UNIVERSITÉ DE LYON INSTITUT CAMILLE JORDAN

A few results in scattering theory :

Time operator, time delay, Mourre theory and topological Levinson's theorems

Mémoire d'habilitation à diriger des recherches
présenté au département de mathématiques de l'Université de Lyon

par

Serge RICHARD

HDR soutenue à Lyon le 16 septembre 2011

Membres du jury

J.-M. Bouclet (Université Paul Sabatier, Toulouse)

S. de Bièvre (Université de Lille 1)

V. Georgescu (Université Cergy-Pontoise)

C. Gérard (Université Paris Sud, Orsay)

J. Kellendonk (Université Claude Bernard, Lyon 1)

C.-A. Pillet (Université du Sud, Toulon)

Rapporteurs

V. Georgescu (Université Cergy-Pontoise)

C.-A. Pillet (Université du Sud, Toulon)

X.-P. Wang (Université de Nantes)

Contents

Preamble

Let us start with a few key facts. This HDR corresponds to 6 years of research (2005–2011), to stays in 3 countries (France, United Kingdom, Japan), to 24 articles ($24 + 4 - 3 - 1$, see the publication list), to a huge number of applications for funds or positions, and to more than twice this number of reference letters ! On the other hand, during that period I deeply benefit from 1 very special collaborator and friend (Rafael), from 3 mentors (Werner, Marius, Johannes), from 5 additional co-authors (Radu, Max, Konstantin, Hiroshi, Tomio), but even more importantly from Claudine and Thomas. Obviously, all this was possible thanks to the generosity of 3 research institutions (CNRS, FNS, JSPS) and thanks to the hospitality of the mathematics departments of the Universities of Lyon, of Cambridge and of Tsukuba. Now, this HDR was completed and submitted while Japan was facing the fear and the unknown consequences of a tragical nuclear accident. So this work is dedicated to the inhabitants of this country.

When I started thinking about this HDR and its content, a natural question occurred to me: how would it be possible to condense 6 years of research in a single document ? How could I link magnetic pseudodifferential calculus and the corresponding twisted crossed product algebras to a topological approach of Levinson's theorem, and add on the top of this applications of Mourre theory and the abstract notion of time delay ? Obviously, this is impossible. I could not find a way of giving an intelligent account on each of these subjects, and I finally gave up with this project. More precisely, I decided to change my point of view, perform a drastic choice between these subjects and present only a few works in their entirety. So, among the publication list presented subsequently I have chosen 5 works, namely the papers [17,19,20,23,24]. Clearly, they do not represent all subjects studied during these 6 years and give only a partial view of my interests. On the the hand, I have chosen them because these works are self-content and rather complete (at least four of them). Chapter 3, which is certainly not complete, stands for the cherry on the cake, or for the opening towards the future.

Let us be more precise. Chapters 1 and 2 correspond to publications [17] and [20]. The first one introduce the notion of time operator and the second one deals with the concept of time delay. Both subjects are treated in a completely abstract framework. Chapter 1 is self-consistency while Chapter 2 is based on the results obtained in Chapter 1. Note that the final result is then complete in the sense that it provides a rather exhaustive relation between 2 notions of time delay, both developed without reference to a special model or setting.

Chapters 4 and 5, which correspond to publications [19] and [23], have the same structure in pair: The first one presents the Aharonov-Bohm model almost from scratch while the second one provides a thorough analysis of Levinson's type theorems for this model based on the result obtained in the previous chapter. Note that a completely new relation between spectral and scattering theory is proposed in this chapter. Namely, the Chern number of a bundle defined by a family of projections on bound states is related to a 3-trace applied on the scattering part of the model.

Let us mention that Chapter 5 is also a good illustration of what we have in mind for a topological approach of Levinson's theorem. Indeed, part of last few years have been devoted to the development of a new approach of Levinson's theorem, based on a construction involving a C^*-algebraic framework. Then, Levinson's theorem can be read as an index theorem, leading to new explanations for the corrections at thresholds. This research also led to new expressions for the wave operators, the key elements in our approach. Obviously, this HDR could have been centered on this project. However, my feeling is that this research is still at a preliminary stage and I am looking for a more general and suitable framework. By mainly concentrating on this subject, the above mentioned criterion of completeness would certainly not be met and too much time would have been devoted to an unfinished work. A more general document on our findings on the topological approach of Levinson's theorem will certainly appear once in the future, but for the time being Chapter 5 is a good illustration on a concrete example.

Finally, Chapter 3 corresponds to a very recent work on the concept of a Mourre estimate in a two-Hilbert spaces setting. Clearly, this work is only a first step in a direction of research which could certainly be developed and lead to further new results. In fact, I enjoyed a lot when working on this short contribution and I wanted to add it to this HDR as an opening to the future. In particular, this initial work could lead to some new insights for the scattering theory of highly anisotropic situations.

As already mentioned, these five chapters, which can be read independently, correspond only to part of my interests and results. For completeness, a short description of my past and current research is presented at the end of this preliminary part (the different works have been divided into 3 main subjects which are very briefly introduced). However, despite this partial picture and the absence of various fields of research, I hope that this document can fully and truly present one thing: my passion for research and for the spread of knowledge.

Tsukuba, July 2011.

Publication list

Refereed Full Papers

24) S. Richard, R. Tiedra de Aldecoa, *A few results on Mourre theory in a two-Hilbert spaces setting*, 13 pages, submitted.

23) J. Kellendonk, K. Pankrashkin, S. Richard, *Levinson's theorem and higher degree traces for Aharonov-Bohm operators*, J. Math. Phys. **52**, 052102 (28 pages), 2011.

22) J. Kellendonk, S. Richard, *On the wave operators and Levinson's theorem for potential scattering in* $\mathbb{R}^3$, 19 pages, to appear in Asian-European Journal of Mathematics.

21) M. Măntoiu, R. Purice, S. Richard, *Positive quantization in the presence of a variable magnetic field*, 15 pages, submitted.

20) S. Richard, R. Tiedra de Aldecoa, *Time delay is a common feature of quantum scattering theory*, 15 pages, to appear in J. Math. Anal. Appl.

19) K. Pankrashkin, S. Richard, *Spectral and scattering theory for the Aharonov-Bohm operators*, Rev. Math. Phys. **23**, 53–81, 2011.

18) M. Măntoiu, R. Purice, S. Richard, *Coherent states in the presence of a variable magnetic field*, International Journal of Geometric Methods in Modern Physics **8**, 187–202, 2011.

17) S. Richard, R. Tiedra de Aldecoa, *New formula relating localisation operators to time operators*, 29 pages, to appear in Contemporary Mathematics Series (AMS).

16) M. Lein, M. Măntoiu, S. Richard, *Magnetic pseudodifferential operators with coefficients in* C^**-algebras*, Publ. RIMS, Kyoto Univ. **46**, 755–788, 2010.

15) S. Richard, R. Tiedra de Aldecoa, *New formulae for the wave operators for a rank one interaction*, Integral Equations and Operator Theory **66**, 283–292, 2010.

14) M. Măntoiu, S. Richard, R. Tiedra de Aldecoa, *The method of the weakly conjugate operator: Extensions and applications to operators on graphs and groups*, University of Ploiesti, Bulletin, Mathematics - informatics - physics Series **LXI**, 1–14, 2009.

13) J. Kellendonk, S. Richard, *Weber-Schafheitlin type integrals with exponent* 1, Integral Transforms and Special Functions **20**, 147–153, 2009.

12) J. Kellendonk, S. Richard, *On the structure of the wave operators in one dimensional potential scattering*, Mathematical Physics Electronic Journal **14**, 1–21, 2008.

11) J. Kellendonk, S. Richard, *The topological meaning of Levinson's theorem, half-bound states included*, J. Phys. A: Math. Theor. **41**, 295207 (7 pages), 2008.

10) S. Richard, R. Tiedra de Aldecoa, *On the spectrum of magnetic Dirac operators with Coulomb-type perturbations*, J. Funct. Ana. **250**, 625–641, 2007.

9) M. Măntoiu, S. Richard, R. Tiedra de Aldecoa, *Spectral analysis for adjacency operators on graphs*, Ann. Henri Poincaré **8**, 1401–1423, 2007.

8) M. Măntoiu, R. Purice, S. Richard, *Spectral and propagation results for magnetic Schrödinger operators; a C^*-algebraic framework*, J. Funct. Ana. **250**, 42–67, 2007.

7) M. Măntoiu, R. Purice, S. Richard, *On the essential spectrum of magnetic pseudodifferential operators*, C. R. Acad. Sci. Paris, Ser. I **344**, 11–14, 2007.

6) J. Kellendonk, S. Richard, *Levinson's theorem for Schrödinger operators with point interaction: a topological approach*, J. Phys. A: Math Gen. **39**, 14397–14403, 2006.

5) S. Richard, *Some improvements in the method of the weakly conjugate operator*, Letters in Mathematical Physics **76**, 27–36, 2006.

4) S. Richard, *Spectral and scattering theory for Schrödinger operators with cartesian anisotropy*, Publ. RIMS, Kyoto Univ. **41**, 73–111, 2005. *(Included in PhD thesis)*

3) S. Richard, R. Tiedra de Aldecoa, *On perturbations of Dirac operators with variable magnetic field of constant direction*, J. Math. Phys. **45**, 4164–4173, 2004. *(Included in PhD thesis)*

2) S. Richard, *Minimal escape velocities for unitary evolution groups*, Ann. Henri Poincaré **5**, 915–928, 2004. *(Included in PhD thesis)*

1) M. Măntoiu, S. Richard, *Absence of singular spectrum for Schrödinger operators with anisotropic potentials and magnetic fields*, J. Math. Phys. **41**, 2732–2740, 2000. *(Corresponds to Diploma Thesis)*

Refereed Conference Publications

b4) S. Richard, *Time delay for an abstract quantum scattering process*, 11 pages, submitted.

b3) S. Richard, *New formulae for the Aharonov-Bohm wave operators*, in Spectral and Scattering Theory for Quantum Magnetic Systems, 159–168, Contemporary Mathematics **500**, AMS, Providence, 2009.

b2) J. Kellendonk, S. Richard, *Topological boundary maps in physics: General theory and applications*, in Perspectives in Operator Algebras and Mathematical Physics, 105–121, Theta, Bucharest, 2008.

b1) M. Măntoiu, R. Purice, S. Richard, *Twisted crossed products and magnetic pseudodifferential operators*, in Advances in Operator Algebras and Mathematical Physics, 137–172, Theta, 2005.

Past and current research

My past and current research can be divided into 3 main subjects. The numbers $[\cdot]$ correspond to the ones in the publication list (articles can be downloaded from my homepage).

1) Levinson's theorem and wave operators [6,11,12,13,15,19,22,23,b2,b3].

Levinson's theorem is a relation between the number of bound states of a quantum mechanical system and an expression related to the scattering part of that system. The latter can be written either in terms of an integral over the time delay, or as an evaluation of the spectral shift function. In the simplest situations, the relation is an equality, but that is not always the case. Depending on the space dimension and the existence of resonances at thresholds, also called half-bound states, corrections to the former equality have to be taken into account. Different explanations for these corrections can be found in the literature, but they often have the flavor of a case-by-case study.

One of my main achievements was to show that Levinson's theorem is a topological theorem, and this includes the corrections. In our approach, we propose a topological explanation by interpreting it as an index theorem. This does not only shed new light on it, but also provides a more coherent and natural way to take the corrections and some regularizations into account. The proof relies on evaluating the index of the wave operator by the winding number of an expression involving not only the scattering operator, but also new operators that describe the system at zero energy and large energy.

The papers [11,b2] give a good account of what we have in mind for the topological Levinson's theorem. Paper [12] contains precise statements and proofs for the example of potential scattering in 1D. Papers [6,15,19,22] and [b3] contain other examples, namely Schrödinger operators with point interaction, the rank one interaction, 3D potential scattering and Schrödinger operators with singular magnetic fields (also called Aharonov-Bohm model). Publication [23] exhibits a generalization of Levinson's theorem involving higher degree traces, and publication [13] contains integrals of Weber-Schaftheitlin type, which are necessary for the calculation of explicit formulae in [b3].

2) Magnetic systems and pseudodifferential calculus [1,3,7,8,10,16,18,21,b1].

In our research, we have investigated various models involving magnetic fields. Papers [3] and [10] are concerned with the spectral analysis of magnetic Dirac operators. In the latter, perturbations of Coulomb-type with the optimal coupling constant are considered. Paper [1] contains the spectral analysis of Schrödinger operators with a rather general magnetic field.

In papers [7,8,16,18,21,b1], we introduce and develop an approach for the magnetic pseudodifferential calculus which depends only on the magnetic field and which does not require the choice of any vector potential. Paper [b1] contains the presentation of the framework which involves twisted crossed product C^*-algebras. In [7] and [8] we show the relevance of this framework for the study of the spectral theory of generalized magnetic Schrödinger operators with highly anisotropic magnetic fields and potentials. In [15] this algebraic framework is extended to incorporate an anisotropic version of the usual Hörmander classes of symbols. These works contain applications to the spectral analysis of general elliptic magnetic pseudodifferential operators. In publications [18,21], we extend the usual notion of coherent states and states quantization in the presence of a magnetic field.

3) Mourre theory and applications [1,2,3,4,5,9,10,14,17,20,24,b4].

Papers [2,3,4,10] contain applications of the usual commutator theory of Mourre, which is one of the most powerful tool in spectral and scattering theory. Limiting absorption principles, refined spectral properties, propagation estimates and minimal escape velocity are some of the outputs obtained. Paper [1] contains an application of a method of the weakly conjugate operator (MWCO) in its original form, and in reference [5] we provide the first attempt to extend the MWCO to operators with additional point spectrum. Papers [9] and [14] are applications of another extension of the MWCO to operators acting on groups and graphs. In references [17,20,b4] we provide an abstract framework for the concept of time delay, a concept very close to experiments, and in [24] we develop few new results in relation with Mourre theory in a very general setting.

Chapter 1

A new formula relating localisation operators to time operators

1.1 Introduction and main results

Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and let T be a linear operator in $\mathcal{H}$. Generally speaking, the operator T is called a time operator for H if it satisfies the canonical commutation relation

$$[T, H] = i, \tag{1.1}$$

or, alternatively, the relation

$$T\,\mathrm{e}^{-itH} = \mathrm{e}^{-itH}(T + t). \tag{1.2}$$

Obviously, these two equations are very formal and not equivalent. So many authors have proposed various sets of conditions in order to give a precise meaning to them. For instance, one has introduced the concept of infinitesimal Weyl relation in the weak or in the strong sense [56], the T-weak Weyl relation [73] or various generalised versions of the Weyl relation (see *e.g.* [14, 53]). However, in most of these publications the pair $\{H, T\}$ is a priori given and the authors are mainly interested in the properties of H and T that can be deduced from a relation like (1.2). In particular, the self-adjointness of T, the spectral nature of H and T, the connection with the survival probability, the form of T in the spectral representation of H, the relation with the theory of irreversibility and many other properties have been extensively discussed in the literature (see [77, Sec. 8], [78, Sec. 3], [13, 42, 49, 50, 113] and references therein).

Our approach is radically different. Starting from a self-adjoint operator H, one wonders if there exists a linear operator T such that (1.1) holds in a suitable sense. And can we find a universal procedure to construct such an operator ? This work is a first attempt to answer these questions.

Our interest in these questions has been recently aroused by a formula put into evidence in [111]. Along the proof of the existence of time delay for hypoelliptic pseudodifferential operators $H := h(P)$ in $\mathsf{L}^2(\mathbb{R}^d)$, the author derives an integral formula linking the time evolution of localisation operators to the derivative with respect to the spectral parameter of H. The formula reads as follows: if Q stands for the family of position operators in $\mathsf{L}^2(\mathbb{R}^d)$

and $f:\mathbb{R}^d \to \mathbb{C}$ is some appropriate function with $f = 1$ in a neighbourhood of 0, then one has on suitable elements $\varphi \in \mathsf{L}^2(\mathbb{R}^d)$

$$\lim_{r\to\infty} \tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big\langle\varphi,\big[\mathrm{e}^{-itH} f(Q/r)\,\mathrm{e}^{itH} - \mathrm{e}^{itH} f(Q/r)\,\mathrm{e}^{-itH}\big]\varphi\big\rangle = \big\langle\varphi, i\tfrac{\mathrm{d}}{\mathrm{d}H}\varphi\big\rangle, \qquad (1.3)$$

where $\frac{\mathrm{d}}{\mathrm{d}H}$ stands for the operator acting as $\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H. So, this formula furnishes a standardized procedure to obtain a time operator T only constructed in terms of H, the position operators Q and the function f.

A review of the methods used in [111] suggested to us that Equation (1.3) could be extended to the case of an abstract pair of operator H and position operators Φ acting in a Hilbert space $\mathcal{H}$, as soon as H and Φ satisfy two appropriate commutation relations. Namely, suppose that you are given a self-adjoint operator H and a family $\Phi \equiv (\Phi_1,\dots,\Phi_d)$ of mutually commuting self-adjoint operators in $\mathcal{H}$. Then, roughly speaking, the first condition requires that for some $\omega \in \mathbb{C}\setminus\mathbb{R}$ the map

$$\mathbb{R}^d \ni x \mapsto \mathrm{e}^{-ix\cdot\Phi}(H-\omega)^{-1}\,\mathrm{e}^{ix\cdot\Phi} \in \mathscr{B}(\mathcal{H})$$

is 3-times strongly differentiable (see Assumption 1.2.2 for a precise statement). The second condition, Assumption 1.2.3, requires that for each $x \in \mathbb{R}^d$, the operators $\mathrm{e}^{-ix\cdot\Phi}\,H\,\mathrm{e}^{ix\cdot\Phi}$ mutually commute. Given this, our main result reads as follows (see Theorem 1.5.5 for a precise statement):

Theorem 1.1.1. *Let H and Φ be as above. Let f be a Schwartz function on $\mathbb{R}^d$ such that $f = 1$ on a neighbourhood of 0 and $f(x) = f(-x)$ for each $x \in \mathbb{R}^d$. Then, for each φ in some suitable subset of $\mathcal{H}$ one has*

$$\lim_{r\to\infty} \tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big\langle\varphi,\big[\mathrm{e}^{-itH} f(\Phi/r)\,\mathrm{e}^{itH} - \mathrm{e}^{itH} f(\Phi/r)\,\mathrm{e}^{-itH}\big]\varphi\big\rangle = \langle\varphi, T_f\varphi\rangle, \qquad (1.4)$$

where the operator T_f acts, in an appropriate sense, as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H.

