised eigenvectors of $\widehat{U_\star}(k)$ with eigenvalues $\lambda_{\star,j}(k)$. In addition, since for $a_\star \in [0, 1)$ one has $\eta_\star(k) > 0$ and $\eta_\star(k) + (-1)^{j-1}\varsigma_\star(k) > 0$, the 2π-periodic map $\mathbb{R} \ni k \mapsto u_{\star,j}(k) \in \mathbb{C}^2$ is of class C^∞.

Our next goal is to construct a conjugate operator for the operator $U_\star$. For this, a few preliminaries are necessary. First, we equip the interval $[0, 2\pi)$ with the addition modulo 2π, and for any $n \in \mathbb{N}$ we define the space $C^n\big([0, 2\pi), \mathbb{C}^2\big) \subset \mathcal{K}$ as the set of functions $[0, 2\pi) \to \mathbb{C}^2$ of class C^n. In particular, we have $u_{\star,j} \in C^\infty\big([0, 2\pi), \mathbb{C}^2\big)$, and the space $\mathscr{F}\mathcal{H}_{\rm fin} \subset C^\infty\big([0, 2\pi), \mathbb{C}^2\big)$ is the set of $\mathbb{C}^2$-valued trigonometric polynomials.

Next, we define the asymptotic velocity operator for the operator $U_\star$. For $j = 1, 2$, we let $v_{\star,j} : [0, 2\pi) \to \mathbb{R}$ be the bounded function given by

$$v_{\star,j}(k) := i\,\lambda'_{\star,j}(k)\big(\lambda_{\star,j}(k)\big)^{-1}, \quad k \in [0, 2\pi). \tag{4.2}$$

Here, $(\,\cdot\,)'$ stands for the derivative with respect to k, and $v_{\star,j}$ is real valued because $\lambda_{\star,j}$ takes values in $\mathbb{T}$. Finally, for all $f \in \mathcal{K}$ and almost every $k \in [0, 2\pi)$, we define the decomposable operator $\widehat{V_\star} \in \mathscr{B}(\mathcal{K})$ by

$$\big(\widehat{V_\star} f\big)(k) := \widehat{V_\star}(k) f(k) \quad \text{where} \quad \widehat{V_\star}(k) := \sum_{j=1}^{2} v_{\star,j}(k)\,\Pi_{\star,j}(k) \in \mathscr{B}(\mathbb{C}^2), \tag{4.3}$$

and we call asymptotic velocity operator the operator $V_\star := \mathscr{F}^*\,\widehat{V_\star}\,\mathscr{F}$. The basic spectral properties of $V_\star$ are collected in the following lemma.

Lemma 4.2 (Spectrum of $V_\star$) *Let $C_\star$ be parameterised as in* (4.1).

(a) *If $a_\star = 0$, then $v_{\star,j} = 0$ for $j = 1, 2$, and $V_\star = 0$.*

(b) *If* $a_\star \in (0,1)$*, then* $v_{\star,j}(k) = \frac{(-1)^j \varsigma_\star(k)}{\eta_\star(k)}$ *for* $j=1,2$ *and* $k \in [0,2\pi)$*,* $\sigma_{\rm p}(V_\star) = \varnothing$ *and*

$$\sigma(V_\star) = \sigma_{\rm c}(V_\star) = [-a_\star, a_\star].$$

(c) *If* $a_\star = 1$*, then* $v_{\star,j} = (-1)^j$ *for* $j = 1,2$*, and* $V_\star$ *has pure point spectrum*

$$\sigma(V_\star) = \sigma_{\rm p}(V_\star) = \{-1, 1\}$$

with each point an eigenvalue of $V_\star$ *of infinite multiplicity.*

Proof The claims follow from simple calculations using the formulas for $\lambda_{\star,j}(k)$ in the proof of Lemma 4.1 and the definition (4.2) of $v_{\star,j}(k)$. □

For any $\xi, \zeta \in C\big([0,2\pi),\mathbb{C}^2\big)$, we define the operator $|\xi\rangle\langle\zeta| : C\big([0,2\pi),\mathbb{C}^2\big) \to C\big([0,2\pi),\mathbb{C}^2\big)$ by

$$\big(|\xi\rangle\langle\zeta| f\big)(k) := \big\langle\zeta(k), f(k)\big\rangle_2\, \xi(k), \quad f \in C\big([0,2\pi),\mathbb{C}^2\big),\ k \in [0,2\pi),$$

where $\langle\,\cdot\,,\,\cdot\,\rangle_2$ is the usual scalar product on $\mathbb{C}^2$. This operator extends continuously to an element of $\mathscr{B}(\mathcal{K})$, with norm satisfying the bound

$$\big\| |\xi\rangle\langle\zeta| \big\|_{\mathscr{B}(\mathcal{K})} \le \|\xi\|_{\mathrm{L}^\infty([0,2\pi),\frac{\mathrm{d}k}{2\pi},\mathbb{C}^2)}\, \|\zeta\|_{\mathrm{L}^\infty([0,2\pi),\frac{\mathrm{d}k}{2\pi},\mathbb{C}^2)}. \tag{4.4}$$

We also define the self-adjoint operator P in $\mathcal{K}$

$$\begin{aligned} Pf &:= -if', \quad f \in \mathcal{D}(P) \\ \mathcal{D}(P) &:= \big\{ f \in \mathcal{K} \mid f \text{ is absolutely continuous, } f' \in \mathcal{K}, \text{ and } f(0) = f(2\pi) \big\}. \end{aligned}$$

With these definitions at hand, we can prove the self-adjointness of an operator useful for the definition of our future the conjugate operator for U:

Lemma 4.3 *The operator*

$$\widehat{X_\star} f := -\sum_{j=1}^{2} \big(|u_{\star,j}\rangle\langle u_{\star,j}| P - i\, |u_{\star,j}\rangle\langle u'_{\star,j}| \big) f, \quad f \in \mathscr{F}\mathcal{H}_{\rm fin},$$

is essentially self-adjoint in $\mathcal{K}$*, with closure denoted by the same symbol. In particular, the Fourier transform* $X_\star := \mathscr{F}^*\widehat{X_\star}\mathscr{F}$ *of* $\widehat{X_\star}$ *is essentially self-adjoint on* $\mathcal{H}_{\rm fin}$ *in* $\mathcal{H}$*.*