One infers from this result that the operator T_f is a time operator. Furthermore, an explicit description of T_f is also available: if H'_j denotes the self-adjoint operator associated with the commutator $i[H,\Phi_j]$ and $H' := (H'_1,\dots,H'_d)$, then T_f is formally given by

$$T_f = -\tfrac{1}{2}\big(\Phi\cdot R'_f(H') + R'_f(H')\cdot\Phi\big), \qquad (1.5)$$

where $R'_f : \mathbb{R}^d \to \mathbb{C}^d$ is some explicit function (see Section 1.4 and Proposition 1.5.2).

In summary, once a family $(\Phi_1,\dots,\Phi_d)$ of mutually commuting self-adjoint operators satisfying Assumptions 1.2.2 and 1.2.3 has been given, then a time operator can be defined either in terms of the l.h.s. of (1.4) or in terms of (1.5). When suitably defined, both expressions lead to the same operator. We also mention that the equality (1.4), with r.h.s. defined by (1.5), provides a crucial preliminary step for the proof of the existence of quantum time delay and Eisenbud-Wigner Formula for abstract scattering pairs $\{H, H+V\}$. In addition, Theorem 1.1.1 establishes a new relation between time dependent scattering theory (l.h.s.)

and stationary scattering theory (r.h.s.) for a general class of operators. We refer to the discussion in Section 1.6 for more information on these issues.

Let us now describe more precisely the content of this work. In Section 1.2 we recall the necessary definitions from the theory of the conjugate operator and define a critical set $\kappa(H)$ for the operator H. In the more usual setup where $H = h(P)$ is a function of the momentum vector operator P and Φ is the position vector operator Q in $\mathsf{L}^2(\mathbb{R}^d)$, it is known that the critical values of h

$$\kappa_h := \big\{\lambda \in \mathbb{R} \mid \exists x \in \mathbb{R}^d \text{ such that } h(x) = \lambda \text{ and } h'(x) = 0\big\}$$

plays an important role (see *e.g.* [7, Sec. 7]). Typically, the operator $h(P)$ has bad spectral properties and bad propagation properties on κ_h. For instance, one cannot obtain a simple Mourre estimate at these values. Such phenomena also occur in the abstract setup. Since the operator H is a priori not a function of an auxiliary operator as $h(P)$, the derivative appearing in the definition of κ_h does not have a direct counterpart. However, the identities $(\partial_j h)(P) = i[h(P), Q_j]$ suggest to define the set of critical values $\kappa(H)$ in terms of the vector operator $H' := \big(i[H, \Phi_1], \ldots, i[H, \Phi_d]\big)$. This is the content of Definition 1.2.5. In Lemma 1.2.6 and Theorem 1.3.6, we show that $\kappa(H)$ is closed, contains the set of eigenvalues of H, and that the spectrum of H in $\sigma(H) \setminus \kappa(H)$ is purely absolutely continuous. The proof of the latter result relies on the construction, described in Section 1.3, of an appropriate conjugate operator for H.

In Section 1.4, we recall some definitions in relation with the function f that appear in Theorem 1.1.1. The function R_f is introduced and some of its properties are presented. Section 1.5 is the core of the work and its most technical part. It contains the definition of T_f and the proof of the precise version of Theorem 1.1.1. Suitable subspaces of $\mathcal{H}$ on which the operators are well-defined and on which the equalities hold are introduced.

An interpretation of our results is proposed in Section 1.6. The relation with the theory of time operators is explained, and various cases are presented. The importance of Theorem 1.5.5 for the proof of the existence of the quantum time delay and Eisenbud-Wigner Formula is also sketched.

In Section 1.7, we show that our results apply to many operators H appearing in physics and mathematics literature. Among other examples, we treat Friedrichs Hamiltonians, Stark Hamiltonians, some Jacobi operators, the Dirac operator, convolution operators on locally compact groups, pseudodifferential operators, adjacency operators on graphs and direct integral operators. In each case, we are able to exhibit a natural family of position operators Φ satisfying our assumptions. The diversity of the examples covered by our theory make us strongly believe that Formula (1.4) is of natural character. Moreover it also suggests that the existence of time delay is a very common feature of quantum scattering theory. We also point out that one by-product of our study is an efficient algorithm for the choice of a conjugate operator for a given self-adjoint operator H (see Section 1.3). This allows us to obtain (or reobtain) non trivial spectral results for various important classes of self-adjoint operators H.

As a final comment, we would like to emphasize that one of the main interest of our study comes from the fact that we do not restrict ourselves to the standard position operators Q and to operators H which are functions of P. Due to this generality, we cannot rely on the usual canonical commutation relation of Q and P and on the subjacent Fourier analysis. This explains the constant use of abstract commutators methods throughout the work.

1.2 Critical values

In this section, we recall some standard notions on the conjugate operator theory and introduce our general framework. The set of critical values is defined and some of its properties are outlined. This subset of the spectrum of the operator under investigation plays an essential role in the sequel.

We first recall some facts principally borrowed from [7]. Let H and A be two self-adjoint operators in a Hilbert space $\mathcal{H}$. Their respective domain are denoted by $\mathcal{D}(H)$ and $\mathcal{D}(A)$, and for suitable $\omega \in \mathbb{C}$ we write R_ω for $(H-\omega)^{-1}$. The operator H is of class $C^1(A)$ if there exists $\omega \in \mathbb{C} \setminus \sigma(H)$ such that the map

$$\mathbb{R} \ni t \mapsto \mathrm{e}^{-itA} R_\omega \, \mathrm{e}^{itA} \in \mathscr{B}(\mathcal{H}) \tag{1.6}$$

is strongly differentiable. In that case, the quadratic form

$$\mathcal{D}(A) \ni \varphi \mapsto \langle A\varphi, R_\omega \varphi\rangle - \langle R_\omega^* \varphi, A\varphi\rangle \in \mathbb{C}$$

extends continuously to a bounded operator denoted by $[A, R_\omega] \in \mathscr{B}(\mathcal{H})$. It also follows from the $C^1(A)$-condition that $\mathcal{D}(H) \cap \mathcal{D}(A)$ is a core for H and that the quadratic form $\mathcal{D}(H) \cap \mathcal{D}(A) \ni \varphi \mapsto \langle H\varphi, A\varphi\rangle - \langle A\varphi, H\varphi\rangle$ is continuous in the topology of $\mathcal{D}(H)$. This form extends then uniquely to a continuous quadratic form $[H, A]$ on $\mathcal{D}(H)$, which can be identified with a continuous operator from $\mathcal{D}(H)$ to $\mathcal{D}(H)^*$. Finally, the following equality holds:

$$[A, R_\omega] = R_\omega [H, A] R_\omega. \tag{1.7}$$

It is also proved in [44, Lemma 2] that if $[H, A]\mathcal{D}(H) \subset \mathcal{H}$, then the unitary group $\{\mathrm{e}^{itA}\}_{t\in\mathbb{R}}$ preserves the domain of H, *i.e.* $\mathrm{e}^{itA}\,\mathcal{D}(H) \subset \mathcal{D}(H)$ for all $t \in \mathbb{R}$. In the sequel, we shall say that $i[H, A]$ is essentially self-adjoint on $\mathcal{D}(H)$ if $[H, A]\mathcal{D}(H) \subset \mathcal{H}$ and if $i[H, A]$ is essentially self-adjoint on $\mathcal{D}(H)$ in the usual sense.

We now extend this framework in two directions: in the number of conjugate operators and in the degree of regularity with respect to these operators. So, let us consider a family $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ of mutually commuting self-adjoint operators in $\mathcal{H}$ (throughout the work, we use the term "commute" for operators commuting in the sense of [86, Sec. VIII.5]). Then we know from [19, Sec. 6.5] that any measurable function $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ defines a bounded operator $f(\Phi)$ in $\mathcal{H}$. In particular, the operator $\mathrm{e}^{ix\cdot\Phi}$, with $x \cdot \Phi \equiv \sum_{j=1}^d x_j \Phi_j$, is unitary for each $x \in \mathbb{R}^d$. Note also that the conjugation

$$C_x : \mathscr{B}(\mathcal{H}) \to \mathscr{B}(\mathcal{H}), \quad B \mapsto \mathrm{e}^{-ix\cdot\Phi}\, B\, \mathrm{e}^{ix\cdot\Phi}$$

defines an automorphism of $\mathscr{B}(\mathcal{H})$.

Within this framework, the operator H is said to be of class $C^m(\Phi)$ for $m = 1, 2, \ldots$ if there exists $\omega \in \mathbb{C} \setminus \sigma(H)$ such that the map

$$\mathbb{R}^d \ni x \mapsto \mathrm{e}^{-ix\cdot\Phi} R_\omega \, \mathrm{e}^{ix\cdot\Phi} \in \mathscr{B}(\mathcal{H}) \tag{1.8}$$

is strongly of class C^m in $\mathcal{H}$. One easily observes that if H is of class $C^m(\Phi)$, then the operator H is of class $C^m(\Phi_j)$ for each j (the class $C^m(\Phi_j)$ being defined similarly).

Remark 1.2.1. A bounded operator $S \in \mathscr{B}(\mathcal{H})$ belongs to $C^1(A)$ if the map (1.6), with R_ω replaced by S, is strongly differentiable. Similarly, $S \in \mathscr{B}(\mathcal{H})$ belongs to $C^m(\Phi)$ if the map (1.8), with R_ω replaced by S, is strongly C^m.

In the sequel, we assume that H is regular with respect to the group $\{e^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$ in the following sense.

Assumption 1.2.2. The operator H is of class $C^1(\Phi)$, and for each $j \in \{1,\ldots,d\}$, $i[H,\Phi_j]$ is essentially self-adjoint on $\mathcal{D}(H)$, with its self-adjoint extension denoted by H'_j. The operator H'_j is of class $C^1(\Phi)$, and for each $k \in \{1,\ldots,d\}$, $i[H'_j,\Phi_k]$ is essentially self-adjoint on $\mathcal{D}(H'_j)$, with its self-adjoint extension denoted by H''_{jk}. The operator H''_{jk} is of class $C^1(\Phi)$, and for each $\ell \in \{1,\ldots,d\}$, $i[H''_{jk},\Phi_\ell]$ is essentially self-adjoint on $\mathcal{D}(H''_{jk})$, with its self-adjoint extension denoted by $H'''_{jk\ell}$.

This assumption implies the invariance of $\mathcal{D}(H)$ under the action of the unitary group $\{e^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$. Indeed, this follows from the condition $[H,\Phi_j]\mathcal{D}(H) \subset \mathcal{H}$ and from [44, Lemma 2] that $e^{it\Phi_j}\,\mathcal{D}(H) \subset \mathcal{D}(H)$ for all $t \in \mathbb{R}$. In fact, one obtains that $e^{it\Phi_j}\,\mathcal{D}(H) = \mathcal{D}(H)$, and since this property holds for each j one also has $e^{ix\cdot\Phi}\,\mathcal{D}(H) = \mathcal{D}(H)$ for all $x \in \mathbb{R}^d$. As a consequence, we obtain in particular that each self-adjoint operator

$$H(x) := e^{-ix\cdot\Phi}\,H\,e^{ix\cdot\Phi} \tag{1.9}$$

(with $H(0) = H$) has domain $\mathcal{D}[H(x)] = \mathcal{D}(H)$.

Similarly, the domains $\mathcal{D}(H'_j)$ and $\mathcal{D}(H''_{jk})$ are left invariant by the action of the unitary group $\{e^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$, and the operators $H'_j(x) := e^{-ix\cdot\Phi}\,H'_j\,e^{ix\cdot\Phi}$ and also the operators $H''_{jk}(x) := e^{-ix\cdot\Phi}\,H''_{jk}\,e^{ix\cdot\Phi}$ are self-adjoint with domains $\mathcal{D}(H'_j)$ and $\mathcal{D}(H''_{jk})$ respectively.

Our second main assumption concerns the family of operators $H(x)$.

Assumption 1.2.3. The operators $\{H(x)\}_{x\in\mathbb{R}^d}$ mutually commute.

Using the fact that the map $\mathbb{R}^d \ni x \mapsto C_x \in \mathsf{Aut}[\mathscr{B}(\mathcal{H})]$ is a group morphism, one easily shows that Assumption 1.2.3 is equivalent the commutativity of each $H(x)$ with H. Furthermore, Assumptions 1.2.2 and 1.2.3 imply additional commutation relations:

Lemma 1.2.4. *The operators $H(x)$, $H'_j(y)$, $H''_{k\ell}(z)$ mutually commute for each $j,k,\ell \in \{1,\ldots,d\}$ and each $x,y,z \in \mathbb{R}^d$.*

Proof. Let $\omega \in \mathbb{C}\setminus\mathbb{R}$, $x,y,z \in \mathbb{R}^d$, $j,k,\ell,m \in \{1,\ldots,d\}$, and set $R(x) := [H(x)-\omega]^{-1}$, $R'_j(x) := [H'_j(x)-\omega]^{-1}$ and $R''_{jk}(x) := [H''_{jk}(x)-\omega]^{-1}$. By assumption, one has the equality

$$R(x)\,\tfrac{R(\varepsilon e_j)-R(0)}{\varepsilon} = \tfrac{R(\varepsilon e_j)-R(0)}{\varepsilon}\,R(x)$$

for each $\varepsilon \in \mathbb{R}\setminus\{0\}$. By taking the strong limit as $\varepsilon \to 0$, and by using (1.7) and Assumption 1.2.3, one obtains

$$R(0)\left[R(x)H'_j - H'_jR(x)\right]R(0) = 0.$$

Since the resolvent $R(0)$ on the left is injective, this implies that $R(x)H'_j - H'_j R(x) = 0$ on $\mathcal{D}(H)$. Furthermore, since $\mathcal{D}(H)$ is a core for H'_j the last equality can be extended to $\mathcal{D}(H'_j)$. So, one gets

$$R'_j(0)R(x) = R'_j(0)R(x)\big(H'_j - \omega\big)R'_j(0) = R(x)R'_j(0).$$

One infers from this that $H(x)$ and $H'_j(y)$ commute by using the morphism property of the map $\mathbb{R}^d \ni x \mapsto C_x \in \mathsf{Aut}[\mathscr{B}(\mathcal{H})]$.

A similar argument leads to the commutativity of the operators $H'_j(x)$ and $H'_k(y)$ by considering the operators $R'_j(x)\frac{R(\varepsilon e_k)-R(0)}{\varepsilon}$ and $\frac{R(\varepsilon e_k)-R(0)}{\varepsilon}R'_j(x)$. The commutativity of $H(x)$ and $H''_{jk}(z)$ is obtained by considering the operators $R(x)\frac{R'_j(\varepsilon e_k)-R'_j(0)}{\varepsilon}$ together with $\frac{R'_j(\varepsilon e_k)-R'_j(0)}{\varepsilon}R(x)$, and the commutativity of $H'_j(y)$ and $H''_{k\ell}(z)$ by considering the operators $R'_j(y)\frac{R'_k(\varepsilon e_\ell)-R'_k(0)}{\varepsilon}$ and $\frac{R'_k(\varepsilon e_\ell)-R'_k(0)}{\varepsilon}R'_j(y)$. Finally, the commutation between $H''_{jk}(x)$ and $H''_{\ell m}(y)$ is obtained by considering $R''_{jk}(x)\frac{R'_\ell(\varepsilon e_m)-R'_\ell(0)}{\varepsilon}$ and $\frac{R'_\ell(\varepsilon e_m)-R'_\ell(0)}{\varepsilon}R''_{jk}(x)$. Details are left to the reader. □

For simplicity, we write H' for the vector operator $(H'_1, \dots, H'_d)$, and define for each measurable function $f : \mathbb{R}^d \to \mathbb{C}$ the operator $f(H')$ by using the d-variables functional calculus. The symbol $E^H(\,\cdot\,)$ denotes the spectral measure of H.

Definition 1.2.5. A number $\lambda \in \mathbb{R}$ is called a regular value of H if there exists $\delta > 0$ such that

$$\lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H\big((\lambda - \delta, \lambda + \delta)\big)\big\| < \infty. \tag{1.10}$$

A number $\lambda \in \mathbb{R}$ that is not a regular value of H is called a critical value of H. We denote by $\kappa(H)$ the set of critical values of H.

From now on, we shall use the shorter notation $E^H(\lambda; \delta)$ for $E^H\big((\lambda - \delta, \lambda + \delta)\big)$. In the next lemma we put into evidence some useful properties of the set $\kappa(H)$.

Lemma 1.2.6. *Let Assumptions 1.2.2 and 1.2.3 be verified. Then the set $\kappa(H)$ possesses the following properties:*

(a) $\kappa(H)$ is closed.

(b) $\kappa(H)$ contains the set of eigenvalues of H.

(c) The limit $\lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(J)\big\|$ is finite for each compact set $J \subset \mathbb{R} \setminus \kappa(H)$.

(d) For each compact set $J \subset \mathbb{R} \setminus \kappa(H)$, there exists a compact set $U \subset (0, \infty)$ such that $E^H(J) = E^{|H'|}(U)E^H(J)$.

Proof. (a) Let λ_0 be a regular value for H, *i.e.* there exists $\delta_0 > 0$ such that (1.10) holds with δ replaced by δ_0. Let $\lambda \in (\lambda_0 - \delta_0, \lambda_0 + \delta_0)$ and let $\delta > 0$ such that

$$(\lambda - \delta, \lambda + \delta) \subset (\lambda_0 - \delta_0, \lambda_0 + \delta_0).$$

Then, since $E^H(\lambda;\delta) = E^H(\lambda_0;\delta_0)E^H(\lambda;\delta)$, one has

$$\lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta) \big\| \le \lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda_0;\delta_0) \big\| < \infty.$$

But this means exactly that λ is a regular value for any $\lambda \in (\lambda_0 - \delta_0, \lambda_0 + \delta_0)$. So the set of regular values is open, and $\kappa(H)$ is closed.

(b) Let $\lambda \in \mathbb{R}$ be an eigenvalue of H, and let φ_λ be an associated eigenvector with norm one. Since H is of class $C^1(\Phi_j)$ for each j, we know from the Virial theorem [7, Prop. 7.2.10] that $E^H(\{\lambda\})H'_j E^H(\{\lambda\}) = 0$ for each j. This, together with Lemma 1.2.4, implies that

$$E^H(\{\lambda\})\big[(H')^2 + \varepsilon\big]^{-1} E^H(\{\lambda\}) = \varepsilon^{-1} E^H(\{\lambda\})$$

for each $\varepsilon > 0$. In particular, we obtain for each $\delta > 0$ the equalities

$$\big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta)\varphi_\lambda = E^H(\{\lambda\})\big[(H')^2 + \varepsilon\big]^{-1} E^H(\{\lambda\})\varphi_\lambda = \varepsilon^{-1}\varphi_\lambda,$$

and

$$\lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta) \big\| \ge \lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta)\varphi_\lambda \big\| = \lim_{\varepsilon \searrow 0} \varepsilon^{-1}\|\varphi_\lambda\| = \infty.$$

Since δ has been chosen arbitrarily, this implies that λ is not a regular value of H.

(c) This follows easily by using a compacity argument.

(d) Let us concentrate first on the lower bound of U. Clearly, if $|H'|$ is strictly positive, then U can be chosen in $(0,\infty)$ and thus is bounded from below by a strictly positive number. So assume now that $|H'|$ is not strictly positive, that is $0 \in \sigma(|H'|)$. By absurd, suppose that U is not bounded from below by a strictly positive number, *i.e.* there does not exist $a > 0$ such that $U \subset (a,\infty)$. Then for $n = 1,2,\ldots$, there exists $\psi_n \in \mathcal{H}$ such that $E^{|H'|}\big([0,1/n)\big)E^H(J)\psi_n \neq 0$, and the vectors

$$\varphi_n := \frac{E^{|H'|}\big([0,1/n)\big)E^H(J)\psi_n}{\|E^{|H'|}\big([0,1/n)\big)E^H(J)\psi_n\|}$$

satisfy $\|\varphi_n\| = 1$, and $E^H(J)\varphi_n = E^{|H'|}\big([0,1/n)\big)\varphi_n = \varphi_n$. It follows by point (c) that

$$\begin{aligned}
\text{Const.} \ge \lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(J) \big\| &\ge \lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^H(J)\varphi_n \big\| \\
&= \lim_{\varepsilon \searrow 0} \big\| \big[(H')^2 + \varepsilon\big]^{-1} E^{|H'|}\big([0,1/n)\big)\varphi_n \big\| \\
&\ge \lim_{\varepsilon \searrow 0} \big(n^{-2} + \varepsilon\big)^{-1}\|\varphi_n\| \\
&= n^2,
\end{aligned}$$

which leads to a contradiction when $n \to \infty$.

Let us now concentrate on the upper bound of U. Clearly, if $|H'|$ is a bounded operator, one can choose a bounded subset U of $\mathbb{R}$ and thus U is upper bounded. So assume now that $|H'|$ is not a bounded operator. By absurd, suppose that U is not bounded from above, *i.e.* there does not exist $b < \infty$ such that $U \subset (0, b)$. Then for $n = 1, 2, \ldots$, there exists $\psi_n \in \mathcal{H}$ such that $E^{|H'|}\big([n,\infty)\big)E^H(J)\psi_n \neq 0$, and the vectors

$$\varphi_n := \frac{E^{|H'|}\big([n,\infty)\big)E^H(J)\psi_n}{\|E^{|H'|}\big([n,\infty)\big)E^H(J)\psi_n\|}$$

satisfy $\|\varphi_n\| = 1$, and $E^H(J)\varphi_n = E^{|H'|}\big([n,\infty)\big)\varphi_n = \varphi_n$. It follows by Assumption 1.2.2 and Lemma 1.2.4 that $|H'|\,E^H(J)$ is a bounded operator, and

$$\text{Const.} \geq \big\||H'|\,E^H(J)\big\| \geq \big\||H'|\,E^H(J)\varphi_n\big\| = \big\||H'|\,E^{|H'|}\big([n,\infty)\big)\varphi_n\big\| \geq n\,\|\varphi_n\|$$

which leads to a contradiction when $n \to \infty$. □

1.3 Locally smooth operators and absolute continuity

In this section we exhibit a large class of locally H-smooth operators. We also show that the operator H is purely absolutely continuous in $\sigma(H) \setminus \kappa(H)$. These results are obtained by using commutators methods as presented in [7].

In order to motivate our choice of conjugate operator for H, we present first a formal calculation. Let A_η be given by

$$A_\eta := \tfrac{1}{2}\big\{\eta(H)H' \cdot \Phi + \Phi \cdot H'\eta(H)\big\},$$

where η is some real function with a sufficiently rapid decrease to 0 at infinity. Then A_η satisfies with H the commutation relation

$$i[H, A_\eta] = \tfrac{i}{2}\textstyle\sum_{j=1}^d \big\{\eta(H)H'_j\,[H,\Phi_j] + [H,\Phi_j]\,H'_j\eta(H)\big\} = (H')^2\eta(H),$$

which provides (in a sense to be specified) a Mourre estimate. So, in the sequel, one only has to justify these formal manipulations and to determinate an appropriate function η.

First of all, one observes that for each $j \in \{1, \ldots, d\}$ and each $\omega \in \mathbb{C} \setminus \sigma(H)$ the operator $H'_j R_\omega \equiv H'_j(H-\omega)^{-1}$ is a bounded operator. Indeed, one has $(H-\omega)^{-1}\mathcal{H} = \mathcal{D}(H) \subset \mathcal{D}(H'_j)$ by Assumption 1.2.2. In the following lemmas, Assumptions 1.2.2 and 1.2.3 are tacitly assumed, and we set $\langle x\rangle := (1+x^2)^{1/2}$ for any $x \in \mathbb{R}^n$.

Lemma 1.3.1. *(a) For $j, k \in \{1, \ldots, d\}$ and each $\gamma, \omega \in \mathbb{C}\setminus\sigma(H)$, the bounded operator $R_\gamma H'_j R_\omega$ belongs to $C^1(\Phi_k)$.*

(b) For $j, k \in \{1, \ldots, d\}$ the bounded self-adjoint operator $\langle H\rangle^{-2}H'_j\langle H\rangle^{-2}$ belongs to $C^1(\Phi_k)$.

(c) For $j, k, \ell \in \{1, \ldots, d\}$, the bounded self-adjoint operator $i\big[\langle H\rangle^{-2}H'_j\langle H\rangle^{-2}, \Phi_k\big]$ belongs to $C^1(\Phi_\ell)$.

(d) The operator H is of class $C^3(\Phi)$.

Proof. (a) Due to Assumption 1.2.2 one has for each $\varphi \in \mathcal{D}(\Phi_k)$

$$\begin{aligned}
&\big\langle \Phi_k\varphi, R_\gamma H_j' R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega} H_j' R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle \\
&= \big\langle \Phi_k\varphi, R_\gamma H_j' R_\omega\varphi\big\rangle - \big\langle \Phi_k R_{\bar\gamma}\varphi, H_j' R_\omega\varphi\big\rangle + \big\langle \Phi_k R_{\bar\gamma}\varphi, H_j' R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega} H_j' R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle \\
&= \big\langle [R_{\bar\gamma}, \Phi_k]\varphi, H_j' R_\omega\varphi\big\rangle + \big\langle \Phi_k R_{\bar\gamma}\varphi, H_j' R_\omega\varphi\big\rangle - \big\langle H_j' R_{\bar\gamma}\varphi, \Phi_k R_\omega\varphi\big\rangle \\
&\quad + \big\langle H_j' R_{\bar\gamma}\varphi, \Phi_k R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega} H_j' R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle \\
&= \big\langle [R_{\bar\gamma}, \Phi_k]\varphi, H_j' R_\omega\varphi\big\rangle + \big\langle [H_j', \Phi_k] R_{\bar\gamma}\varphi, R_\omega\varphi\big\rangle + \big\langle H_j' R_{\bar\gamma}\varphi, [\Phi_k, R_\omega]\varphi\big\rangle.
\end{aligned}$$

This implies that there exists $\mathrm{c} < \infty$ such that

$$\big|\big\langle \Phi_k\varphi, R_\gamma H_j' R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega} H_j' R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle\big| \le \mathrm{c}\,\|\varphi\|^2.$$

for each $\varphi \in \mathcal{D}(\Phi_k)$, and thus the statement follows from [7, Lem. 6.2.9].

(b) Since $\langle H\rangle^{-2} = R_{-i}R_i$, the operator $\langle H\rangle^{-2} H_j' \langle H\rangle^{-2}$ is clearly bounded and self-adjoint. Furthermore, by observing that

$$\langle H\rangle^{-2} H_j' \langle H\rangle^{-2} = R_i\big(R_{-i} H_j' R_i\big) R_{-i}$$

one concludes from (a) that $\langle H\rangle^{-2} H_j' \langle H\rangle^{-2}$ is the product of three operators belonging to $C^1(\Phi_k)$, and thus belongs to $C^1(\Phi_k)$ due to [7, Prop. 5.1.5].

(c) Taking Lemma 1.2.4 into account, one gets

$$i\big[\langle H\rangle^{-2} H_j' \langle H\rangle^{-2}, \Phi_k\big] = -2(R_i H_k' R_i)(R_{-i} H_j' R_{-i})(R_i + R_{-i}) + \langle H\rangle^{-2} H_{jk}'' \langle H\rangle^{-2}.$$

The first term is a product of operators which belong to $C^1(\Phi_\ell)$, and thus it belongs to $C^1(\Phi_\ell)$. For the second term, a calculation similar to the one presented in (a) using Assumption 1.2.2 shows that this term also belongs to $C^1(\Phi_\ell)$, and so the claim is proved.

(d) In this part of the proof, we freely use the notations of [7] for some regularity classes with respect to the group generated by Φ_ℓ. Let us set $\mathcal{G} := \mathcal{D}(H)$, and consider $z \in \mathbb{C}\setminus\sigma(H)$ and $j, k, \ell \in \{1, \dots, d\}$. We know from the proof of (a) that the equality

$$i\big[i[R_z, \Phi_j], \Phi_k\big] = -i[R_z, \Phi_k] H_j' R_z - R_z H_{jk}'' R_z - H_j' R_z i[R_z, \Phi_k] \tag{1.11}$$

holds on $\mathcal{H}$. We also know from Assumption 1.2.2 and [7, Lemma 5.1.2.(b)] that $R_z \in C^1(\Phi_\ell; \mathcal{H}, \mathcal{G})$, that H_j' belongs to $C^1(\Phi_\ell; \mathcal{G}, \mathcal{H})$ and that H_{jk}'' belongs to $C^1(\Phi_\ell; \mathcal{G}, \mathcal{H})$. So, each term of the r.h.s. of (1.11) belongs to $C^1(\Phi_\ell)$, due to [7, Lemma 5.1.5]. This implies that $i\big[i[R_z, \Phi_j], \Phi_k\big] \in C^1(\Phi_\ell)$, which proves the claim. □

We can now give a precise definition of the conjugate operator A we will use, and prove its self-adjointness. For that purpose, we consider the family

$$\Pi_j := \langle H\rangle^{-2} H_j' \langle H\rangle^{-2}, \qquad j = 1, \dots, d,$$

of mutually commuting bounded self-adjoint operators, and write $\Pi := (\Pi_1, \dots, \Pi_d)$ for the associated vector operator. Due to Lemma 1.3.1.(b), each operator Π_j belongs to $C^1(\Phi_j)$. Therefore the operator

$$A := \tfrac{1}{2}\big(\Pi\cdot\Phi + \Phi\cdot\Pi\big)$$

is well-defined and symmetric on $\bigcap_{j=1}^d \mathcal{D}(\Phi_j)$. For the next lemma, we note that this set contains the domain $\mathcal{D}(\Phi^2)$ of Φ^2.

Lemma 1.3.2. *The operator A is essentially self-adjoint on $\mathcal{D}(\Phi^2)$.*

Proof. We use the criterion of essential self-adjointness [87, Thm. X.37].

Given $a > 1$, we define the self-adjoint operator $N := \Phi^2 + \Pi^2 + a$ with domain $\mathcal{D}(N) \equiv \mathcal{D}(\Phi^2)$ and observe that in the form sense on $\mathcal{D}(N)$ one has

$$\begin{aligned} N^2 &= \Phi^4 + \Pi^4 + a^2 + 2a\Phi^2 + 2a\Pi^2 + \Phi^2\Pi^2 + \Pi^2\Phi^2 \\ &= \Phi^4 + \Pi^4 + a^2 + 2a\Phi^2 + 2a\Pi^2 + \sum_{j,k} \big\{\Phi_j \Pi_k^2 \Phi_j + \Pi_k \Phi_j^2 \Pi_k\big\} + R \end{aligned}$$

with $R := \sum_{j,k} \big\{\Pi_k[\Pi_k, \Phi_j]\Phi_j + \Phi_j[\Phi_j, \Pi_k]\Pi_k + [\Pi_k, \Phi_j]^2\big\}$. Now, the following inequality holds

$$\sum_{j,k} \big\{\Pi_k[\Pi_k, \Phi_j]\Phi_j + \Phi_j[\Phi_j, \Pi_k]\Pi_k\big\} \geq -d\Phi^2 - \sum_{j,k} \big(\Pi_k[\Pi_k, \Phi_j]\big)^2.$$

Thus there exists $c > 0$ such that $R \geq -d\Phi^2 - c$. Altogether, we have shown that in the form sense on $\mathcal{D}(N)$

$$N^2 \geq \Phi^4 + \Pi^4 + (a^2 - c) + (2a - d)\Phi^2 + 2a\Pi^2 + \sum_{j,k} \big\{\Phi_j \Pi_k^2 \Phi_j + \Pi_k \Phi_j^2 \Pi_k\big\},$$

where the r.h.s. is a sum of positive terms for a large enough. In particular, one has for $\varphi \in \mathcal{D}(N)$

$$\|N\varphi\|^2 \geq \big\|\Pi_j \Phi_j \varphi\big\|^2 + \big\|\Phi_j \Pi_j \varphi\big\|^2,$$

which implies that

$$\|A\varphi\| \leq \tfrac{1}{2} \sum_j \big\{\big\|\Pi_j \Phi_j \varphi\big\| + \big\|\Phi_j \Pi_j \varphi\big\|\big\} \leq d\,\|N\varphi\|.$$

It remains to estimate the commutator $[A, N]$. In the form sense on $\mathcal{D}(N)$, one has

$$\begin{aligned} 2[A, N] = \sum_{j,k} \big\{&[\Pi_j, \Phi_k]\Phi_j\Phi_k + \Phi_k[\Pi_j, \Phi_k]\Phi_j + \Phi_j[\Pi_j, \Phi_k]\Phi_k + \Phi_j\Phi_k[\Pi_j, \Phi_k] \\ &+ \Pi_j[\Phi_j, \Pi_k]\Pi_k + \Pi_j\Pi_k[\Phi_j, \Pi_k] + [\Phi_j, \Pi_k]\Pi_j\Pi_k + \Pi_k[\Phi_j, \Pi_k]\Pi_j\big\}. \end{aligned}$$

The last four terms are bounded. For the other terms, Lemma 1.3.1.(c), together with the bound

$$|\langle \Phi_j\varphi, B\Phi_k\varphi\rangle| \leq \|B\|\,\langle \varphi, \Phi^2\varphi\rangle \leq \|B\|\,\langle \varphi, N\varphi\rangle, \quad \varphi \in \mathcal{D}(N),\ B \in \mathscr{B}(\mathcal{H}),$$

leads to the desired estimate, *i.e.* $\langle \varphi, [A, N]\varphi\rangle \leq \text{Const.}\,\langle \varphi, N\varphi\rangle$. □

Lemma 1.3.3. *The operator H is of class $C^2(A)$ and the sesquilinear form $i[H, A]$ on $\mathcal{D}(H)$ extends to the bounded positive operator $\langle H\rangle^{-2}(H')^2\langle H\rangle^{-2}$.*

Proof. One has for each $\varphi \in \mathcal{D}(\Phi^2)$ and each $\omega \in \mathbb{C} \setminus \sigma(H)$

$$\begin{aligned} &2\big\{\big\langle R_{\bar\omega}\varphi, A\varphi\big\rangle - \big\langle A\varphi, R_\omega\varphi\big\rangle\big\} \\ &= \sum_j \big\{\big\langle R_{\bar\omega}\varphi, \big(\Pi_j\Phi_j + \Phi_j\Pi_j\big)\varphi\big\rangle - \big\langle\big(\Pi_j\Phi_j + \Phi_j\Pi_j\big)\varphi, R_\omega\varphi\big\rangle\big\} \\ &= \sum_j \big\{\big\langle \Pi_j\varphi, [R_\omega, \Phi_j]\,\varphi\big\rangle + \big\langle\, [\Phi_j, R_{\bar\omega}]\,\varphi, \Pi_j\varphi\big\rangle\big\}. \end{aligned} \tag{1.12}$$

Since all operators in the last equality are bounded and since $\mathcal{D}(\Phi^2)$ is a core for A, this implies that H is of class $C^1(A)$ [7, Lem. 6.2.9].