Proof The proof simply consists in checking the assumptions of Nelson's commutator theorem [36, Thm. X.37] applied with the comparison operator $N := P^2 + 1$. □

The main relations between the operators introduced so far are summarised in the following proposition whose proof is left to the reader. To state it, we need one more decomposable operator $\widehat{H_\star} \in \mathscr{B}(\mathcal{K})$ defined for all $f \in \mathcal{K}$ and almost every $k \in [0, 2\pi)$ by

$$\big(\widehat{H_\star} f\big)(k) := \widehat{H_\star}(k) f(k) \quad \text{where} \quad \widehat{H_\star}(k) := -\sum_{j=1}^{2} v'_{\star,j}(k)\, \Pi_{\star,j}(k) \in \mathscr{B}(\mathbb{C}^2).$$

We also need the inverse Fourier transform $H_\star := \mathscr{F}^* \widehat{H_\star} \mathscr{F}$ of $\widehat{H_\star}$.

Proposition 4.4 (a) *One has the equality* $[iX_\star, V_\star] = H_\star$ *in the form sense on* $\mathcal{H}_{\text{fin}}$.
(b) $U_\star$, $V_\star$ *and* $H_\star$ *are mutually commuting.*
(c) *One has the equality* $[X_\star, U_\star] = U_\star V_\star$ *in the form sense on* $\mathcal{H}_{\text{fin}}$.

Since $X_\star$ is essentially self-adjoint on $\mathcal{H}_{\text{fin}}$, Proposition 4.4(a) implies that $V_\star \in C^1(X_\star)$. Therefore,

$$A_\star \Psi := \tfrac{1}{2}\big(X_\star V_\star + V_\star X_\star\big)\Psi, \quad \Psi \in \mathcal{D}(A_\star) := \big\{\Psi \in \mathcal{H} \mid V_\star \Psi \in \mathcal{D}(X_\star)\big\},$$

is self-adjoint in $\mathcal{H}$, and essentially self-adjoint on $\mathcal{H}_{\text{fin}}$ (see [44, Lemma 2.4]). We can now state and prove the main results of this section. The symbols $\operatorname{Int}(\Theta)$ and $\partial\Theta$ denote the interior and the boundary of a set $\Theta \subset \mathbb{T}$.

Proposition 4.5 (a) $U_\star \in C^1(A_\star)$ *with* $U_\star^{-1}[A_\star, U_\star] = V_\star^2$.
(b) $\varrho_{U_\star}^{A_\star} = \widetilde{\varrho}_{U_\star}^{A_\star}$, *and*
 (i) *if* $a_\star = 0$, *then* $\widetilde{\varrho}_{U_\star}^{A_\star}(\theta) = 0$ *for* $\theta \in \big\{i\,\mathrm{e}^{i\delta_\star/2}, -i\,\mathrm{e}^{i\delta_\star/2}\big\}$ *and* $\widetilde{\varrho}_{U_\star}^{A_\star}(\theta) = \infty$ *otherwise,*
 (ii) *if* $a_\star \in (0,1)$, *then* $\widetilde{\varrho}_{U_\star}^{A_\star}(\theta) > 0$ *for* $\theta \in \operatorname{Int}\big(\sigma(U_\star)\big)$, $\widetilde{\varrho}_{U_\star}^{A_\star}(\theta) = 0$ *for* $\theta \in \partial\sigma(U_\star)$, *and* $\widetilde{\varrho}_{U_\star}^{A_\star}(\theta) = \infty$ *otherwise,*
 (iii) *if* $a_\star = 1$, *then* $\widetilde{\varrho}_{U_\star}^{A_\star}(\theta) = 1$ *for all* $\theta \in \mathbb{T}$.
(c) (i) *If* $a_\star \in (0,1)$, *then* $U_\star$ *has purely absolutely continuous spectrum*

$$\sigma(U_\star) = \sigma_{\text{ac}}(U_\star) = \big\{\mathrm{e}^{i\gamma} \mid \gamma \in [\delta_\star/2 + \theta_\star, \pi + \delta_\star/2 - \theta_\star] \cup [\pi + \delta_\star/2 + \theta_\star, 2\pi + \delta_\star/2 - \theta_\star]\big\}.$$

 (ii) *If* $a_\star = 1$, *then* $U_\star$ *has purely absolutely continuous spectrum* $\sigma(U_\star) = \sigma_{\text{ac}}(U_\star) = \mathbb{T}$.

Proof (a) A calculation in the forme sense on $\mathcal{H}_{\text{fin}}$ using points (b) and (c) of Proposition 4.4 gives

$$[A_\star, U_\star] = \tfrac{1}{2}\big(V_\star[X_\star, U_\star] + [X_\star, U_\star]V_\star\big) = U_\star V_\star^2.$$

Since $A_\star$ is essentially self-adjoint on $\mathcal{H}_{\text{fin}}$, this implies that $U_\star \in C^1(A_\star)$ with $U_\star^{-1}[A_\star, U_\star] = V_\star^2$.

(b) Take $\theta \in \mathbb{T}$ and $\varepsilon > 0$. Then, the result of point (a) and (4.3) imply for almost every $k \in [0, 2\pi)$

$$\begin{aligned}\big(\mathscr{F} E^{U_\star}(\theta;\varepsilon) U_\star^{-1}[A_\star, U_\star] E^{U_\star}(\theta;\varepsilon)\mathscr{F}^*\big)(k) &= \big(\mathscr{F} E^{U_\star}(\theta;\varepsilon)\, V_\star^2 E^{U_\star}(\theta;\varepsilon)\mathscr{F}^*\big)(k)\\ &= E^{\widehat{U_\star}(k)}(\theta;\varepsilon)\, \widehat{V_\star}(k)^2 E^{\widehat{U_\star}(k)}(\theta;\varepsilon)\\ &\geq \min\big\{v_{\star,1}(k)^2, v_{\star,2}(k)^2\big\} E^{\widehat{U_\star}(k)}(\theta;\varepsilon).\end{aligned}$$

Then, the definition (4.2) of $v_{\star,j}(k)$ shows that $v_{\star,j}(k) = 0$ if and only if $\lambda'_{\star,j}(k) = 0$, which occurs when $\lambda_{\star,j}(k) \in \partial\sigma(U_\star)$. Therefore, one gets $\varrho_{U_\star}^{A_\star} = \widetilde{\varrho}_{U_\star}^{A_\star}$ by Lemma 3.3(d), and to conclude one just has to take into account the form of the boundary sets $\sigma(U_\star)$ given in Lemma 4.1.