Now observe that the following equalities hold on $\mathcal{H}$

$$i[R_\omega, A] = \tfrac{i}{2}\textstyle\sum_j \big\{\Pi_j[R_\omega, \Phi_j] + [R_\omega, \Phi_j]\Pi_j\big\} = -R_\omega\, \langle H\rangle^{-2}\, (H')^2\, \langle H\rangle^{-2}\, R_\omega.$$

Therefore the sesquilinear form $i[H, A]$ on $\mathcal{D}(H)$ extends to the bounded positive operator $\langle H\rangle^{-2}\, (H')^2\, \langle H\rangle^{-2}$. Finally, the operator $i[R_\omega, A]$ can be written as a product of factors in $C^1(\Phi_\ell)$ for each ℓ, namely

$$i[R_\omega, A] = -\textstyle\sum_j R_\omega \left(R_{-i}H_j'R_i\right)\left(R_{-i}H_j'R_i\right) R_\omega.$$

So $i[R_\omega, A]$ also belongs to $C^1(\Phi_\ell)$ for each ℓ, and thus a calculation similar to the one of (1.12) shows that $i[R_\omega, A]$ belongs to $C^1(A)$. This implies that H is of class $C^2(A)$. □

Definition 1.3.4. A number $\lambda \in \mathbb{R}$ is called a A-regular value of H if there exist numbers $a, \delta > 0$ such that $(H')^2E^H(\lambda;\delta) \geq a\,E^H(\lambda;\delta)$. The complement of this set in $\mathbb{R}$ is denoted by $\kappa^A(H)$.

The set of A-regular values corresponds to the Mourre set with respect to A. Indeed, if λ is a A-regular value, then $(H')^2E^H(\lambda;\delta) \geq a\,E^H(\lambda;\delta)$ for some $a, \delta > 0$ and

$$E^H(\lambda;\delta)i[H, A]E^H(\lambda;\delta) = E^H(\lambda;\delta)\,\langle H\rangle^{-2}\,(H')^2\,\langle H\rangle^{-2}\,E^H(\lambda;\delta) \geq a' E^H(\lambda;\delta),$$

where $a' := a \cdot \inf_{\mu\in(\lambda-\delta,\lambda+\delta)}\langle\mu\rangle^{-4}$. In the framework of Mourre theory, this means that the operator A is strictly conjugate to H at the point λ [7, Sec. 7.2.2].

Lemma 1.3.5. *The sets $\kappa(H)$ and $\kappa^A(H)$ are equal.*

Proof. Let λ be a A-regular value of H. Then there exist $a, \delta > 0$ such that

$$E^H(\lambda;\delta) \leq a^{-1}(H')^2E^H(\lambda;\delta),$$

and we obtain for $\varepsilon > 0$:

$$\begin{aligned} &\big\|\big[(H')^2 + \varepsilon\big]^{-1}E^H(\lambda;\delta)\big\|^2 \\ &= \sup_{\varphi\in\mathcal{H},\, \|\varphi\|=1} \big\langle\big[(H')^2 + \varepsilon\big]^{-1}\varphi, E^H(\lambda;\delta)\big[(H')^2 + \varepsilon^2\big]^{-1}\varphi\big\rangle \\ &\leq a^{-2} \sup_{\varphi\in\mathcal{H},\, \|\varphi\|=1} \big\langle\big[(H')^2 + \varepsilon\big]^{-1}\varphi, E^H(\lambda;\delta)(H')^4[(H')^2 + \varepsilon]^{-1}\varphi\big\rangle \\ &\leq a^{-2}\big\|(H')^2[(H')^2 + \varepsilon]^{-1}\big\|^2 \\ &\leq a^{-2}, \end{aligned}$$

which implies, by taking the limit $\lim_{\varepsilon\searrow 0}$, that λ is a regular value.

Now, let λ be a regular value of H. Then there exists $\delta > 0$ such that

$$\begin{aligned}\text{Const.} &\geq \lim_{\varepsilon\searrow 0} \big\| \big[(H')^2+\varepsilon\big]^{-1} E^H(\lambda;\delta)\big\| \\ &= \lim_{\varepsilon\searrow 0} \big\| E^H(\lambda;\delta)\big[(H')^2 E^H(\lambda;\delta)+\varepsilon\big]^{-1} E^H(\lambda;\delta)\big\| \\ &= \lim_{\varepsilon\searrow 0} \big\| \big[(H')^2 E^H(\lambda;\delta)+\varepsilon\big]^{-1}\big\|_{\mathscr{B}(\mathcal{H}_{\lambda,\delta})}, \end{aligned} \tag{1.13}$$

where $\mathcal{H}_{\lambda,\delta} := E^H(\lambda;\delta)\mathcal{H}$. But we have

$$\big\| \big[(H')^2 E^H(\lambda;\delta)+\varepsilon\big]^{-1}\big\|_{\mathscr{B}(\mathcal{H}_{\lambda,\delta})} = (a+\varepsilon)^{-1},$$

where the number $a \geq 0$ is the infimum of the spectrum of $(H')^2E^H(\lambda;\delta)$, considered as an operator in $\mathcal{H}_{\lambda,\delta}$. Therefore, Formula (1.13) entails the bound $a^{-1} \leq \text{Const.}$, which implies that $a > 0$. In consequence, the operator $(H')^2E^H(\lambda;\delta)$ is strictly positive in $\mathcal{H}_{\lambda,\delta}$, namely,

$$(H')^2 E^H(\lambda;\delta) \geq a E^H(\lambda;\delta)$$

with $a > 0$. This implies that λ is a A-regular value of H, and $\kappa(H)$ is equal to $\kappa^A(H)$. □

We shall now state our main result on the nature of the spectrum of H, and exhibit a class of locally H-smooth operators. The space $\big(\mathcal{D}(A),\mathcal{H}\big)_{1/2,1}$, defined by real interpolation [7, Sec. 3.4.1], is denoted by $\mathscr{K}$. Since for each $j \in \{1,\dots,d\}$ the operator Π_j belongs to $C^1(\Phi_j)$, we have $\mathcal{D}(\langle\Phi\rangle) \subset \mathcal{D}(A)$, and it follows from [7, Thm. 2.6.3] and [7, Thm. 3.4.3.(a)] that for $s > 1/2$ the continuous embeddings hold:

$$\mathcal{D}(\langle\Phi\rangle^s) \subset \mathscr{K} \subset \mathcal{H} \subset \mathscr{K}^* \subset \mathcal{D}(\langle\Phi\rangle^{-s}). \tag{1.14}$$

The symbol $\mathbb{C}_\pm$ stands for the half-plane $\mathbb{C}_\pm := \{\omega \in \mathbb{C} \mid \pm\Im(\omega) > 0\}$.

Theorem 1.3.6. *Let H satisfy Assumptions 1.2.2 and 1.2.3. Then,*

(a) the spectrum of H in $\sigma(H) \setminus \kappa(H)$ is purely absolutely continuous,

(b) each operator $T \in \mathscr{B}\big(\mathcal{D}(\langle\Phi\rangle^{-s}),\mathcal{H}\big)$, with $s > 1/2$, is locally H-smooth on $\mathbb{R}\setminus\kappa(H)$.

Proof. (a) This is a direct application of [101, Thm. 0.1] which takes Lemmas 1.3.3 and 1.3.5 into account.

(b) We know from [101, Thm. 0.1] that the map $\omega \mapsto R_\omega \in \mathscr{B}(\mathscr{K},\mathscr{K}^*)$, which is holomorphic on the half-plane $\mathbb{C}_\pm$, extends to a weak*-continuous function on $\mathbb{C}_\pm \cup \{\mathbb{R} \setminus \kappa(H)\}$. Now, consider $T \in \mathscr{B}(\mathscr{K}^*,\mathcal{H})$. Then one has $T^* \in \mathscr{B}(\mathcal{H},\mathscr{K})$, and it follows from the above continuity that for each compact subset $J \subset \mathbb{R}\setminus\kappa(H)$ there exists a constant $\mathrm{c} \geq 0$ such that for all $\omega \in \mathbb{C}$ with $\Re(\omega) \in J$ and $\Im(\omega) \in (0,1)$ one has

$$\|TR_\omega T^*\| + \|TR_{\bar\omega}T^*\| \leq \mathrm{c}.$$

A fortiori, one also has $\sup_\omega \|T(R_\omega - R_{\bar\omega})T^*\| \leq \mathrm{c}$, where the supremum is taken over the same set of complex numbers. This last property is equivalent to the local H-smoothness of T on $\mathbb{R}\setminus\kappa(H)$. The claim is then obtained by using the last embedding of (1.14). □

1.4 Averaged localisation functions

In this section we recall some properties of a class of averaged localisation functions which appears naturally when dealing with quantum scattering theory. These functions, which are denoted R_f, are constructed in terms of functions $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ of localisation around the origin 0 of $\mathbb{R}^d$. They were already used, in one form or another, in [45], [110], and [111].

Assumption 1.4.1. The function $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ satisfies the following conditions:

(i) There exists $\rho > 0$ such that $|f(x)| \le \mathrm{Const.}\,\langle x\rangle^{-\rho}$ for a.e. $x \in \mathbb{R}^d$.

(ii) $f = 1$ on a neighbourhood of 0.

It is clear that $\operatorname{s-lim}_{r\to\infty} f(\Phi/r) = 1$ if f satisfies Assumption 1.4.1. Furthermore, one has for each $x \in \mathbb{R}^d \setminus \{0\}$

$$\left|\int_0^\infty \frac{\mathrm{d}\mu}{\mu}\,\big[f(\mu x) - \chi_{[0,1]}(\mu)\big]\right| \le \int_0^1 \frac{\mathrm{d}\mu}{\mu}\,|f(\mu x) - 1| + \mathrm{Const.}\int_1^{+\infty} \mathrm{d}\mu\,\mu^{-(1+\rho)} < \infty,$$

where $\chi_{[0,1]}$ denotes the characteristic function for the interval $[0,1]$. Therefore the function $R_f : \mathbb{R}^d \setminus \{0\} \to \mathbb{C}$ given by

$$R_f(x) := \int_0^{+\infty} \frac{\mathrm{d}\mu}{\mu}\,\big[f(\mu x) - \chi_{[0,1]}(\mu)\big]$$

is well-defined. If $\mathbb{R}_+^* := (0,\infty)$, endowed with the multiplication, is seen as a Lie group with Haar measure $\frac{\mathrm{d}\mu}{\mu}$, then R_f is the renormalised average of f with respect to the (dilation) action of $\mathbb{R}_+^*$ on $\mathbb{R}^d$.

In the next lemma we recall some differentiability and homogeneity properties of R_f. We also give the explicit form of R_f when f is a radial function. The reader is referred to [111, Sec. 2] for proofs and details. The symbol $\mathscr{S}(\mathbb{R}^d)$ stands for the Schwartz space on $\mathbb{R}^d$.

Lemma 1.4.2. *Let f satisfy Assumption 1.4.1.*

(a) Assume that $(\partial_j f)(x)$ exists for all $j \in \{1,\dots,d\}$ and $x \in \mathbb{R}^d$, and suppose that there exists some $\rho > 0$ such that $|(\partial_j f)(x)| \le \mathrm{Const.}\,\langle x\rangle^{-(1+\rho)}$ for each $x \in \mathbb{R}^d$. Then R_f is differentiable on $\mathbb{R}^d \setminus \{0\}$, and its derivative is given by

$$R_f'(x) = \int_0^\infty \mathrm{d}\mu\, f'(\mu x).$$

In particular, if $f \in \mathscr{S}(\mathbb{R}^d)$ then R_f belongs to $C^\infty(\mathbb{R}^d \setminus \{0\})$.

(b) Assume that R_f belongs to $C^m(\mathbb{R}^d \setminus \{0\})$ for some $m \ge 1$. Then one has for each $x \in \mathbb{R}^d \setminus \{0\}$ and $t > 0$ the homogeneity properties

$$x \cdot R_f'(x) = -1, \tag{1.15}$$

$$t^{|\alpha|}(\partial^\alpha R_f)(tx) = (\partial^\alpha R_f)(x), \tag{1.16}$$

where $\alpha \in \mathbb{N}^d$ is a multi-index with $1 \le |\alpha| \le m$.

(c) *Assume that f is radial,* i.e. *there exists $f_0 \in \mathsf{L}^\infty(\mathbb{R})$ such that $f(x) = f_0(|x|)$ for a.e. $x \in \mathbb{R}^d$. Then R_f belongs to $C^\infty(\mathbb{R}^d \setminus \{0\})$, and $R_f'(x) = -x^{-2}x$.*

Obviously, one can show as in Lemma 1.4.2.(a) that R_f is of class $C^m(\mathbb{R}^d \setminus \{0\})$ if one has for each $\alpha \in \mathbb{N}^d$ with $|\alpha| \le m$ that $(\partial^\alpha f)(x)$ exists and that $|(\partial^\alpha f)(x)| \le \text{Const.}\, \langle x\rangle^{-(|\alpha|+\rho)}$ for some $\rho > 0$. However, this is not a necessary condition. In some cases (as in Lemma 1.4.2.(c)), the function R_f is very regular outside the point 0 even if f is not continuous.

1.5 Integral formula

In this section we prove our main result on the relation between the evolution of the localisation operators $f(\Phi/r)$ and the time operator T_f defined below. We begin with a technical lemma that will be used subsequently. Since this result could also be useful in other situations, we present here a general version of it. The symbol $\mathscr{F}$ stands for the Fourier transformation, and the measure $\underline{\mathrm{d}}x$ on $\mathbb{R}^n$ is chosen so that $\mathscr{F}$ extends to a unitary operator in $\mathsf{L}^2(\mathbb{R}^n)$.

Proposition 1.5.1. *Let $C \equiv (C_1, \dots, C_n)$ and $D \equiv (D_1, \dots, D_d)$ be two families of mutually commuting self-adjoint operators in a Hilbert space $\mathscr{H}$. Let $k \ge 1$ be an integer, and assume that each C_j is of class $C^k(D)$. Let $f \in \mathsf{L}^\infty(\mathbb{R}^n)$, set $g(x) := f(x)\, \langle x_1\rangle^{2k} \cdots \langle x_n\rangle^{2k}$, and suppose that the functions g and*

$$x \mapsto (\mathscr{F}g)(x)\, \langle x_1\rangle^{k+1} \cdots \langle x_n\rangle^{k+1}$$

are in $\mathsf{L}^1(\mathbb{R}^n)$. Then the operator $f(C)$ belongs to $C^k(D)$. In particular, if $f \in \mathscr{S}(\mathbb{R}^n)$ then $f(C)$ belongs to $C^k(D)$.

Proof. For each $y \in \mathbb{R}^d$, we set $D_y := \frac{1}{i|y|}(\mathrm{e}^{iy\cdot D} - 1)$. Then we know from [7, Lem. 6.2.3.(a)] that it is sufficient to prove that $\big\| \operatorname{ad}^k_{D_y} \big(f(C)\big)\big\|$ is bounded by a constant independent of y. By using the linearity of $\operatorname{ad}^k_{D_y}(\,\cdot\,)$ and [7, Eq. 5.1.16], we get

$$\begin{aligned}
&\operatorname{ad}^k_{D_y} \big(f(C)\big) \\
&= \operatorname{ad}^k_{D_y} \big(g(C)\, \langle C_1\rangle^{-2k} \cdots \langle C_n\rangle^{-2k}\big) \\
&= \int_{\mathbb{R}^n} \underline{\mathrm{d}}x\, (\mathscr{F}g)(x)\, \operatorname{ad}^k_{D_y} \big(\mathrm{e}^{ix_1C_1} \langle C_1\rangle^{-2k} \cdots \mathrm{e}^{ix_2C_n} \langle C_n\rangle^{-2k}\big) \\
&= \sum_{k_1+\cdots+k_n=k} \mathrm{c}_{k_1\cdots k_n} \int_{\mathbb{R}^n} \underline{\mathrm{d}}x\, (\mathscr{F}g)(x)\, \operatorname{ad}^{k_1}_{D_y} \big(\mathrm{e}^{ix_1C_1} \langle C_1\rangle^{-2k}\big) \cdots \operatorname{ad}^{k_n}_{D_y} \big(\mathrm{e}^{ix_2C_n} \langle C_n\rangle^{-2k}\big),
\end{aligned}$$

where $\mathrm{c}_{k_1\cdots k_n} > 0$ is some explicit constant. Furthermore, since C_j is of class $C^k(D)$, we know from [7, Eq. 6.2.13] that

$$\big\| \operatorname{ad}^{k_j}_{G_y} \big(\mathrm{e}^{ix_jC_j} \langle C_j\rangle^{-2k}\big)\big\| \le \mathrm{c}_{k_j} \langle x_j\rangle^{k+1},$$

where $c_{k_j} \geq 0$ is independent of y and x_j. This implies that

$$\left\| \operatorname{ad}_{D_y}^k \big(f(C)\big)\right\| \leq \text{Const.} \int_{\mathbb{R}^n} \underline{\mathrm{d}}x \, |(\mathscr{F}g)(x)| \, \langle x_1 \rangle^{k+1} \cdots \langle x_n \rangle^{k+1} \leq \text{Const.}\,,$$

and the claim is proved. □

In Lemma 1.2.6.(a) we have shown that the set $\kappa(H)$ is closed. So we can define for each $t \geq 0$ the set

$$\mathscr{D}_t := \big\{\varphi \in \mathcal{D}(\langle \Phi \rangle^t) \mid \varphi = \eta(H)\varphi \text{ for some } \eta \in C_c^\infty\big(\mathbb{R} \setminus \kappa(H)\big)\big\}.$$

The set $\mathscr{D}_t$ is included in the subspace $\mathcal{H}_{\mathrm{ac}}(H)$ of absolute continuity of H, due to Theorem 1.3.6.(a), and $\mathscr{D}_{t_1} \subset \mathscr{D}_{t_2}$ if $t_1 \geq t_2$. We refer the reader to Section 1.6 for an account on density properties of the sets $\mathscr{D}_t$.

In the sequel we shall consider the set of operators $\big\{H''_{jk}\big\}$ as the components of a d-dimensional (Hessian) matrix which we denote by H'' (H''^{T} stands for its matrix transpose). Furthermore we shall sometimes write C^{-1} for an operator C a priori not invertible. In such a case, the operator C^{-1} will always be restricted to a set where it is well-defined. Namely, if $\mathcal{D}$ is a set on which C is invertible, then we shall simply write "C^{-1} acting on $\mathcal{D}$" instead of using the notation $C^{-1}|_{\mathcal{D}}$.

Proposition 1.5.2. *Let H and Φ satisfy Assumptions 1.2.2 and 1.2.3. Let f satisfy Assumption 1.4.1 and assume that R_f belongs to $C^1(\mathbb{R}^d \setminus \{0\})$. Then the map*

$$t_f : \mathscr{D}_1 \to \mathbb{C}, \quad \varphi \mapsto t_f(\varphi) := -\tfrac{1}{2} \sum_j \big\{\big\langle \Phi_j \varphi, (\partial_j R_f)(H')\varphi \big\rangle + \big\langle \big(\partial_j R_{\overline{f}}\big)(H')\varphi, \Phi_j \varphi \big\rangle\big\},$$

is well-defined. Moreover, if $(\partial_j R_f)(H')\varphi$ belongs to $\mathcal{D}(\Phi_j)$ for each j, then the linear operator $T_f : \mathscr{D}_1 \to \mathcal{H}$ defined by

$$T_f \varphi := -\tfrac{1}{2}\Big(\Phi \cdot R_f'(H') + R_f'\big(\tfrac{H'}{|H'|}\big) \cdot \Phi \, |H'|^{-1} + i R_f'\big(\tfrac{H'}{|H'|}\big) \cdot \big(H''^{\mathsf{T}} H'\big) \, |H'|^{-3}\Big)\varphi \quad (1.17)$$

satisfies $t_f(\varphi) = \langle \varphi, T_f \varphi \rangle$ for each $\varphi \in \mathscr{D}_1$. In particular, T_f is a symmetric operator if f is real and if $\mathscr{D}_1$ is dense in $\mathcal{H}$.

Remark 1.5.3. Formula (1.17) is a priori rather complicated and one could be tempted to replace it by the simpler formula $-\frac{1}{2}\big(\Phi \cdot R_f'(H') + R_f'(H') \cdot \Phi\big)$. Unfortunately, a precise meaning of this expression is not available in general, and its full derivation can only be justified in concrete examples.

Remark 1.5.4. If $\varphi \in \mathscr{D}_1$ and if f either belongs to $\mathscr{S}(\mathbb{R}^d)$ or is radial, then the assumption $(\partial_j R_f)(H')\varphi \in \mathcal{D}(\Phi_j)$ holds for each j. Indeed, by Lemma 1.2.6.(d) there exists $\eta \in C_c^\infty\big((0,\infty)\big)$ such that $(\partial_j R_f)(H')\varphi = (\partial_j R_f)(H')\eta\big((H')^2\big)\varphi$. By Lemma 1.4.2 and Proposition 1.5.1, it then follows that $(\partial_j R_f)(H')\eta\big((H')^2\big) \in C^1(\Phi_j)$, which implies the statement.

Proof of Proposition 1.5.2. Let $\varphi \in \mathscr{D}_1$. Then Lemma 1.2.6.(d) implies that there exists a function $\eta \in C_c^\infty\big((0,\infty)\big)$ such that

$$(\partial_j R_f)(H')\varphi = (\partial_j R_f)(H')\eta\big((H')^2\big)\varphi.$$

Thus $\|(\partial_j R_f)(H')\varphi\| \le \mathrm{Const.}\,\|\varphi\|$, and we have

$$|t_f(\varphi)| \le \mathrm{Const.}\,\|\varphi\| \cdot \|\langle\Phi\rangle\varphi\|,$$

which implies the first part of the claim.

For the second part of the claim, it is sufficient to show that

$$\sum_j \big\langle\big(\partial_j R_{\overline{f}}\big)(H')\varphi, \Phi_j\varphi\big\rangle = \big\langle\varphi, \big\{R_f'\big(\tfrac{H'}{|H'|}\big)\cdot\Phi\,|H'|^{-1} + iR_f'\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)\,|H'|^{-3}\big\}\varphi\big\rangle.$$

Using Formula (1.16), Lemma 1.2.6.(d), and [34, Eq. 4.3.2], one gets

$$\begin{aligned}
&\sum_j \big\langle\big(\partial_j R_{\overline{f}}\big)(H')\varphi, \Phi_j\varphi\big\rangle\\
&= \sum_j \big\langle(\partial_j R_{\overline{f}})\big(\tfrac{H'}{|H'|}\big)|H'|^{-1}\varphi, \Phi_j\varphi\big\rangle\\
&= \sum_j \lim_{\varepsilon\searrow 0}\lim_{\delta\to 0}\big\langle\big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi, [(H')^2+\varepsilon]^{-1/2}\Phi_j(1+i\delta\Phi_j)^{-1}\varphi\big\rangle\\
&= \big\langle\varphi, R_f'\big(\tfrac{H'}{|H'|}\big)\cdot\Phi\,|H'|^{-1}\varphi\big\rangle\\
&\quad + \pi^{-1}\sum_j \lim_{\varepsilon\searrow 0}\lim_{\delta\to 0}\int_0^\infty \mathrm{d}t\, t^{-1/2}\big\langle\big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi, \big[[(H')^2+\varepsilon+t]^{-1}, \Phi_j(1+i\delta\Phi_j)^{-1}\big]\varphi\big\rangle.
\end{aligned} \tag{1.18}$$

Now, using Assumption 1.2.2, Lemma 1.2.4 and the usual mollifiers technics, one obtains that

$$\lim_{\delta\to 0}\big[[(H')^2+\varepsilon+t]^{-1}, \Phi_j(1+i\delta\Phi_j)^{-1}\big]\varphi = 2i\big[(H')^2+\varepsilon+t\big]^{-2}\big(H''^{\mathsf{T}}H'\big)_j\,\varphi.$$

So, the term (1.18) is equal to

$$\begin{aligned}
&\pi^{-1}\sum_j \lim_{\varepsilon\searrow 0}\int_0^\infty \mathrm{d}t\, t^{-1/2}\big\langle\big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi, 2i[(H')^2+\varepsilon+t]^{-2}\big(H''^{\mathsf{T}}H'\big)_j\varphi\big\rangle\\
&= \sum_j \lim_{\varepsilon\searrow 0}\big\langle\big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi, i[(H')^2+\varepsilon]^{-3/2}\big(H''^{\mathsf{T}}H'\big)_j\varphi\big\rangle\\
&= \big\langle\varphi, iR_f'\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)\,|H'|^{-3}\varphi\big\rangle,
\end{aligned}$$

and thus

$$\sum_j \big\langle\big(\partial_j R_{\overline{f}}\big)(H')\varphi, \Phi_j\varphi\big\rangle = \big\langle\varphi, \big\{R_f'\big(\tfrac{H'}{|H'|}\big)\cdot\Phi\,|H'|^{-1} + iR_f'\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)\,|H'|^{-3}\big\}\varphi\big\rangle.$$

□

Suppose for a while that f is radial. Then one has $(\partial_j R_f)(x) = -x^{-2}x_j$ due to Lemma 1.4.2.(c), and Formula (1.17) holds by Remark 1.5.4. This implies that T_f is equal to

$$T := \tfrac{1}{2}\Big(\Phi \cdot \tfrac{H'}{(H')^2} + \tfrac{H'}{|H'|} \cdot \Phi |H'|^{-1} + \tfrac{iH'}{(H')^4} \cdot \big(H''^{\mathsf{T}} H'\big)\Big) \tag{1.19}$$

on $\mathscr{D}_1$.

The next theorem is our main result; it relates the evolution of localisation operators $f(\Phi/r)$ to the operator T_f. In its proof, we freely use the notations of [7] for some regularity classes with respect to the unitary group generated by Φ. For us, a function $f : \mathbb{R}^d \to \mathbb{C}$ is even if $f(x) = f(-x)$ for *a.e.* $x \in \mathbb{R}^d$.

Theorem 1.5.5. *Let H and Φ satisfy Assumptions 1.2.2 and 1.2.3. Let $f \in \mathscr{S}(\mathbb{R}^d)$ be an even function such that $f = 1$ on a neighbourhood of 0. Then we have for each $\varphi \in \mathscr{D}_2$*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \, \big\langle \varphi, \big[\mathrm{e}^{-itH} f(\Phi/r)\, \mathrm{e}^{itH} - \mathrm{e}^{itH} f(\Phi/r)\, \mathrm{e}^{-itH}\big]\varphi \big\rangle = t_f(\varphi). \tag{1.20}$$

Note that the integral on the l.h.s. of (1.20) is finite for each $r > 0$ since $f(\Phi/r)$ can be factorized as

$$f(\Phi/r) \equiv |f(\Phi/r)|^{1/2} \cdot \mathrm{sgn}[f(\Phi/r)] \cdot |f(\Phi/r)|^{1/2},$$

with $|f(\Phi/r)|^{1/2}$ locally H-smooth on $\mathbb{R} \setminus \kappa(H)$ by Theorem 1.3.6. Furthermore, since Remark 1.5.4 applies, the r.h.s. can also be written as the expectation value $\langle \varphi, T_f \varphi\rangle$.

Proof. (i) Let $\varphi \in \mathscr{D}_2$, take a real $\eta \in C_{\mathrm{c}}^\infty\big(\mathbb{R} \setminus \kappa(H)\big)$ such that $\eta(H)\varphi = \varphi$, and set $\eta_t(H) := \mathrm{e}^{itH}\,\eta(H)$. Then we have

$$\begin{aligned}
&\big\langle \varphi, \big[\mathrm{e}^{itH} f(\Phi/r)\, \mathrm{e}^{-itH} - \mathrm{e}^{-itH} f(\Phi/r)\, \mathrm{e}^{itH}\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}^d} \underline{\mathrm{d}}x \, (\mathscr{F} f)(x) \big\langle \varphi, \big[\eta_t(H)\, \mathrm{e}^{i\frac{x}{r}\cdot\Phi}\, \eta_{-t}(H) - \eta_{-t}(H)\, \mathrm{e}^{i\frac{x}{r}\cdot\Phi}\, \eta_t(H)\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}^d} \underline{\mathrm{d}}x \, (\mathscr{F} f)(x) \big\langle \varphi, \big[\, \mathrm{e}^{i\frac{x}{r}\cdot\Phi}\, \eta_t\big(H(\tfrac{x}{r})\big)\eta_{-t}(H) - \eta_{-t}(H)\eta_t\big(H(-\tfrac{x}{r})\big)\, \mathrm{e}^{i\frac{x}{r}\cdot\Phi}\,\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}^d} \underline{\mathrm{d}}x \, (\mathscr{F} f)(x) \big\langle \varphi, \big\{\big(\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi} - 1\big)\eta_t\big(H(\tfrac{x}{r})\big)\eta_{-t}(H) \\
&\qquad + \eta_{-t}(H)\big[\eta_t\big(H(\tfrac{x}{r})\big) - \eta_t\big(H(-\tfrac{x}{r})\big)\big] - \eta_{-t}(H)\eta_t\big(H(-\tfrac{x}{r})\big)\big(\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi} - 1\big)\big\}\varphi\big\rangle.
\end{aligned} \tag{1.21}$$

Since f is even, $\mathscr{F} f$ is also even, and

$$\int_{\mathbb{R}^d} \underline{\mathrm{d}}x \, (\mathscr{F} f)(x) \,\big\langle \varphi, \eta_{-t}(H)\big[\eta_t\big(H(\tfrac{x}{r})\big) - \eta_t\big(H(-\tfrac{x}{r})\big)\big]\varphi\big\rangle = 0.$$

Thus Formula (1.21), Lemma 1.2.4, and the change of variables $\mu := t/r$, $\nu := 1/r$, give

$$\begin{aligned}
&\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \, \big\langle \varphi, \big[\,\mathrm{e}^{-itH} f(\Phi/r)\, \mathrm{e}^{itH} - \mathrm{e}^{itH} f(\Phi/r)\, \mathrm{e}^{-itH}\,\big]\varphi\big\rangle \\
&= -\tfrac{1}{2} \lim_{\nu\searrow 0} \int_0^\infty \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x \, K(\nu,\mu,x),
\end{aligned} \tag{1.22}$$

where

$$K(\nu,\mu,x) := (\mathscr{F}f)(x)\big\langle\varphi,\big\{\tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi}-1\big)\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]} - \eta(H(-\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(-\nu x)-H]}\,\tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi}-1\big)\big\}\varphi\big\rangle.$$

(ii) To prove the statement, we shall show that one may interchange the limit and the integrals in (1.22), by invoking Lebesgue's dominated convergence theorem. This will be done in (iii) below. Here we pursue the calculations assuming that these interchanges are justified.

There exists a bounded interval $J\subset\mathbb{R}$ such that $\varphi = E^H(J)\varphi$. Thus

$$\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi = \mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]E^H(J)}\,\varphi.$$

Furthermore, it follows from Assumption 1.2.2 and [7, Lem. 5.1.2.(b)] that $H\in C^2(\Phi,\mathcal{G},\mathcal{H})$, where $\mathcal{G}$ denotes the space $\mathcal{D}(H)$ endowed with the graph topology. In particular, we have $H\in C^1_{\mathrm{u}}(\Phi,\mathcal{G},\mathcal{H})$ (see [7, Sec. 5.2.2]), and therefore the map

$$\mathbb{R}\setminus\{0\}\ni\nu\mapsto i\tfrac{\mu}{\nu}[H(\nu x)-H]E^H(J)\in\mathscr{B}(\mathcal{H})$$

extends to a continuous map defined on $\mathbb{R}$ and taking value $i\mu x\cdot HE^H(J)$ at $\nu=0$. Since the exponential $B\mapsto\mathrm{e}^{iB}$ is continuous from $\mathscr{B}(\mathcal{H})$ to $\mathscr{B}(\mathcal{H})$, the composed map

$$\mathbb{R}\ni\nu\mapsto\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]E^H(J)}\in\mathscr{B}(\mathcal{H})$$

is also continuous, and takes value $\mathrm{e}^{i\mu x\cdot H'E^H(J)}$ at $\nu=0$. Summing up, we obtain that

$$\lim_{\nu\searrow 0}\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi = \mathrm{e}^{i\mu x\cdot H'}\,\varphi.$$

This identity, together with the symmetry of f, Lemma 1.4.2.(a), and Proposition 1.5.2, implies that for $\varphi\in\mathscr{D}_2$

$$\begin{aligned}
&\lim_{r\to\infty}\tfrac12\int_0^\infty\mathrm{d}t\,\big\langle\varphi,\big[\,\mathrm{e}^{-itH}f(\Phi/r)\,\mathrm{e}^{itH}-\mathrm{e}^{itH}f(\Phi/r)\,\mathrm{e}^{-itH}\big]\varphi\big\rangle\\
&=-\tfrac{i}{2}\int_0^\infty\mathrm{d}\mu\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\{\big\langle(x\cdot\Phi)\,\varphi,\mathrm{e}^{i\mu x\cdot H'}\,\varphi\big\rangle-\big\langle\varphi,\mathrm{e}^{-i\mu x\cdot H'}\,(x\cdot\Phi)\,\varphi\big\rangle\big\}\\
&=-\tfrac12\sum_j\int_0^\infty\mathrm{d}\mu\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,[\mathscr{F}(\partial_jf)](x)\big[\big\langle\Phi_j\varphi,\mathrm{e}^{i\mu x\cdot H'}\,\varphi\big\rangle+\big\langle\varphi,\mathrm{e}^{i\mu x\cdot H'}\,\Phi_j\varphi\big\rangle\big]\\
&=-\tfrac12\sum_j\int_0^\infty\mathrm{d}\mu\,\big[\big\langle\Phi_j\varphi,(\partial_jf)\big(\mu H'\big)\varphi\big\rangle+\big\langle\big(\partial_j\overline{f}\big)\big(\mu H'\big)\varphi,\Phi_j\varphi\big\rangle\big]\\
&=t_f(\varphi).
\end{aligned}$$

(iii) To interchange the limit $\nu\searrow 0$ and the integration over μ in (1.22), one has to bound $\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,K(\nu,\mu,x)$ uniformly in ν by a function in $\mathsf{L}^1\big((0,\infty),\mathrm{d}\mu\big)$. We begin with the first term of $\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,K(\nu,\mu,x)$:

$$K_1(\nu,\mu) := \int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\,\Big\langle\langle\Phi\rangle^2\varphi,\tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi}-1\big)\langle\Phi\rangle^{-2}\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi\Big\rangle\,.$$

Observe that for each multi-index $\alpha \in \mathbb{N}^d$ with $|\alpha| \le 2$ one has

$$\big\|\partial_x^\alpha \tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2}\big\| \le \mathrm{Const.}\,\langle x\rangle, \tag{1.23}$$

where the derivatives are taken in the strong topology and where the constant is independent of $\nu \in (-1,1)$. Since $\mathscr{F}f \in \mathscr{S}(\mathbb{R}^d)$ it follows that

$$\big|K_1(\nu,\mu)\big| \le \mathrm{Const.}, \tag{1.24}$$

and thus $K_1(\nu,\mu)$ is bounded uniformly in ν by a function in $\mathsf{L}^1\big((0,1],\mathrm{d}\mu\big)$.