(c) We know from point (a) that $U_\star \in C^1(A_\star)$ with $U_\star^{-1}[A_\star, U_\star] = V_\star^2$, and Proposition 4.4(a) implies that $V_\star \in C^1(A_\star)$. Thus, $U_\star \in C^2(A_\star)$. Therefore, if $a_\star \in (0,1)$, we infer from point (b.ii) and Theorem 3.5 that $U_\star$ has no singular continuous spectrum in $\mathrm{Int}\big(\sigma(U_\star)\big)$. This, together with Lemma 4.1(b), implies the claim in the case $a_\star \in (0,1)$. The claim in the case $a_\star = 1$ is proved in a similar way.□

4.2 Mourre estimate for U

In this section, we use the Mourre estimate for the asymptotic operators U_ℓ, U_r to derive a Mourre estimate for U. To achieve this, we apply the abstract construction introduced in Sect. 3.2, starting by choosing $\mathcal{H}_0 := \mathcal{H} \oplus \mathcal{H}$ as second Hilbert space and $U_0 := U_\ell \oplus U_\mathrm{r}$ as second unitary operator in $\mathcal{H}_0$.

The spectral properties of U_0 are obtained as a consequence of Lemma 4.1(a), Proposition 4.5(c) and the direct sum decomposition of U_0 :

Lemma 4.6 (Spectrum of U_0) *One has $\sigma(U_0) = \sigma(U_\ell) \cup \sigma(U_\mathrm{r})$ and $\sigma_{\mathrm{sc}}(U_0) = \varnothing$. Furthermore,*

(a) *if $a_\ell = a_\mathrm{r} = 0$, then U_0 has pure point spectrum*

$$\sigma(U_0) = \sigma_\mathrm{p}(U_0) = \sigma_\mathrm{p}(U_\ell) \cup \sigma_\mathrm{p}(U_\mathrm{r}) = \big\{i\,\mathrm{e}^{i\delta_\ell/2}, -i\,\mathrm{e}^{i\delta_\ell/2}, i\,\mathrm{e}^{i\delta_\mathrm{r}/2}, -i\,\mathrm{e}^{i\delta_\mathrm{r}/2}\big\}$$

with each point an eigenvalue of U_0 of infinite multiplicity,

(b) *if $a_\ell = 0$ and $a_\mathrm{r} \in (0,1]$, then $\sigma_{\mathrm{ac}}(U_0) = \sigma_{\mathrm{ac}}(U_\mathrm{r})$ with $\sigma_{\mathrm{ac}}(U_\mathrm{r})$ as in Proposition* 4.5(c)*, and*

$$\sigma_\mathrm{p}(U_0) = \sigma_\mathrm{p}(U_\ell) = \big\{i\,\mathrm{e}^{i\delta_\ell/2}, -i\,\mathrm{e}^{i\delta_\ell/2}\big\}$$

with each point an eigenvalue of U_0 of infinite multiplicity,

(c) *if $a_\ell \in (0,1]$ and $a_\mathrm{r} = 0$, then $\sigma_{\mathrm{ac}}(U_0) = \sigma_{\mathrm{ac}}(U_\ell)$ with $\sigma_{\mathrm{ac}}(U_\ell)$ as in Proposition* 4.5(c)*, and*

$$\sigma_\mathrm{p}(U_0) = \sigma_\mathrm{p}(U_\mathrm{r}) = \big\{i\,\mathrm{e}^{i\delta_\mathrm{r}/2}, -i\,\mathrm{e}^{i\delta_\mathrm{r}/2}\big\}$$

with each point an eigenvalue of U_0 of infinite multiplicity,

(d) *if* $a_\ell, a_{\rm r} \in (0,1]$*, then* U_0 *has purely absolutely continuous spectrum*

$$\sigma(U_0) = \sigma_{\rm ac}(U_0) = \sigma_{\rm ac}(U_\ell) \cup \sigma_{\rm ac}(U_{\rm r})$$

with $\sigma_{\rm ac}(U_\ell)$ *and* $\sigma_{\rm ac}(U_{\rm r})$ *as in Proposition* 4.5(c).

Also, as intuition suggests and as already stated in Theorem 2.2, the spectrum of U_0 coincides with the essential spectrum of U, namely $\sigma_{\rm ess}(U) = \sigma(U_\ell) \cup \sigma(U_{\rm r}) = \sigma(U_0)$.

Proof of Theorem 2.2 The proof is based on an argument using crossed product C^*-algebras inspired from [32]. Let $\mathcal{A}$ be the algebra of functions $\mathbb{Z} \to \mathscr{B}(\mathbb{C}^2)$ admitting limits at $\pm\infty$, and let $\mathcal{A}_0$ be the ideal of $\mathcal{A}$ consisting in functions $\mathbb{Z} \to \mathscr{B}(\mathbb{C}^2)$ vanishing at $\pm\infty$. Since $\mathcal{A}$ is equipped with an action of $\mathbb{Z}$ by translation, namely

$$\big(T_y\varphi\big)(x) := \varphi(x+y), \quad x, y \in \mathbb{Z},\ \varphi \in \mathcal{A},$$

we can consider the crossed product algebra $\mathcal{A} \rtimes \mathbb{Z}$, and the functoriality of the crossed product implies the identities

$$\begin{aligned}(\mathcal{A} \rtimes \mathbb{Z})/(\mathcal{A}_0 \rtimes \mathbb{Z}) &\cong (\mathcal{A}/\mathcal{A}_0) \rtimes \mathbb{Z} = \big(\mathscr{B}(\mathbb{C}^2) \oplus \mathscr{B}(\mathbb{C}^2)\big) \rtimes \mathbb{Z} \\ &= \big(\mathscr{B}(\mathbb{C}^2) \rtimes \mathbb{Z}\big) \oplus \big(\mathscr{B}(\mathbb{C}^2) \rtimes \mathbb{Z}\big), \end{aligned} \tag{4.5}$$

where the equality $\mathcal{A}/\mathcal{A}_0 = \mathscr{B}(\mathbb{C}^2) \oplus \mathscr{B}(\mathbb{C}^2)$ is obtained by evaluation of the functions $\varphi \in \mathcal{A}$ at $\pm\infty$.

Now, the algebras $\mathcal{A} \rtimes \mathbb{Z}$ and $\mathcal{A}_0 \rtimes \mathbb{Z}$ can be faithfully represented in $\mathcal{H}$ by mapping the elements of $\mathcal{A}$ and $\mathcal{A}_0$ to multiplication operators in $\mathcal{H}$ and the elements of $\mathbb{Z}$ to the shifts T_z. Writing $\mathfrak{A}$ and $\mathfrak{A}_0$ for these representations of $\mathcal{A} \rtimes \mathbb{Z}$ and $\mathcal{A}_0 \rtimes \mathbb{Z}$ in $\mathcal{H}$, we can note three facts. First, $\mathfrak{A}_0$ is equal to the ideal of compact operators $\mathscr{K}(\mathcal{H})$. Secondly, the operator U belongs to $\mathfrak{A}$, since

$$U = SC = T_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} C + T_{-1} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} C$$

with T_1, T_{-1} shifts and $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right) C$, $\left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right) C$ multiplication operators in $\mathcal{H}$. Thirdly, the essential spectrum of U in $\mathfrak{A}$ is equal to the spectrum of the image of U in the quotient algebra $\mathfrak{A}/\mathscr{K}(\mathcal{H}) = \mathfrak{A}/\mathfrak{A}_0$. These facts, together with (4.5) and Lemma 4.6, imply the equalities

$$\sigma_{\rm ess}(U) = \sigma\big(SC(-\infty) \oplus SC(+\infty)\big) = \sigma\big(SC_\ell \oplus SC_{\rm r}\big) = \sigma(U_\ell) \cup \sigma(U_{\rm r}) = \sigma(U_0),$$

which prove the claim. □

Next, we define the identification operator $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ by

$$J(\Psi_\ell, \Psi_{\rm r}) := j_\ell \Psi_\ell + j_{\rm r} \Psi_{\rm r}, \quad (\Psi_\ell, \Psi_{\rm r}) \in \mathcal{H}_0,$$

where

$$j_{\rm r}(x) := \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x \leq -1 \end{cases} \quad \text{and} \quad j_\ell := 1 - j_{\rm r}.$$

The adjoint operator $J^* \in \mathscr{B}(\mathcal{H}, \mathcal{H}_0)$ satisfies $J^*\Psi = (j_\ell \Psi, j_{\rm r} \Psi)$ for $\Psi \in \mathcal{H}$. Using the same notation for the functions j_ℓ, $j_{\rm r}$ and the associated multiplication operators in $\mathcal{H}$, one directly gets:

Lemma 4.7 *$J^*J = j_\ell \oplus j_{\rm r}$ is an orthogonal projection, and $JJ^* = 1_{\mathcal{H}}$.*

The first result of the next lemma is an analogue of Proposition 4.5(a) in the Hilbert space $\mathcal{H}_0$. To state it, we need to introduce the operator $A_0 := A_\ell \oplus A_{\rm r}$ (which will be used as a conjugate operator for U_0) and the operator $V_0 := V_\ell \oplus V_{\rm r}$.

Lemma 4.8 (a) *$U_0 \in C^1(A_0)$ with $U_0^{-1}[A_0, U_0] = V_0^2$.*
(b) *$B := JU_0 - UJ \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$ and $B_* := JU_0^* - U^*J \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$.*

Proof The proof of point (a) is similar to the proof of Proposition 4.5(a); one just has to replace the operators $U_\star, A_\star, V_\star$ in $\mathcal{H}$ by the operators U_0, A_0, V_0 in $\mathcal{H}_0$. For point (b), a direct computation with $(\Psi_\ell, \Psi_{\rm r}) \in \mathcal{H}_0$ gives

$$\begin{aligned} B(\Psi_\ell, \Psi_{\rm r}) &= \big(j_\ell U_\ell \Psi_\ell + j_{\rm r} U_{\rm r} \Psi_{\rm r}\big) - U\big(j_\ell \Psi_\ell + j_{\rm r} \Psi_{\rm r}\big) \\ &= \big([j_\ell, U_\ell] - (U - U_\ell)\, j_\ell\big)\Psi_\ell + \big([j_{\rm r}, U_{\rm r}] - (U - U_{\rm r})\, j_{\rm r}\big)\Psi_{\rm r} \\ &= \big([j_\ell, S]C_\ell - S(C - C_\ell)\, j_\ell\big)\Psi_\ell + \big([j_{\rm r}, S]C_{\rm r} - S(C - C_{\rm r})\, j_{\rm r}\big)\Psi_{\rm r}. \end{aligned} \tag{4.6}$$

Since we have $[j_\star, S] \in \mathscr{K}(\mathcal{H})$ and $(C - C_\star)\, j_\star \in \mathscr{K}(\mathcal{H})$ as a consequence of Assumption 2.1, it follows that $B \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$. The inclusion $B_* \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$ is proved in a similar way. □

The next step is to define a conjugate operator A for U by using the conjugate operator A_0 for U_0. For this, we consider the operator JA_0J^* which is well-defined and symmetric on $\mathcal{H}_{\rm fin}$. We have the equality

$$JA_0J^* = j_\ell A_\ell j_\ell + j_{\rm r} A_{\rm r} j_{\rm r} \quad \text{on} \quad \mathcal{H}_{\rm fin}, \tag{4.7}$$

and JA_0J^* is essentially self-adjoint on $\mathcal{H}_{\rm fin}$:

Lemma 4.9 (Conjugate operator for U) *The operator JA_0J^* is essentially self-adjoint on $\mathcal{H}_{\rm fin}$, with corresponding self-adjoint extension denoted by A.*