For the case $\mu > 1$ we first remark that there exists a compact set $J \subset \mathbb{R}\setminus\kappa(H)$ such that $\varphi = E^H(J)\varphi$. There also exists $\zeta \in C_{\mathrm{c}}^\infty\big((0,\infty)\big)$ such that $\zeta\big((H')^2\big)\eta(H) = \eta(H)$ due to Lemma 1.2.6.(d). It then follows that

$$\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi = \zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi.$$

Moreover, from Assumption 1.2.3, we also get that

$$B_{\nu,\mu}^J(x)\varphi := E^H(J)\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,E^H(J)\varphi = \mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi.$$

So, $K_1(\nu,\mu)$ can be rewritten as

$$\int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\,\big\langle\langle\Phi\rangle^2\varphi, \tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2}\zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))B_{\nu,\mu}^J(x)\varphi\big\rangle\,.$$

Now, it is easily shown by using Assumption 1.2.2 and Lemma 1.2.4 that the function $B_{\nu,\mu}^J : \mathbb{R}^d \to \mathscr{B}(\mathcal{H})$ is differentiable with derivative equal to

$$\big(\partial_j B_{\nu,\mu}^J\big)(x) = i\mu H_j'(\nu x)B_{\nu,\mu}^J(x).$$

Furthermore, the bounded operator

$$A_{j,\nu}(x) := (\mathscr{F}f)(x)\tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2}H_j'(\nu x)|H'(\nu x)|^{-2}\zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))$$

satisfies for each integer $k \ge 1$ the bound

$$\big\|A_{j,\nu}(x)\big\| \le \mathrm{Const.}\,\langle x\rangle^{-k},$$

due to Assumption 1.2.2, Lemma 1.2.4, Equation (1.23) and the rapid decay of $\mathscr{F}f$. Thus $K_1(\nu,\mu)$ can be written as

$$K_1(\nu,\mu) = -i\mu^{-1}\sum_j \int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,\big\langle\langle\Phi\rangle^2\varphi, A_{j,\nu}(x)\big(\partial_j B_{\nu,\mu}^J\big)(x)\varphi\big\rangle\,.$$

Now, calculations as in the proof of Lemma 1.3.1.(d) show that each operator H_j' is of class $C^2(\Phi)$. So, the factor $H_j'(\nu x)|H'(\nu x)|^{-2}\zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))$ in $A_{j,\nu}(x)$ can be rewritten as $\mathrm{e}^{-i\nu x\cdot\Phi}\,g(H,H_1',\dots,H_d')\,\mathrm{e}^{i\nu x\cdot\Phi}$, with $g \in \mathscr{S}(\mathbb{R}^{d+1})$ and $H, H_1',\dots,H_d'$ mutually commuting and of class $C^2(\Phi)$. It follows by Equation (1.23) and Proposition 1.5.1 that the map $\mathbb{R}^d \ni x \mapsto A_{j,\nu}(x) \in \mathscr{B}(\mathcal{H})$ is twice strongly differentiable and satisfies

$$\big\|(\partial_j A_{j,\nu})(x)\big\| \le \mathrm{Const.}\,\langle x\rangle^{-k}$$

and

$$\big\|\partial_\ell\big\{(\partial_j A_{j,\nu})H'_\ell(\nu\,\cdot)(H'(\nu\,\cdot))^{-2}\big\}(x)\big\| \le \text{Const.}\,(1+|\nu|)\,\langle x\rangle^{-k} \tag{1.25}$$

for any integer $k \ge 1$. Therefore one can perform two successive integrations by parts (with vanishing boundary contributions) and obtain

$$\begin{aligned} K_1(\nu,\mu) &= i\mu^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big\langle\langle\Phi\rangle^2\varphi,(\partial_j A_{j,\nu})(x)B^J_{\nu,\mu}(x)\varphi\big\rangle \\ &= -\mu^{-2}\sum_{j,\ell}\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,\big\langle\langle\Phi\rangle^2\varphi,\partial_\ell\big\{(\partial_j A_{j,\nu})H'_\ell(\nu\,\cdot)(H'(\nu\,\cdot))^{-2}\big\}(x)B^J_{\nu,\mu}(x)\varphi\big\rangle. \end{aligned}$$

This together with Formula (1.25) implies for each $\nu < 1$ and each $\mu > 1$ that

$$\big|K_1(\nu,\mu)\big| \le \text{Const.}\,\mu^{-2}. \tag{1.26}$$

The combination of the bounds (1.24) and (1.26) shows that $K_1(\nu,\mu)$ is bounded uniformly for $\nu < 1$ by a function in $\mathsf{L}^1\big((0,\infty),\mathrm{d}\mu\big)$. Since similar arguments shows that the same holds for the second term of $\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,K(\nu,\mu,x)$, one can interchange the limit $\nu \searrow 0$ and the integration over μ in (1.22).

The interchange of the limit $\nu \searrow 0$ and the integration over x in (1.22) is justified by the bound

$$\big|K(\nu,\mu,x)\big| \le \text{Const.}\,\big|x(\mathscr{F}f)(x)\big|,$$

which follows from Formula (1.23). □

When the localisation function f is radial, the operator T_f is equal to the operator T, which is independent of f. The next result, which depicts this situation of particular interest, is a direct consequence of Lemma 1.4.2.(c) and Theorem 1.5.5.

Corollary 1.5.6. *Let H and Φ satisfy Assumptions 1.2.2 and 1.2.3. Let $f \in \mathscr{S}(\mathbb{R}^d)$ be a radial function such that $f = 1$ on a neighbourhood of 0. Then we have for each $\varphi \in \mathscr{D}_2$*

$$\lim_{r\to\infty}\tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big\langle\varphi,\big[\,\mathrm{e}^{-itH}f(\Phi/r)\,\mathrm{e}^{itH}-\mathrm{e}^{itH}f(\Phi/r)\,\mathrm{e}^{-itH}\,\big]\varphi\big\rangle = \langle\varphi,T\varphi\rangle, \tag{1.27}$$

with T defined by (1.19).

1.6 Interpretation of the integral formula

This section is devoted to the interpretation of Formula (1.20) and to the description of the sets $\mathscr{D}_t$. We begin by stressing some properties of the subspace $\mathcal{K} := \ker\big((H')^2\big)$ of $\mathcal{H}$, which plays an important role in the sequel.

Lemma 1.6.1. *(a) The eigenvectors of H belong to $\mathcal{K}$,*

(b) If $\varphi \in \mathcal{K}$, then the spectral support of φ with respect to H is contained in $\kappa(H)$,

(c) For each $t \ge 0$, the set $\mathcal{K}$ is orthogonal to $\mathscr{D}_t$,

(d) *For each* $t \geq 0$*, the set* $\mathscr{D}_t$ *is dense in* $\mathcal{H}$ *only if* $\mathcal{K}$ *is trivial.*

Proof. As observed in the proof of Lemma 1.2.6.(b), if λ is an eigenvalue of H then one has $E^H(\{\lambda\})H'_j E^H(\{\lambda\}) = 0$ for each j. If φ_λ is some corresponding eigenvector, it follows that $H'_j\varphi_\lambda = E^H(\{\lambda\})H'_j E^H(\{\lambda\})\varphi_\lambda = 0$. Thus, all eigenvectors of H belong to the kernel of H'_j, and a fortiori to the kernels of $(H'_j)^2$ and $(H')^2$.

Now, let $\varphi \in \mathcal{K}$ and let J be the minimal closed subset of $\mathbb{R}$ such that $E^H(J)\varphi = \varphi$. It follows then from Definition 1.2.5 that $J \subset \kappa(H)$. This implies that $\varphi \perp \mathscr{D}_t$, and thus $\mathcal{K} \perp \mathscr{D}_t$. The last statement is a straightforward consequence of point (c). □

Let us now proceed to the interpretation of Formula (1.20). We consider first the term $t_f(\varphi)$ on the r.h.s., and recall that f is an even element of $\mathscr{S}(\mathbb{R}^d)$ with $f = 1$ in a neighbourhood of 0. We also assume that f is real.

Due to Remark 1.5.4 with $\varphi \in \mathscr{D}_1$, the term $t_f(\varphi)$ reduces to the expectation value $\langle \varphi, T_f\varphi\rangle$, with T_f given by (1.17). Now, a direct calculation using Formulas (1.15), (1.16), and (1.17) shows that the operators T_f and H satisfy in the form sense on $\mathscr{D}_1$ the canonical commutation relation

$$\big[T_f, H\big] = i. \tag{1.28}$$

Therefore, since the group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ leaves $\mathscr{D}_1$ invariant, the following equalities hold in the form sense on $\mathscr{D}_1$:

$$\begin{aligned} T_f\,\mathrm{e}^{-itH} &= \mathrm{e}^{-itH}\,T_f + \big[T_f, \mathrm{e}^{-itH}\,\big] \\ &= \mathrm{e}^{-itH}\,T_f - i\int_0^t \mathrm{d}s\ \mathrm{e}^{-i(t-s)H}\,\big[T_f, H\big]\,\mathrm{e}^{-isH} \\ &= \mathrm{e}^{-itH}\,\big(T_f + t\big). \end{aligned}$$

In other terms, one has

$$\big\langle \psi, T_f\,\mathrm{e}^{-itH}\,\varphi\big\rangle = \big\langle \psi, \mathrm{e}^{-itH}\,\big(T_f + t\big)\varphi\big\rangle \tag{1.29}$$

for each $\psi, \varphi \in \mathscr{D}_1$, and the operator T_f satisfies on $\mathscr{D}_1$ the so-called infinitesimal Weyl relation in the weak sense [56, Sec. 3]. Note that we have not supposed that $\mathscr{D}_1$ is dense. However, if $\mathscr{D}_1$ is dense in $\mathcal{H}$, then the infinitesimal Weyl relation in the strong sense holds:

$$T_f\,\mathrm{e}^{-itH}\,\varphi = \mathrm{e}^{-itH}\,\big(T_f + t\big)\varphi, \qquad \varphi \in \mathscr{D}_1. \tag{1.30}$$

This relation, also known as T_f-weak Weyl relation [73, Def. 1.1], has deep implications on the spectral nature of H and on the form of T_f in the spectral representation of H. Formally, it suggests that $T_f = i\frac{\mathrm{d}}{\mathrm{d}H}$, and thus $-iT_f$ can be seen as the operator of differentiation with respect to the Hamiltonian H. Moreover, being a weak version of the usual Weyl relation, Relation (1.30) also suggests that the spectrum of H may not differ too much from a purely absolutely continuous spectrum. These properties are now discussed more rigorously in particular situations. In the first two cases, the density of $\mathscr{D}_1$ in $\mathcal{H}$ is assumed, and so the point spectrum of H is empty by Lemma 1.6.1.

Case 1 (T_f essentially self-adjoint): If the set $\mathscr{D}_1$ is dense in $\mathcal{H}$, and T_f is essentially self-adjoint on $\mathscr{D}_1$, then it has been shown in [56, Lemma 4] that (1.30) implies that the pair $\{\overline{T_f}, H\}$ satisfies the usual Weyl relation, *i.e.*

$$\mathrm{e}^{isH}\,\mathrm{e}^{it\overline{T_f}} = \mathrm{e}^{ist}\,\mathrm{e}^{it\overline{T_f}}\,\mathrm{e}^{isH}, \qquad s,t \in \mathbb{R}.$$

It follows by the Stone-von Neumann theorem [86, VIII.14] that there exists a unitary operator $\mathscr{U} : \mathcal{H} \to \mathsf{L}^2(\mathbb{R};\mathbb{C}^N, \mathrm{d}\lambda)$, with N finite or infinite, such that $\mathscr{U}\,\mathrm{e}^{it\overline{T_f}}\,\mathscr{U}^*$ is the operator of translation by t, and $\mathscr{U}\,\mathrm{e}^{isH}\,\mathscr{U}^*$ is the operator of multiplication by $\mathrm{e}^{is\lambda}$. In terms of the generator H, this means that $\mathscr{U} H \mathscr{U}^* = \lambda$, where "$\lambda$" stands for the multiplication operator by λ in $\mathsf{L}^2(\mathbb{R};\mathbb{C}^N, \mathrm{d}\lambda)$. Therefore the spectrum of H is purely absolutely continuous and covers the whole real line. Moreover, we have for each $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{D}_1$

$$\langle \psi, T_f\varphi\rangle = \langle \psi, \overline{T_f}\varphi\rangle = \int_{\mathbb{R}} \mathrm{d}\lambda\,\big\langle (\mathscr{U}\psi)(\lambda), i\,\tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda)\big\rangle_{\mathbb{C}^N},$$

where $\frac{\mathrm{d}}{\mathrm{d}\lambda}$ denotes the distributional derivative (see for instance [8, Rem. 1] for an interpretation of the derivative $\frac{\mathrm{d}}{\mathrm{d}\lambda}$).

Case 2 (T_f symmetric): If the set $\mathscr{D}_1$ is dense in $\mathcal{H}$, then we know from Proposition 1.5.2 and Remark 1.5.4 that T_f is symmetric. In such a situation, (1.30) once more implies that the spectrum of H is purely absolutely continuous [73, Thm. 4.4], but it may not cover the whole real line. We expect that the operator T_f is still equal to $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ (on a suitable subspace) in the spectral representation of H, but we have not been able to prove it in this generality. However, this property holds in most of the examples presented below. If T_f and H satisfy more assumptions, then more can be said (see for instance [104]).

Case 3 (T_f not densely defined): If $\mathscr{D}_1$ is not dense in $\mathcal{H}$, then we are not aware of general works using a relation like (1.29) to deduce results on the spectral nature of H or on the form of T_f in the spectral representation of H. In such a case, we only know from Theorem 1.3.6 that the spectrum of H is purely absolutely continuous in $\sigma(H)\backslash\kappa(H)$, but we have no general information on the form of T_f in the spectral representation of H. However, with a suitable additional assumption the analysis can be continued. Indeed, consider the orthogonal decomposition $\mathcal{H} := \mathcal{K} \oplus \mathcal{G}$, with $\mathcal{K} \equiv \ker\big((H')^2\big)$. Then the operators H, H'_j, and $H''_{k\ell}$ are all reduced by this decomposition, due to Lemma 1.2.4. If we assume additionally that $T_f\mathscr{D}_1 \subset \mathcal{G}$, then the analysis can be performed in the subspace $\mathcal{G}$.

Since $\mathscr{D}_1 \subset \mathcal{G}$ by Lemma 1.6.1, the additional hypothesis allows us to consider the restriction of T_f to $\mathcal{G}$, which we denote by T_f. Let also H, H'_j, and $\mathsf{H}''_{k\ell}$ denote the restrictions of the corresponding operators in $\mathcal{G}$. We then set

$$\mathsf{D}_t := \big\{\varphi \in \mathcal{D}(\langle\Phi\rangle^t) \cap \mathcal{G} \mid \varphi = \eta(\mathsf{H})\varphi \text{ for some } \eta \in C^\infty_{\mathrm{c}}\big(\mathbb{R}\setminus\kappa(H)\big)\big\} \subset \mathcal{G},$$

and observe that the equality (1.28) holds in the form sense on D_1. In other words, (1.28) can be considered in the reduced Hilbert space $\mathcal{G}$ instead of $\mathcal{H}$. The interest of the above decomposition comes from the following fact: If D_1 is dense in $\mathcal{G}$ (which is certainly more likely than in $\mathcal{H}$), then T_f is symmetric and the situation reduces to the case 2 with the operators H and T_f. If in addition T_f is essentially self-adjoint on D_1, the situation even reduces to the case 1 with the operators H and T_f. In both situations, the spectrum of H is purely absolutely continuous. In Section 1.7, we shall present 2 examples corresponding to these situations.

Remark 1.6.2. The implicit condition $T_f \mathscr{D}_1 \subset \mathcal{G}$ can be made more explicit. For example, if the collection Φ is reduced by the decomposition $\mathcal{H} = \mathcal{K} \oplus \mathcal{G}$, then the condition holds (and (1.20) also holds on D_2). More generally, if $\Phi_j \mathscr{D}_1 \subset \mathcal{G}$ for each j, then the condition holds. Indeed, if $\varphi \in \mathscr{D}_1$ one knows from Remark 1.5.4 that $(\partial_j R_f)(H')\varphi \in \mathcal{D}(\langle\Phi\rangle)$, and one can prove similarly that $|H'|^{-1}\varphi \in \mathcal{D}(\langle\Phi\rangle)$. Furthermore, there exists $\eta \in C_c^\infty\big(\mathbb{R} \setminus \kappa(H)\big)$ such that $(\partial_j R_f)(H')\varphi = \eta(H)(\partial_j R_f)(H')\varphi$ and $|H'|^{-1}\varphi = \eta(H)|H'|^{-1}\varphi$, which means that both vectors $\partial_j R_f(H')\varphi$ and $|H'|^{-1}\varphi$ belong to $\mathscr{D}_1$. It follows that $T_f\varphi \in \mathcal{G}$ by taking the explicit form (1.17) of T_f into account.

Let us now concentrate on the other term in Formula (1.20). If we consider the operators Φ_j as the components of an abstract position operator Φ, then the l.h.s. of Formula (1.20) has the following meaning: For r fixed, it can be interpreted as the difference of times spent by the evolving state $\mathrm{e}^{-itH}\varphi$ in the past (first term) and in the future (second term) within the region defined by the localisation operator $f(\Phi/r)$. Thus, Formula (1.20) shows that this difference of times tends as $r \to \infty$ to the expectation value in φ of the operator T_f.

On the other hand, let us consider a quantum scattering pair $\{H, H+V\}$, with V an appropriate perturbation of H. Let us also assume that the corresponding scattering operator S is unitary, and recall that S commute with H. In this framework, the global time delay $\tau(\varphi)$ for the state φ defined in terms of the localisation operators $f(\Phi/r)$ can usually be reexpressed as follows: it is equal to the l.h.s. of (1.20) minus the same quantity with φ replaced by $S\varphi$. Therefore, if φ and $S\varphi$ are elements of $\mathscr{D}_2$, then the time delay for the scattering pair $\{H, H+V\}$ should satisfy the equation

$$\tau(\varphi) = -\langle \varphi, S^*[T_f, S]\varphi\rangle. \tag{1.31}$$

In addition, if T_f acts in the spectral representation of H as a differential operator $i\frac{\mathrm{d}}{\mathrm{d}H}$, then $\tau(\varphi)$ would verify, in our complete abstract setting, the Eisenbud-Wigner formula

$$\tau(\varphi) = \big\langle \varphi, -iS^* \tfrac{\mathrm{d}S}{\mathrm{d}H}\,\varphi\big\rangle.$$

Summing up, as soon as the position operator Φ and the operator H satisfy Assumptions 1.2.2 and 1.2.3, then our study establishes a preliminary relation between time operators T_f given by (1.17) and the theory of quantum time delay. Many concrete examples discussed in the literature [8, 9, 10, 45, 74, 109, 111] turn out to fit in the present framework, and several old or new examples are presented in the following section. Further investigations in relation with the abstract Formula (1.31) will be considered in the next chapter.

Now, most of the above discussion depends on the size of $\mathscr{D}_1$ in $\mathcal{H}$, and implicitly on the size of $\kappa(H)$ in $\sigma(H)$. We collect some information about these sets. It has been proved in Lemma 1.2.6.(d) that $\kappa(H)$ is closed and corresponds to the complement in $\sigma(H)$ of the Mourre set (see the comment after Definition 1.3.4). It always contains the eigenvalues of H. Furthermore, since the spectrum of H is absolutely continuous on $\sigma(H) \setminus \kappa(H)$, the support of the singularly continuous spectrum, if any, is contained in $\kappa(H)$. In particular, if $\kappa(H)$ is discrete, then H has no singularly continuous spectrum. Thus, the determination of the size of $\kappa(H)$ is an important issue for the spectral analysis of H. More will be said in the concrete examples of the next section.