Proof The operator $\widehat{j_\star} := \mathscr{F} j_\star \mathscr{F}^* \in \mathscr{B}(\mathcal{K})$ satisfies $\widehat{j_\star}\mathcal{D}(P) \subset \mathcal{D}(P)$ and $[\widehat{j_\star}, P] = 0$ on $\mathcal{D}(P)$. Therefore, we have the following equalities on $\mathscr{F}\mathcal{H}_{\rm fin}$

$$\begin{aligned} \mathscr{F} j_\star A_\star j_\star \mathscr{F}^* &= \tfrac{1}{2} \mathscr{F} j_\star \big(X_\star V_\star + V_\star X_\star\big)\, j_\star \mathscr{F}^* \\ &= \tfrac{1}{2}\, \widehat{j_\star}\big(\widehat{X_\star}\widehat{V_\star} + \widehat{V_\star}\widehat{X_\star}\big)\, \widehat{j_\star} \end{aligned}$$

$$= \widehat{j_\star}\big(\widehat{V_\star}\widehat{X_\star} - \tfrac{i}{2}\widehat{H_\star}\big)\,\widehat{j_\star}$$
$$= -\sum_{j=1}^{2}\Big(\widehat{j_\star}\big|v_{\star,j}u_{\star,j}\big\rangle\!\big\langle u_{\star,j}\big|\,\widehat{j_\star}\,P - i\,\widehat{j_\star}\big|v_{\star,j}u_{\star,j}\big\rangle\!\big\langle u'_{\star,j}\big|\,\widehat{j_\star}\Big) - \tfrac{i}{2}\,\widehat{j_\star}\widehat{H_\star}\widehat{j_\star}.$$

which give on $\mathscr{F}\mathcal{H}_{\rm fin}$

$$\mathscr{F}JA_0J^*\mathscr{F}^* = -\sum_{j=1}^{2}\sum_{\star\in\{\ell,{\rm r}\}}\widehat{j_\star}\big|v_{\star,j}u_{\star,j}\big\rangle\!\big\langle u_{\star,j}\big|\,\widehat{j_\star}\,P$$
$$+i\sum_{j=1}^{2}\sum_{\star\in\{\ell,{\rm r}\}}\widehat{j_\star}\big|v_{\star,j}u_{\star,j}\big\rangle\!\big\langle u'_{\star,j}\big|\,\widehat{j_\star} - \tfrac{i}{2}\sum_{\star\in\{\ell,{\rm r}\}}\widehat{j_\star}\widehat{H_\star}\widehat{j_\star}.$$

The rest of the proof consists in an application of Nelson's commutator theorem [36, Thm. X.37] with the comparison operator $N := P^2 + 1$. As a consequence, it follows that $\mathscr{F}JA_0J^*\mathscr{F}^*$ is essentially self-adjoint on $\mathscr{F}\mathcal{H}_{\rm fin}$, and thus that JA_0J^* is essentially self-adjoint on $\mathcal{H}_{\rm fin}$. □

We are thus in the set-up of Assumption 3.9 with $\mathscr{D} = \mathcal{H}_{\rm fin}$. So, the next step is to show the inclusion $U \in C^1(A)$. For this, we use Corollary 3.10. Using Corollary 3.11, we also get an additional compacity result:

Lemma 4.10 *$U \in C^1(A)$ and $JU_0^{-1}[A_0, U_0]J^* - U^{-1}[A, U] \in \mathscr{K}(\mathcal{H})$.*

Proof First, we recall that $U_0 \in C^1(A_0)$ due to Lemma 4.8(a), and that Assumption 3.9 holds with $\mathscr{D} = \mathcal{H}_{\rm fin}$. Next, we note that the expression for $B(\Psi_\ell, \Psi_{\rm r})$ with $(\Psi_\ell, \Psi_{\rm r}) \in \mathcal{H}_0$ is given in (4.6), and that

$$B_*(\Psi_\ell, \Psi_{\rm r}) = \big(C^*[j_\ell, S^*] - (C^* - C_\ell^*)\,j_\ell S^*\big)\Psi_\ell + \big(C^*[j_{\rm r}, S^*] - (C^* - C_{\rm r}^*)\,j_{\rm r} S^*\big)\Psi_{\rm r}.$$

Furthermore, we know from Lemma 4.8(b) that $B, B_* \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$. In consequence, due to Corollaries 3.10–3.11, the claims will follow if we show that $\overline{BA_0 \restriction \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ and $\overline{B_*A_0 \restriction \mathcal{D}(A_0)} \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$. For this, we first note that computations as in the proof of Lemma 4.9 imply on $\mathcal{H}_{\rm fin}$ the equalities

$$A_\star = -\mathscr{F}^*\Big\{P\sum_{j=1}^{2}\Big(\big|u_{\star,j}\big\rangle\!\big\langle v_{\star,j}u_{\star,j}\big| + i\,\big|u'_{\star,j}\big\rangle\!\big\langle v_{\star,j}u_{\star,j}\big|\Big)\Big\}\mathscr{F} + \tfrac{i}{2}H_\star$$
$$= Q\,\mathscr{F}^*\Big\{\sum_{j=1}^{2}\Big(\big|u_{\star,j}\big\rangle\!\big\langle v_{\star,j}u_{\star,j}\big| + i\,\big|u'_{\star,j}\big\rangle\!\big\langle v_{\star,j}u_{\star,j}\big|\Big)\Big\}\mathscr{F} + \tfrac{i}{2}H_\star \qquad (4.8)$$

with Q the self-adjoint multiplication operator defined by

$$\big(Q\Psi\big)(x) = x\,\Psi(x), \quad x \in \mathbb{Z}, \;\; \Psi \in \mathcal{D}(Q) := \big\{\Psi \in \mathcal{H} \mid \|Q\Psi\|_{\mathcal{H}} < \infty\big\}. \qquad (4.9)$$

Therefore, since all the operators on the right of Q in (4.8) are bounded, it is sufficient to show that

$$\overline{B(Q \oplus Q) \upharpoonright \mathcal{D}(Q) \oplus \mathcal{D}(Q)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$$
$$\text{and} \quad \overline{B_*(Q \oplus Q) \upharpoonright \mathcal{D}(Q) \oplus \mathcal{D}(Q)} \in \mathscr{K}(\mathcal{H}_0, \mathcal{H}).$$

But, this can be deduced from the Assumption 2.1 once the following observations are made: $\big[j_\star, S\big] = S m_\star$ with $m_\star : \mathbb{Z} \to \mathscr{B}(\mathbb{C}^2)$ a function with compact support, $[j_\star, S^*] = S^* n_\star$ with $n_\star : \mathbb{Z} \to \mathscr{B}(\mathbb{C}^2)$ a function with compact support, and $S^* Q = Q S^* + b$ with $b \in \mathrm{L}^\infty\big(\mathbb{Z}, \mathscr{B}(\mathbb{C}^2)\big)$. □

Recall that the set $\tau(U) = \partial\sigma(U_\ell) \cup \partial\sigma(U_\mathrm{r})$ has been introduced in Sect. 2. Due to Lemma 4.1, $\tau(U)$ contains at most 8 values. Moreover, since we show in the next proposition that a Mourre estimate holds outside $\tau(U)$, it is natural to interpret $\tau(U)$ as the set of thresholds in the spectrum of U.