Let us now turn to the density properties of the sets $\mathscr{D}_t$. For this, we recall that a subset $K \subset \mathbb{R}$ is said to be uniformly discrete if

$$\inf\{|x-y| \mid x, y \in K \text{ and } x \neq y\} > 0.$$

Lemma 1.6.3. *Assume that $\kappa(H)$ is uniformly discrete. Then*

(a) $\mathscr{D}_0$ is dense in $\mathcal{H}_{\rm ac}(H)$,

(b) If $\sigma_{\rm p}(H) = \varnothing$ and if H is of class $C^k(\Phi)$ for some integer k, then $\mathscr{D}_t$ is dense in $\mathcal{H}$ for any $t \in [0, k)$.

Proof. (a) Let $\varphi \in \mathcal{H}_{\rm ac}(H)$ and $\varepsilon > 0$. Then there exists a finite interval $[a, b]$ such that $\big\|\big[1-E^H([a,b])\big]\varphi\big\| \leq \varepsilon/2$. Since $\kappa(H)$ is uniformly discrete, the set $\kappa(H) \cap (a, b)$ contains only a finite number N of points $x_1 < x_2 < \cdots < x_N$. Let us set $x_0 := a$ and $x_{N+1} := b$. Since $\varphi \in \mathcal{H}_{\rm ac}$, there exists $\delta > 0$ such that $x_j + \delta < x_{j+1} - \delta$ for each $j \in \{0, \dots, N\}$, and $\|E^H(L_\delta)\varphi\| \leq \varepsilon/2$, where

$$L_\delta := \{x \in [a, b] \mid |x - x_j| \leq \delta \text{ for each } j = 0, 1, \dots, N+1\}.$$

Now, for any $j \in \{0, \dots, N\}$ there exist $\eta_j, \widetilde{\eta}_j \in C_{\rm c}^\infty\big((x_j, x_{j+1}); [0,1]\big)$ such that $\widetilde{\eta}_j(x) = 1$ for $x \in [x_j + \delta, x_{j+1} - \delta]$ and $\eta_j \widetilde{\eta}_j = \widetilde{\eta}_j$. Therefore, if $\eta := \sum_{j=0}^N \eta_j$, $\widetilde{\eta} := \sum_{j=0}^N \widetilde{\eta}_j$ and $\psi := \widetilde{\eta}(H)\varphi$, one verifies that $\eta \in C_{\rm c}^\infty\big((a,b); [0,1]\big) \subset C_{\rm c}^\infty\big(\mathbb{R} \setminus \kappa(H)\big)$ and that $\psi = \eta(H)\psi$, which imply that $\psi \in \mathscr{D}_0$. Moreover, one has

$$\begin{aligned}
\|\varphi - \psi\| &\leq \big\|[1-\widetilde{\eta}(H)]E^H([a,b])\varphi\big\| + \big\|[1-\widetilde{\eta}(H)]\big[1-E^H([a,b])\big]\varphi\big\| \\
&\leq \big\|[1-\widetilde{\eta}(H)]E^H(L_\delta)\varphi\big\| + \big\|\big[1-E^H([a,b])\big]\varphi\big\| \\
&\leq \tfrac{\varepsilon}{2} + \tfrac{\varepsilon}{2}\,.
\end{aligned}$$

Thus $\|\varphi - \psi\| \leq \varepsilon$ for $\psi \in \mathscr{D}_0$, and the claim is proved.

(b) If $\sigma_{\rm p}(H) = \varnothing$, then it follows from the above discussion that $\mathcal{H}_{\rm ac}(H) = \mathcal{H}$. In view of what precedes, it is enough to show that the vector $\psi \equiv \widetilde{\eta}(H)\varphi$ of point (a) belongs to $\mathcal{D}(\langle\Phi\rangle^t)$: The operator $\widetilde{\eta}(H)$ belongs to $C^k(\Phi)$, since H is of class $C^k(\Phi)$ and $\widetilde{\eta} \in C_{\rm c}^\infty(\mathbb{R})$ (see [7, Thm. 6.2.5]). So, we obtain from [7, Prop. 5.3.1] that $\langle\Phi\rangle^t\,\widetilde{\eta}(H)\,\langle\Phi\rangle^{-t}$ is bounded on $\mathcal{H}$, which implies the claim. ☐

1.7 Examples

In this section we show that Assumptions 1.2.2 and 1.2.3 are satisfied in various general situations. In these situations all the results of the preceding sections such as Theorem 1.3.6 or Formula (1.20) hold. However, it is usually impossible to determine explicitly the set $\kappa(H)$ when the framework is too general. Therefore, we also illustrate our approach with some concrete examples for which everything can be computed explicitly. When possible, we also relate these examples with the different cases presented in Section 1.6. For that purpose, we shall always assume that f is a real and even function in $\mathscr{S}(\mathbb{R}^d)$ with $f = 1$ on a neighbourhood of 0.

The configuration space of the system under consideration will sometimes be $\mathbb{R}^n$, and the corresponding Hilbert space $\mathsf{L}^2(\mathbb{R}^n)$. In that case, the notations $Q \equiv (Q_1, \dots, Q_n)$ and $P \equiv (P_1, \dots, P_n)$ refer to the families of position operators and momentum operators. More precisely, for suitable $\varphi \in \mathsf{L}^2(\mathbb{R}^n)$ and each $j \in \{1, \dots, n\}$, we have $(Q_j\varphi)(x) = x_j\varphi(x)$ and $(P_j\varphi)(x) = -i(\partial_j\varphi)(x)$ for each $x \in \mathbb{R}^n$.

1.7.1 H' constant

Suppose that H is of class $C^1(\Phi)$, and assume that there exists $v \in \mathbb{R}^d \setminus \{0\}$ such that $H' = v$. Then H is of class $C^\infty(\Phi)$, Assumption 1.2.2 is directly verified, and one has on $\mathcal{D}(H)$

$$H(x) = H(0) + \int_0^1 \mathrm{d}t \, \big(x \cdot H'(tx)\big) = H + \int_0^1 \mathrm{d}t \; \mathrm{e}^{-itx\cdot\Phi} \left(x \cdot H'\right) \mathrm{e}^{itx\cdot\Phi} = H + x \cdot v.$$

This implies Assumption 1.2.3. Furthermore $\kappa(H) = \varnothing$, and $\sigma(H) = \sigma_{\rm ac}(H)$ due to Theorem 1.3.6. So, the set $\mathscr{D}_t$ is dense in $\mathcal{H}$ for each $t \geq 0$, due to Lemma 1.6.3.(b). The operator $R'_f(H')$ reduces to the constant vector $R'_f(v)$. Therefore, we have the equality $T_f = -R'_f(v) \cdot \Phi$ on $\mathscr{D}_1$, and it is easily shown that T_f is essentially self-adjoint on $\mathscr{D}_1$. It follows from the case 1 of Section 1.6 that the spectrum of H covers the whole real line, and there exists a unitary operator $\mathscr{U} : \mathcal{H} \to \mathsf{L}^2(\mathbb{R}; \mathbb{C}^N, \mathrm{d}\lambda)$ such that

$$\langle \psi, T_f \varphi \rangle = \int_{\mathbb{R}} \mathrm{d}\lambda \left\langle (\mathscr{U}\psi)(\lambda), i \, \tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda) \right\rangle_{\mathbb{C}^N}$$

for each $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{D}_1$.

Typical examples of operators H and Φ fitting into this construction are Friedrichs-type Hamiltonians and position operators. For illustration, we mention the case $H := v{\cdot}P+V(Q)$ and $\Phi := Q$ in $\mathsf{L}^2(\mathbb{R}^d)$, with $v \in \mathbb{R}^d \setminus \{0\}$ and $V \in \mathsf{L}^\infty(\mathbb{R}^d; \mathbb{R})$ (see also [111, Sec. 5] for informations on quantum time delay in a similar case).

Stark Hamiltonians and momentum operators also fit into the construction, for example $H := P^2 + v \cdot Q$ in $\mathsf{L}^2(\mathbb{R}^d)$ with $v \in \mathbb{R}^d \setminus \{0\}$, and $\Phi := P$. We refer to [85, 97, 98] for previous accounts on the theory of time operators and quantum time delay in similar situations.

Note that these first two examples are interesting since the operators H contain not only a kinetic part, but also a potential perturbation.

Another example is provided by the Jacobi operator related to the family of Hermite polynomials (see [102, Appendix A] for details). In the Hilbert space $\mathcal{H} := \ell^2(\mathbb{N})$, consider the Jacobi operator given for $\varphi \in \mathcal{H}$ by

$$(H\varphi)(n) := \tfrac{\sqrt{n-1}}{2} \, \varphi(n-1) + \tfrac{\sqrt{n}}{2} \, \varphi(n+1),$$

with the convention that $\varphi(0) = 0$. The operator H is essentially self-adjoint on ℓ^2_0, the subspace of sequences in $\mathcal{H}$ with only finitely many non-zero components. As operator Φ (with one component), take

$$(\Phi\varphi)(n) := -i\big\{\sqrt{n-1}\,\varphi(n-1) - \sqrt{n}\,\varphi(n+1)\big\},$$

which is also essentially self-adjoint on ℓ^2_0. Then H is of class $C^1(\Phi)$ and $H' \equiv i[H,\Phi] = 1$, and so the preceding results hold.

1.7.2 $H' = H$

Suppose that Φ has only one component, and assume that H is Φ-homogeneous of degree 1, *i.e.* $H(x) \equiv \mathrm{e}^{-ix\Phi}\, H\, \mathrm{e}^{ix\Phi} = \mathrm{e}^{x}\, H$ for all $x \in \mathbb{R}$. This implies that H is of class $C^\infty(\Phi)$ and that $H' = H$. So, Assumptions 1.2.2 and 1.2.3 are readily verified. Moreover, since $\kappa(H) = \{0\}$, Theorem 1.3.6 implies that H is purely absolutely continuous except at the origin, where it may have the eigenvalue 0.

Now, let us show that the formal formula of Remark 1.5.3 holds in this case. For any $\varphi \in \mathscr{D}_1$ one has by Remark 1.5.4 that $R_f'(H')\varphi \equiv R_f'(H)\varphi$ belongs to $\mathcal{D}(\Phi)$. On another hand, we have

$$\Phi\varphi = \big\{H\Phi + [\Phi, H]\big\}H^{-1}\varphi = H(\Phi + i)H^{-1}\varphi,$$

which implies that $R_f'(H)\Phi\varphi = R_f'\big(\tfrac{H}{|H|}\big)\tfrac{H}{|H|}(\Phi + i)H^{-1}\varphi \in \mathcal{H}$. In consequence, the operator

$$T_f = -\tfrac{1}{2}\big(\Phi R_f'(H) + R_f'(H)\Phi\big)$$

is well-defined on $\mathscr{D}_1$. In particular, if 0 is not an eigenvalue of H, then T_f is a symmetric operator and the discussion of the case 2 of Section 1.6 is relevant (if T_f is essentially self-adjoint, the case 1 is relevant).

We now give two examples of pairs $\{H, \Phi\}$ satisfying the preceding assumptions. Other examples are presented in [22, Sec. 10]. Suppose that $H := P^2$ is the free Schrödinger operator in $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^n)$ and $\Phi := \frac{1}{4}(Q\cdot P + P\cdot Q)$ is the generator of dilations in $\mathcal{H}$. Then the relation $\mathrm{e}^{-ix\Phi}\, H\, \mathrm{e}^{ix\Phi} = \mathrm{e}^{x}\, H$ is satisfied, and $\sigma(H) = \sigma_{\mathrm{ac}}(H) = [0,\infty)$. Furthermore, for $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{F}C^\infty_{\mathrm{c}}\big(\mathbb{R}^n \setminus \{0\}\big) \subset \mathscr{D}_1$ a direct calculation using Formula (1.15) shows that

$$\langle \psi, T_f\varphi\rangle = \big\langle \psi, \tfrac{1}{4}\big(Q\cdot PP^{-2} + PP^{-2}\cdot Q\big)\varphi\big\rangle = \int_0^\infty \mathrm{d}\lambda\, \big\langle (\mathscr{U}\psi)(\lambda), i\,\tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda)\big\rangle_{\mathsf{L}^2(\mathbb{S}^{n-1})},$$

where $\mathscr{U} : \mathcal{H} \to \int^\oplus_{[0,\infty)} \mathrm{d}\lambda\, \mathsf{L}^2(\mathbb{S}^{n-1})$ is the spectral transformation for P^2. This example corresponds to the case 2 of Section 1.6.

Another example of Φ-homogeneous operator is provided by the Jacobi operator related to the family of Laguerre polynomials (see [102, Appendix A] for details). In the Hilbert space $\mathcal{H} := \ell^2(\mathbb{N})$, consider the Jacobi operator given for $\varphi \in \mathcal{H}$ by

$$(H\varphi)(n) := (n-1)\varphi(n-1) + (2n-1)\varphi(n) + n\varphi(n+1),$$

with the convention that $\varphi(0) = 0$. The operator H is essentially self-adjoint on ℓ^2_0. As operator Φ (with one component), take

$$(\Phi\varphi)(n) := -\tfrac{i}{2}\big\{(n-1)\varphi(n-1) - n\varphi(n+1)\big\}.$$

Then one has $H' \equiv i[H,\Phi] = H$, which implies that H is Φ-homogeneous of degree 1 and so the preceding results hold.

1.7.3 Dirac operator

In the Hilbert space $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$ we consider the Dirac operator for a spin-$\frac{1}{2}$ particle of mass $m > 0$

$$H := \alpha \cdot P + \beta m,$$

where $\alpha \equiv (\alpha_1, \alpha_2, \alpha_3)$ and β denote the usual 4×4 Dirac matrices. It is known that H has domain $\mathcal{H}^1(\mathbb{R}^3;\mathbb{C}^4)$, that $|H| = (P^2 + m^2)^{1/2}$ and that $\sigma(H) = \sigma_{\rm ac}(H) = (-\infty, -m] \cup [m, \infty)$.

We also let $\Phi := \mathscr{U}_{\rm FW}^{-1} Q \mathscr{U}_{\rm FW} \equiv Q_{\rm NW}$ be the Wigner-Newton position operator, with $\mathscr{U}_{\rm FW}$ the usual Foldy-Wouthuysen transformation [108, Sec. 1.4.3]. Then a direct calculation shows that

$$H(x) = \sqrt{\tfrac{(P+x)^2+m^2}{P^2+m^2}}\, H$$

for each $x \in \mathbb{R}^3$, and thus Assumptions 1.2.2 and 1.2.3 are easily verified. Furthermore, since $H_j' = P_j H^{-1}$ for each $j = 1, 2, 3$, it follows that

$$(H')^2 = P^2 H^{-2} = (H^2 - m^2) H^{-2}.$$

Clearly, $\ker\big((H')^2\big) = \{0\}$ and one infers from Definition 1.2.5 that $\kappa(H) = \{\pm m\}$, and from Lemma 1.6.3.(b) that the sets

$$\mathscr{D}_t = \big\{\varphi \in \mathscr{U}_{\rm FW}^{-1} \mathcal{D}\big(\langle Q\rangle^t\big) \mid \eta(H)\varphi = \varphi \text{ for some } \eta \in C_{\rm c}^\infty\big(\mathbb{R} \setminus \{\pm m\}\big)\big\},$$

are dense in $\mathcal{H}$. So the discussion of the case 2 of Section 1.6 is relevant.

We now show that the formal formula of Remark 1.5.3 holds if f is radial. Indeed, each $\varphi \in \mathscr{D}_1$ satisfies $\varphi = \eta(H) \mathscr{U}_{\rm FW}^{-1} \psi$ for some $\eta \in C_{\rm c}^\infty\big(\mathbb{R} \setminus \{\pm m\}\big)$ and some $\psi \in \mathcal{D}(\langle Q\rangle)$. So, we have

$$\begin{aligned} H'(H')^{-2} \cdot Q_{\rm NW}\varphi &= PP^{-2}H \cdot \mathscr{U}_{\rm FW}^{-1} Q \mathscr{U}_{\rm FW} \eta(H) \mathscr{U}_{\rm FW}^{-1}\psi \\ &= \mathscr{U}_{\rm FW}^{-1} PP^{-2}\beta|H| \cdot Q\eta(\beta|H|)\psi \in \mathcal{H}, \end{aligned}$$

and the operator T of (1.19) is symmetric and can be written on $\mathscr{D}_1$ in the simpler form

$$T = \tfrac{1}{2}\big\{Q_{\rm NW} \cdot H'(H')^{-2} + H'(H')^{-2} \cdot Q_{\rm NW}\big\} \equiv \tfrac{1}{2}\big\{Q_{\rm NW} \cdot PP^{-2}H + PP^{-2}H \cdot Q_{\rm NW}\big\}.$$

Now let $h : \mathbb{R}^3 \to \mathbb{R}$ be defined by $h(\xi) := (\xi^2 + m^2)^{1/2}$. Then it is known that $\mathscr{U}_{\rm FW} H \mathscr{U}_{\rm FW}^{-1} = \beta h(P)$, and a direct calculation shows that

$$\begin{aligned} \mathscr{U}_{\rm FW} T \mathscr{U}_{\rm FW}^{-1} &= \tfrac{1}{2}\beta\big\{Q \cdot PP^{-2}(P^2+m^2)^{1/2} + PP^{-2}(P^2+m^2)^{1/2} \cdot Q\big\} \\ &= \tfrac{1}{2}\beta\big\{Q \cdot \frac{h'(P)}{h'(P)^2} + \frac{h'(P)}{h'(P)^2} \cdot Q\big\} \end{aligned}$$

on $\mathscr{U}_{\rm FW}\mathscr{D}_1$. Furthermore there exists a spectral transformation

$$\mathscr{U}_0 : \mathsf{L}^2(\mathbb{R}^3) \to \int_{[m,\infty)}^{\oplus} \mathrm{d}\lambda\, \mathsf{L}^2(\mathbb{S}^2)$$

for $h(P)$ such that

$$\mathscr{U}_0\big\{Q \cdot \tfrac{h'(P)}{h'(P)^2} + \tfrac{h'(P)}{h'(P)^2} \cdot Q\big\}\mathscr{U}_0^{-1}$$

is equal to the operator $2i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ of differentiation with respect to the spectral parameter λ of $h(P)$ (see [111, Lemma 3.6] for a precise statement). Combining the preceding transformations we obtain for each $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{D}_1$ that

$$\langle \psi, T\varphi \rangle = \int_{\sigma(H)} \mathrm{d}\lambda \, \big\langle (\mathscr{U}\psi)(\lambda), i\,\tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda) \big\rangle_{\mathsf{L}^2(\mathbb{S}^2;\mathbb{C}^2)},$$

where $\mathscr{U} : \mathcal{H} \to \int_{\sigma(H)}^{\oplus} \mathrm{d}\lambda \, \mathsf{L}^2(\mathbb{S}^2;\mathbb{C}^2)$ is the spectral transformation for the free Dirac operator H.