Proposition 4.11 *(Mourre estimate for U) We have* $\widetilde{\varrho}_U^A \ge \widetilde{\varrho}_{U_0}^{A_0}$ *with* $\widetilde{\varrho}_{U_0}^{A_0} = \min\big\{\widetilde{\varrho}_{U_\ell}^{A_\ell}, \widetilde{\varrho}_{U_\mathrm{r}}^{A_\mathrm{r}}\big\}$ *and* $\widetilde{\varrho}_{U_\ell}^{A_\ell}, \widetilde{\varrho}_{U_\mathrm{r}}^{A_\mathrm{r}}$ *given in Proposition 4.5. In particular,* $\widetilde{\varrho}_{U_0}^{A_0}(\theta) > 0$ *if* $\theta \in \{\sigma(U_\ell) \cup \sigma(U_\mathrm{r})\} \setminus \tau(U)$.

Proof The first claim follows from Theorem 3.6, with the assumptions of this theorem verified in Lemmas 4.7–4.10. The second claim follows from Proposition 4.5 and standard results on the function $\widetilde{\varrho}_{U_0}^{A_0}$ when A_0 and U_0 are direct sums of operators (see [3, Prop. 8.3.5] for a proof in the case of direct sums of self-adjoint operators). □

4.3 Spectral properties of U

In order to go one step further in the study of U, a regularity property of U with respect to A stronger than $U \in C^1(A)$ has to be established. This regularity property will be obtained by considering first the operator $J U_0 J^*$, and then by analysing the difference $U - J U_0 J^*$. We note that $J U_0 J^*$ and $U - J U_0 J^*$ satisfy the equalities

$$J U_0 J^* = j_\ell \, U_\ell \, j_\ell + j_\mathrm{r} \, U_\mathrm{r} \, j_\mathrm{r} \tag{4.10}$$

and

$$U - J U_0 J^* = j_\ell (U - U_\ell) \, j_\ell + j_\mathrm{r} (U - U_\mathrm{r}) \, j_\mathrm{r} + j_\ell \, U \, j_\mathrm{r} + j_\mathrm{r} \, U \, j_\ell. \tag{4.11}$$

Lemma 4.12 $J U_0 J^* \in C^2(A)$.

Proof The proof is based on standard results from toroidal pseudodifferential calculus, as presented for example in [40, Chap. 4]. The normalisation we use for the Fourier transform differs from the one used in [40], but the difference is harmless.

(i) First, we note that $\widehat{j_\star}$ is a toroidal pseudodifferential operator on $\mathscr{F}\mathcal{H}_{\mathrm{fin}}$ with symbol in $S^0_{\rho,0}(\mathbb{T} \times \mathbb{Z})$ for each $\rho > 0$ (see the definitions 4.1.7 and 4.1.9 of [40]). Similarly, Eq. (4.8) shows that $\widehat{A_\star}$ is a first-order differential operator on $\mathscr{F}\mathcal{H}_{\mathrm{fin}}$ with matrix coefficients in $\mathrm{M}\big(2, C^\infty(\mathbb{T})\big) \subset \mathrm{M}\big(2, S^0_{\rho,0}(\mathbb{T}\times\mathbb{Z})\big)$ for each $\rho > 0$. In consequence, it follows from [40, Thm. 4.7.10] that the commutator $\big[\widehat{j_\star}, \widehat{A_\star}\big]$ on $\mathscr{F}\mathcal{H}_{\rm fin}$ is well-defined and equal to a toroidal pseudodifferential operator with matrix coefficients in $\mathrm{M}\big(2, S^{1-\rho}_{\rho,0}(\mathbb{T}\times\mathbb{Z})\big)$ for each $\rho > 0$. This implies that $\big[\widehat{j_\star}, \widehat{A_\star}\big]$ is bounded on $\mathscr{F}\mathcal{H}_{\rm fin}$, and thus that $\widehat{j_\star} \in C^1(\widehat{A_\star})$ since $\mathscr{F}\mathcal{H}_{\rm fin}$ is dense in $\mathcal{D}(\widehat{A_\star})$. By Fourier transform, it follows that $j_\star \in C^1(A_\star)$.

(ii) A calculation in the form sense on $\mathcal{H}_{\rm fin}$ using Eqs. (4.7) and (4.10) and the identities $j_\ell\, j_{\rm r} = 0 = j_{\rm r}\, j_\ell$ gives

$$\begin{aligned}\big[JU_0J^*, A\big] &= \big[j_\ell\, U_\ell\, j_\ell,\, j_\ell\, A_\ell\, j_\ell\big] + \big[j_{\rm r}\, U_{\rm r}\, j_{\rm r},\, j_{\rm r}\, A_{\rm r}\, j_{\rm r}\big]\\ &= \sum_{\star\in\{\ell,{\rm r}\}} j_\star\big(U_\star\, j_\star A_\star - A_\star\, j_\star U_\star\big)\, j_\star\\ &= \sum_{\star\in\{\ell,{\rm r}\}} j_\star\big(\big[U_\star, j_\star\big]A_\star + \big[j_\star U_\star, A_\star\big]\big)\, j_\star. \end{aligned}\tag{4.12}$$

Since $j_\star U_\star \in C^1(A_\star)$ by Proposition 4.5(a), point (i) and [3, Prop. 5.1.5], the second term on the r.h.s. of (4.12) belongs to $\mathscr{B}(\mathcal{H})$. Furthermore, a calculation using the definition of the shift operator S shows that $\big[U_\star, j_\star\big] = \big[S, j_\star\big]C_\star = B_\star m_\star$ with $B_\star \in \mathscr{B}(\mathcal{H})$ and $m_\star : \mathbb{Z} \to \mathscr{B}(\mathbb{C}^2)$ a function with compact support. It follows from (4.8) that $\big[U_\star, j_\star\big]A_\star$ is bounded on $\mathcal{H}_{\rm fin}$. Therefore, both terms on the r.h.s. of (4.12) are bounded on $\mathcal{H}_{\rm fin}$, and thus we infer from the density of $\mathcal{H}_{\rm fin}$ in $\mathcal{D}(A)$ that $JU_0J^* \in C^1(A)$.

(iii) To show that $JU_0J^* \in C^2(A)$, one has to commute the r.h.s. of (4.12) once more with A. Doing this in the form sense on $\mathcal{H}_{\rm fin}$ with the notation $\sum_{\star\in\{\ell,{\rm r}\}} j_\star D_\star\, j_\star$ with $D_\star := [U_\star, j_\star]A_\star + [j_\star U_\star, A_\star]$ for the r.h.s. of (4.12), one gets that $JU_0J^* \in C^2(A)$ if the operators $[D_\star, A_\star]$, $[D_\star, j_\star]A_\star$ and $A_\star[D_\star, j_\star]$ defined in the form sense on $\mathcal{H}_{\rm fin}$ extend continuously to elements of $\mathscr{B}(\mathcal{H})$.

For the first operator, we have in the form sense on $\mathcal{H}_{\rm fin}$ the equalities

$$\begin{aligned}[D_\star, A_\star] &= \big[[U_\star, j_\star]A_\star + j_\star[U_\star, A_\star] + [j_\star, A_\star]U_\star, A_\star\big]\\ &= \big[[U_\star, j_\star]A_\star, A_\star\big] + j_\star\big[[U_\star, A_\star], A_\star\big] + [j_\star, A_\star][U_\star, A_\star]\\ &\quad + [j_\star, A_\star][U_\star, A_\star] + \big[[j_\star, A_\star], A_\star\big]U_\star. \end{aligned}\tag{4.13}$$

Then, simple adaptations of the arguments presented in points (i) and (ii) show that the operators $[j_\star, A_\star], [U_\star, j_\star] \in \mathscr{B}(\mathcal{H})$ can be multiplied in the form sense on $\mathcal{H}_{\rm fin}$ by several operators $A_\star$ on the left and/or on the right and that the resultant operators extend continuously to elements of $\mathscr{B}(\mathcal{H})$. Therefore, the first, the third, the fourth, and the fifth terms in (4.13) extend continuously to elements of $\mathscr{B}(\mathcal{H})$. For the second term, we note from Propositions 4.4(a) and 4.5(a) that $U_\star, V_\star \in C^1(A_\star)$ with $[U_\star, A_\star] = -U_\star V_\star^2$. In consequence, we have $U_\star V_\star^2 \in C^1(A_\star)$ by [3, Prop. 5.1.5] and

$$j_\star\big[[U_\star, A_\star], A_\star\big] = -j_\star\big[U_\star V_\star^2, A_\star\big] \in \mathscr{B}(\mathcal{H}).$$

The proof that the operators $[D_\star, j_\star]A_\star$ and $A_\star[D_\star, j_\star]$ defined in the form sense on $\mathcal{H}_{\rm fin}$ extend continuously to elements of $\mathscr{B}(\mathcal{H})$ is similar. The only noticeable difference is the appearance of terms $[U_\star V_\star^2, j_\star]A_\star$ and $A_\star[U_\star V_\star^2, j_\star]$. However, by observing that $V_\star^2 \in C^1(A_\star)$ and that $[V_\star^2, j_\star]$ is a toroidal pseudodifferential operator with matrix coefficients in $\mathrm{M}\big(2, S^{-\rho}_{\rho,0}(\mathbb{T}\times\mathbb{Z})\big)$ for each $\rho > 0$, one infers that $[U_\star V_\star^2, j_\star]A_\star$ and $A_\star[U_\star V_\star^2, j_\star]$ extend continuously to elements of $\mathscr{B}(\mathcal{H})$. □

In the next lemma, we prove that U satisfies sufficient regularity with respect to A, namely that $U \in C^{1+\varepsilon}(A)$ for some $\varepsilon \in (0,1)$. We recall from Sect. 3.1 that the sets $C^2(A)$, $C^{1+\varepsilon}(A)$, $C^{1+0}(A)$ and $C^{1,1}(A)$ satisfy the continuous inclusions $C^2(A) \subset C^{1+\varepsilon}(A) \subset C^{1+0}(A) \subset C^{1,1}(A)$.

Lemma 4.13 *$U \in C^{1+\varepsilon}(A)$ for each $\varepsilon \in (0,1)$ with $\varepsilon \le \min\{\varepsilon_\ell, \varepsilon_{\rm r}\}$.*

Proof (i) Since $JU_0J^* \in C^2(A)$ by Lemma 4.12 and $C^2(A) \subset C^{1+\varepsilon}(A)$, it is sufficient to show that $U - JU_0J^* \in C^{1+\varepsilon}(A)$, with $U - JU_0J^*$ given by (4.11). Moreover, calculations as in the proof of Lemma 4.12 show that the last two terms $j_\ell\, U\, j_{\rm r}$ and $j_{\rm r}\, U\, j_\ell$ of (4.11) belong to $C^2(A)$. So, it only remains to show that $j_\ell(U - U_\ell)\, j_\ell + j_{\rm r}(U - U_{\rm r})\, j_{\rm r} \in C^{1+\varepsilon}(A)$.

(ii) In order to show this inclusion, we first observe from (2.1) and (4.7) that we have in the form sense on $\mathcal{H}_{\rm fin}$ the equalities

$$\begin{aligned}\big[j_\ell(U-U_\ell)\, j_\ell + j_{\rm r}(U-U_{\rm r})\, j_{\rm r}, A\big] &= \sum_{\star\in\{\ell,{\rm r}\}} \big[j_\star(U-U_\star)\, j_\star, j_\star A_\star\, j_\star\big]\\ &= \sum_{\star\in\{\ell,{\rm r}\}} \big(j_\star S(C-C_\star)\, j_\star A_\star\, j_\star\\ &\qquad - j_\star A_\star\, j_\star S(C-C_\star)\, j_\star\big).\end{aligned} \tag{4.14}$$

Then, using Assumption 2.1, the formula (4.8) for $A_\star$ on $\mathcal{H}_{\rm fin}$, and a similar formula with the operator Q on the right (recall that Q is the position operator defined in (4.9)), one obtains that the operator on the r.h.s. of (4.14) defined as

$$D_\star := j_\star S(C-C_\star)\, j_\star A_\star\, j_\star - j_\star A_\star\, j_\star S(C-C_\star)\, j_\star$$

extends continuously to an element of $\mathscr{B}(\mathcal{H})$. Since $\mathcal{H}_{\rm fin}$ is dense in $\mathcal{D}(A)$, this implies that $j_\ell(U-U_\ell)\, j_\ell + j_{\rm r}(U-U_{\rm r})\, j_{\rm r} \in C^1(A)$.

(iii) To show that $j_\ell(U-U_\ell)\, j_\ell + j_{\rm r}(U-U_{\rm r})\, j_{\rm r} \in C^{1+\varepsilon}(A)$, it remains to check that

$$\big\|\,\mathrm{e}^{-itA}\, D_\star\, \mathrm{e}^{itA} - D_\star\big\|_{\mathscr{B}(\mathcal{H})} \le \mathrm{Const.}\, t^\varepsilon \quad \text{for all } t \in (0,1).$$

But, algebraic manipulations as presented in [3, pp. 325–326] show that for all $t \in (0,1)$

$$\big\|\,\mathrm{e}^{-itA}\, D_\star\, \mathrm{e}^{itA} - D_\star\big\|_{\mathscr{B}(\mathcal{H})} \le \mathrm{Const.}\big(\|\sin(tA)D_\star\|_{\mathscr{B}(\mathcal{H})} + \|\sin(tA)(D_\star)^*\|_{\mathscr{B}(\mathcal{H})}\big)$$

$$\leq \text{Const.}\big(\|tA\,(tA+i)^{-1}D_\star\|_{\mathscr{B}(\mathcal{H})} + \|tA\,(tA+i)^{-1}(D_\star)^*\|_{\mathscr{B}(\mathcal{H})}\big).$$

Furthermore, if we set $A_t := tA\,(tA+i)^{-1}$ and $\Lambda_t := t\langle Q\rangle(t\langle Q\rangle + i)^{-1}$, we obtain that

$$A_t = \big(A_t + i(tA+i)^{-1}A\,\langle Q\rangle^{-1}\big)\Lambda_t$$

with $A\langle Q\rangle^{-1} \in \mathscr{B}(\mathcal{H})$ due to (4.7)–(4.8). Thus, since $\big\|A_t+i(tA+i)^{-1}A\,\langle Q\rangle^{-1}\big\|_{\mathscr{B}(\mathcal{H})}$ is bounded by a constant independent of $t \in (0,1)$, it is sufficient to prove that

$$\|\Lambda_t D_\star\|_{\mathscr{B}(\mathcal{H})} + \|\Lambda_t(D_\star)^*\|_{\mathscr{B}(\mathcal{H})} \leq \text{Const.}\, t^\varepsilon \quad \text{for all } t \in (0,1).$$

Now, this estimate will hold if we show that the operators $\langle Q\rangle^\varepsilon D_\star$ and $\langle Q\rangle^\varepsilon(D_\star)^*$ defined in the form sense on $\mathcal{H}_{\rm fin}$ extend continuously to elements of $\mathscr{B}(\mathcal{H})$. For this, we fix $\varepsilon \in (0,1)$ with $\varepsilon \leq \min\{\varepsilon_\ell, \varepsilon_{\rm r}\}$, and note that $\langle Q\rangle^{1+\varepsilon}(C - C_\star)\, j_\star \in \mathscr{B}(\mathcal{H})$. With this inclusion and the fact that $\langle Q\rangle^{-1}A_\star$ defined in the form sense on $\mathcal{H}_{\rm fin}$ extend continuously to elements of $\mathscr{B}(\mathcal{H})$, one readily obtains that $\langle Q\rangle^\varepsilon D_\star$ and $\langle Q\rangle^\varepsilon(D_\star)^*$ defined in the form sense on $\mathcal{H}_{\rm fin}$ extend continuously to elements of $\mathscr{B}(\mathcal{H})$, as desired. □

With what precedes, we can now prove our last two main results on U which have been stated in Sect. 2.

Proof of Theorem 2.3 Theorem 3.4, whose assumptions are verified in Proposition 4.11 and Lemma 4.13, implies that each $T \in \mathscr{B}(\mathcal{H},\mathcal{G})$ which extends continuously to an element of $\mathscr{B}\big(\mathcal{D}(\langle A\rangle^s)^*,\mathcal{G}\big)$ for some $s > 1/2$ is locally U-smooth on $\Theta\setminus\sigma_{\rm p}(U)$. Moreover, we know from the proof of Lemma 4.13 that $\mathcal{D}(Q) \subset \mathcal{D}(A)$. Therefore, we have $\mathcal{D}(\langle Q\rangle^s) \subset \mathcal{D}(\langle A\rangle^s)$ for each $s > 1/2$, and it follows by duality that $\mathcal{D}(\langle A\rangle^s)^* \subset \mathcal{D}(\langle Q\rangle^s)^* \equiv \mathcal{D}(\langle Q\rangle^{-s})$ for each $s > 1/2$. In consequence, any operator $T \in \mathscr{B}(\mathcal{H},\mathcal{G})$ which extends continuously to an element of $\mathscr{B}\big(\mathcal{D}(\langle Q\rangle^{-s}),\mathcal{G}\big)$ some $s > 1/2$ also extends continuously to an element of $\mathscr{B}\big(\mathcal{D}(\langle A\rangle^s)^*,\mathcal{G}\big)$. This concludes the proof. □

Proof of Theorem 2.4 The claim follows from Theorem 3.5, whose hypotheses are verified in Lemma 4.13 and Proposition 4.11. □

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