1.7.4 Convolution operators on locally compact groups

This example is partially inspired from [69], where the spectral nature of convolution operators on locally compact groups is studied.

Let G be a locally compact group with identity e and a left Haar measure ρ. In the Hilbert space $\mathcal{H} := \mathsf{L}^2(G, \mathrm{d}\rho)$ we consider the operator H_μ of convolution by $\mu \in \mathsf{M}(G)$, where $\mathsf{M}(G)$ is the set of complex bounded Radon measures on G. Namely, for $\varphi \in \mathcal{H}$ one sets

$$(H_\mu \varphi)(g) := (\mu * \varphi)(g) \equiv \int_G \mathrm{d}\mu(h)\, \varphi(h^{-1}g) \quad \text{for } a.e.\ g \in G,$$

where the notation *a.e.* stands for "almost everywhere" and refers to the Haar measure ρ. The operator H_μ is bounded with norm $\|H_\mu\| \le |\mu|(G)$, and it is self-adjoint if μ is symmetric, *i.e.* $\mu(E) = \overline{\mu(E^{-1})}$ for each Borel subset E of G. For simplicity, we also assume that μ is central and with compact support, where central means that $\mu(h^{-1}Eh) = \mu(E)$ for each $h \in G$ and each Borel subset E of G.

We recall that given two measures $\mu, \nu \in \mathsf{M}(G)$, their convolution $\mu * \nu \in \mathsf{M}(G)$ is defined by the relation [41, Eq. 2.34]

$$\int_G \mathrm{d}(\mu * \nu)(g)\, \psi(g) := \int_G \int_G \mathrm{d}\mu(g)\mathrm{d}\nu(h)\, \psi(gh) \qquad \forall \psi \in C_0(G),$$

where $C_0(G)$ denotes the C^*-algebra of continuous complex functions on G vanishing at infinity. If $\mu \in \mathsf{M}(G)$ has compact support and $\zeta : G \to \mathbb{C}$ is continuous, then the linear functional

$$C_0(G) \ni \psi \mapsto \int_G \mathrm{d}\mu(g)\, \zeta(g)\psi(g) \in \mathbb{C}$$

is bounded, and there exists a unique measure with compact support associated with it, due to the Riesz-Markov representation theorem. We write $\zeta\mu$ for this measure.

A natural choice for the family of operators $\Phi \equiv (\Phi_1, \dots, \Phi_d)$ are, if they exist, real characters $\Phi_j \in \mathrm{Hom}(G;\mathbb{R})$, *i.e.* continuous group morphisms from G to $\mathbb{R}$. With this choice, one obtains that

$$[H_\mu(x)\varphi](g) \equiv \big(\mathrm{e}^{-ix\cdot\Phi}\, H_\mu\, \mathrm{e}^{ix\cdot\Phi}\, \varphi\big)(g) = \int_G \mathrm{d}\mu(h)\; \mathrm{e}^{-ix\cdot\Phi(h)}\, \varphi(h^{-1}g)$$

for each $x \in \mathbb{R}^d$, $\varphi \in \mathcal{H}$, and *a.e.* $g \in G$. Namely, $H_\mu(x)$ is equal to the operator of convolution by the measure $\mathrm{e}^{-ix\cdot\Phi}\,\mu$, *i.e.* $H_\mu(x) = H_{\mathrm{e}^{-ix\cdot\Phi}\,\mu}$. Since μ has compact support and each Φ_j is continuous, this implies that H_μ is of class $C^\infty(\Phi)$, with all the operators $(H_\mu)'_j, (H_\mu)''_{jk}, (H_\mu)'''_{jk\ell}$ belonging to $\mathscr{B}(\mathcal{H})$. So Assumption 1.2.2 is satisfied. Furthermore, the commutativity of central measures with respect to the convolution product implies that $\mu * \mathrm{e}^{-ix\cdot\Phi}\,\mu = \mathrm{e}^{-ix\cdot\Phi}\,\mu * \mu$ or equivalently that $HH(x) = H(x)H$. So Assumption 1.2.3 is satisfied. Finally, the equality $H_\mu(x) = H_{\mathrm{e}^{-ix\cdot\Phi}\,\mu}$ readily implies that $(H'_\mu)_j = H_{-i\Phi_j\mu}$.

Since both Assumptions 1.2.2 and 1.2.3 are satisfied, the general results of the previous sections apply. However, it is very complicated to describe the set $\kappa(H_\mu)$ in the present generality. Therefore, we shall now assume that the group G is abelian in order to use the Fourier transformation to determine some properties of $\kappa(H_\mu)$. So let us assume that G is a locally compact abelian group. Then any measure on G is automatically central, and thus we only need to suppose that μ is symmetric and with compact support. For a suitably normalised Haar measure $\rho_\wedge$ on the dual group $\widehat{G}$, the Fourier transformation $\mathscr{F}$ defines a unitary isomorphism from $\mathcal{H}$ onto $\mathsf{L}^2(\widehat{G}, \mathrm{d}\rho_\wedge)$. It maps unitarily H_μ on the operator M_m of multiplication with the bounded continuous real function $m := \mathscr{F}(\mu)$ on $\widehat{G}$. Furthermore, one has

$$\sigma(H_\mu) = \sigma(M_m) = \overline{m(\widehat{G})}, \quad \sigma_\mathrm{p}(H_\mu) = \sigma_\mathrm{p}(M_m) = \overline{\big\{s \in \mathbb{R} \mid \rho_\wedge\big(m^{-1}(s)\big) > 0\big\}}, \tag{1.32}$$

where the overlines denote the closure in $\mathbb{R}$.

Let us recall that there is an almost canonical identification of $\mathrm{Hom}(G, \mathbb{R})$ with the vector space $\mathrm{Hom}(\mathbb{R}, \widehat{G})$ of all continuous one-parameter subgroups of $\widehat{G}$. Given the real character Φ_j, we denote by $\Upsilon_j \in \mathrm{Hom}(\mathbb{R}, \widehat{G})$ the unique element satisfying

$$\big\langle g, \Upsilon_j(t)\big\rangle = \mathrm{e}^{it\Phi_j(g)} \quad \text{for all } t \in \mathbb{R} \text{ and } g \in G,$$

where $\langle\cdot,\cdot\rangle : G \times \widehat{G} \to \mathbb{C}$ is the duality between G and $\widehat{G}$.

Definition 1.7.1. A function $m : \widehat{G} \to \mathbb{C}$ is *differentiable at* $\xi \in \widehat{G}$ *along the one-parameter subgroup* $\Upsilon_j \in \mathrm{Hom}(\mathbb{R}, \widehat{G})$ if the function $\mathbb{R} \ni t \mapsto m\big(\xi + \Upsilon_j(t)\big) \in \mathbb{C}$ is differentiable at $t = 0$. In such a case we write $(d_j m)(\xi)$ for $\frac{\mathrm{d}}{\mathrm{d}t}\, m\big(\xi + \Upsilon_j(t)\big)\big|_{t=0}$. Higher order derivatives, when existing, are denoted by $d_j^k m$, $k \in \mathbb{N}$.

We refer to [95] for more details on differential calculus on locally compact groups. Here we only note that (since μ has compact support) the function $m = \mathscr{F}(\mu)$ is differentiable at any point ξ along the one-parameter subgroup Υ_j, and $-i\mathscr{F}(\Phi_j\mu) = d_j m$ [95, p. 68]. This implies that the operator $(H'_\mu)_j$ is mapped unitarily by $\mathscr{F}$ on the multiplication operator $M_{d_j m}$, and thus $(H'_\mu)^2$ is unitarily equivalent to the operator of multiplication by the function $\sum_j (d_j m)^2$. It follows that

$$\kappa(H_\mu) \supset \big\{\lambda \in \mathbb{R} \mid \exists \xi \in \widehat{G} \text{ such that } m(\xi) = \lambda \text{ and } \textstyle\sum_j (d_j m)(\xi)^2 = 0\big\}.$$

This property of $\kappa(H_\mu)$ suggests a way to justify the formal formula of Remark 1.5.3 and to write nice formulas for the operator T given by (1.19). Indeed, since $\mathscr{F}\Phi_j\mathscr{F}^{-1}$ acts as the differential operator id_j in $\mathsf{L}^2(\widehat{G}, \mathrm{d}\rho_\wedge)$, it follows that Φ_j leaves invariant the complement of the support of the functions on which it acts. Therefore, the set $\Phi_j\mathscr{D}_1 \equiv \mathscr{F}^{-1}(id_j)\mathscr{F}\mathscr{D}_1$ is included in the domain of the operator

$$\tfrac{(H'_\mu)_j}{(H'_\mu)^2} \equiv \mathscr{F}^{-1}\frac{M_{d_jm}}{M_{\sum_k(d_km)^2}}\,\mathscr{F}.$$

Thus the formula (1.19) takes the form

$$T = \tfrac{1}{2}\textstyle\sum_j\left\{\Phi_j\frac{H_{-i\Phi_j\mu}}{\sum_k(H_{-i\Phi_k\mu})^2} + \frac{H_{-i\Phi_j\mu}}{\sum_k(H_{-i\Phi_k\mu})^2}\,\Phi_j\right\}$$

on $\mathscr{D}_1$, or alternatively the form

$$\mathscr{F}T\mathscr{F}^{-1} = \tfrac{i}{2}\textstyle\sum_j\left\{d_j\frac{M_{d_jm}}{M_{\sum_k(d_km)^2}} + \frac{M_{d_jm}}{M_{\sum_k(d_km)^2}}\,d_j\right\} \tag{1.33}$$

on $\mathscr{F}\mathscr{D}_1$ (note that the last expression is well-defined on $\mathscr{F}\mathscr{D}_1$, since $m = \mathscr{F}(\mu)$ is of class C^2 in the sense of Definition 1.7.1).

In simple situations, everything can be calculated explicitly. For instance, when $G = \mathbb{Z}^d$, the Haar measure ρ is the counting measure, and the most natural real characters Φ_j are the position operators given by

$$(\Phi_j\varphi)(g) := g_j\varphi(g), \qquad \varphi \in \mathsf{L}^2(\mathbb{Z}^d),$$

where g_j is the j-th component of $g \in \mathbb{Z}^d$. The operators H_μ and $(H'_\mu)^2$ are unitarily equivalent to multiplication operators on $\widehat{G} = (-\pi,\pi]^d$. Since the measures μ and $\Phi_j\mu$ have compact (and thus finite) support, these operators are just multiplication operators by polynomials of finite degree in the variables $\mathrm{e}^{-i\xi_1},\dots,\mathrm{e}^{-i\xi_d}$, with $\xi_j \in (-\pi,\pi]$. So, the set $\kappa(H_\mu)$ is finite, and the characterisation (1.32) of the point spectrum of H_μ implies that $\sigma_{\rm p}(H_\mu) = \varnothing$ if $\operatorname{supp}(\mu) \neq \{e\}$. By taking into account Lemma 1.6.3.(b) and Theorem 1.3.6, we infer that the sets $\mathscr{D}_t$ are dense in $\mathcal{H}$ for each $t \geq 0$, and thus the case 2 of Section 1.6 applies. Finally, we mention as a corollary the following spectral result:

Corollary 1.7.2. *Let μ be a symmetric measure on $\mathbb{Z}^d$ with finite support. If one has $\operatorname{supp}(\mu) \neq \{e\}$, then the convolution operator H_μ in $\mathcal{H} := \mathsf{L}^2(\mathbb{Z}^d)$ is purely absolutely continuous.*

1.7.5 $H = h(P)$

Consider in $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^d)$ the dispersive operator $H := h(P)$, where $h \in C^3(\mathbb{R}^d;\mathbb{R})$ satisfies the following condition: For each multi-indices $\alpha,\beta \in \mathbb{N}^d$ with $\alpha > \beta$, $|\alpha| = |\beta| + 1$, and $|\alpha| \leq 3$, we have

$$|\partial^\alpha h| \leq \mathrm{Const.}\big(1 + |\partial^\beta h|\big). \tag{1.34}$$

Note that this class of operators $h(P)$ contains all the usual elliptic free Hamiltonians appearing in physics.

Take for the family $\Phi \equiv (\Phi_1,\dots,\Phi_d)$ the position operators $Q \equiv (Q_1,\dots,Q_d)$. Then we have for each $x \in \mathbb{R}^d$

$$H(x) = \mathrm{e}^{-ix\cdot Q}\,H_\mu\,\mathrm{e}^{ix\cdot Q} = h(P + x),$$

and $H' = h'(P)$. So Assumption 1.2.3 is directly verified and Assumption 1.2.2 follows from (1.34). Therefore all the results of the previous sections are valid. We do not give more details since many aspects of this example, including the existence of time delay, have already been extensively discussed in [111]. We only add some comments in relation with the case 3 of Section 1.6.

Assume that there exist $\lambda \in \mathbb{R}$ and a maximal subset $\Omega \subset \mathbb{R}^d$ of strictly positive Lebesgue measure such that $h(x) = \lambda$ for all $x \in \Omega$. Then any φ in $\mathcal{H}_\Omega := \{\psi \in \mathcal{H} \mid \operatorname{supp}(\mathscr{F}\psi) \subset \Omega\}$ is an eigenvector of $h(P)$ with eigenvalue λ. Furthermore, one has $\mathscr{F}^{-1}\mathcal{H}_\Omega \subset \mathcal{K} \equiv \ker\big(h'(P)^2\big)$, and for simplicity we assume that the first inclusion is an equality. Then, an application of the Fourier transformation shows that $Q_j\mathscr{D}_1 \subset \mathcal{G}$ for each j, where $\mathcal{G}$ is the orthocomplement of $\mathcal{K}$ in $\mathcal{H}$. Thus Remark 1.6.2 applies, and one can consider the restrictions of H and T_f to the subspace $\mathcal{G}$, as described in the case 3 of Section 1.6. In favorable situations, we expect that the restriction of T_f to $\mathcal{G}$ acts as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of the restriction of H to $\mathcal{G}$.

1.7.6 Adjacency operators on admissible graphs

Let $(X, \sim)$ be a graph X with no multiple edges or loops. We write $g \sim h$ whenever the vertices g and h of X are connected. In the Hilbert space $\mathcal{H} := \ell^2(X)$ we consider the adjacency operator

$$(H\varphi)(g) := \sum_{h\sim g} \varphi(h), \quad \varphi \in \mathcal{H},\ g \in X.$$

We denote by $\deg(g) := \#\{h \in X \mid h \sim g\}$ the degree of the vertex g. Under the assumption that $\deg(X) := \sup_{g\in X} \deg(g)$ is finite, H is a bounded self-adjoint operator in $\mathcal{H}$. The spectral analysis of the adjacency operator on some general graphs has been performed in [68]. Here we consider only a subclass of such graphs called admissible graphs.

A directed graph $(X, \sim, <)$ is a graph $(X, \sim)$ and a relation $<$ on the graph such that, for any $g, h \in X$, $g \sim h$ is equivalent to $g < h$ or $h < g$, and one cannot have both $h < g$ and $g < h$. We also write $h > g$ for $g < h$. For a fixed g, we denote by $N^-(g) \equiv \{h \in X \mid g < h\}$ the set of fathers of g and by $N^+(g) \equiv \{h \in X \mid h < g\}$ the set of sons of g. The set $\{h \in X \mid g \sim h\}$ of neighbours of g is denoted by $N(g) \equiv N^-(g) \cup N^+(g)$. When using drawings, one has to choose a direction (an arrow) for any edge. By convention, we set $g \leftarrow h$ if $g < h$, *i.e.* any arrow goes from a son to a father. When directions have been fixed, we use the simpler notation $(X, <)$ for the directed graph $(X, \sim, <)$.

Definition 1.7.3. A directed graph $(X, <)$ is called admissible if

(a) any closed path in X has index zero (the index of a path is the difference between the number of positively oriented edges in the path and that of the negatively oriented ones),

(b) for any $g, h \in X$, one has $\#\{N^-(g) \cap N^-(h)\} = \#\{N^+(g) \cap N^+(h)\}$.

It is proved in [68, Lemma 5.3] that for admissible graphs there exists a unique (up to constant) map $\Phi : X \to \mathbb{Z}$ satisfying $\Phi(h) + 1 = \Phi(g)$ whenever $h < g$. With this choice of operator Φ, one obtains that

$$[H(x)\varphi](g) = \sum_{h\sim g} \mathrm{e}^{ix[\Phi(h)-\Phi(g)]}\,\varphi(h) \tag{1.35}$$

for each $x \in \mathbb{R}$, $\varphi \in \mathcal{H}$, and $g \in X$. Therefore, the commutativity of H and $H(x)$ is equivalent to the condition

$$\sum_{h\in N(g)\cap N(\ell)} \big(\mathrm{e}^{ix[\Phi(\ell)-\Phi(h)]} - \mathrm{e}^{ix[\Phi(h)-\Phi(g)]}\big) = 0$$

for each $g, \ell \in X$. By taking into account the growth property of Φ and Hypothesis (b) of Definition 1.7.3, one obtains that the parts $h \in N^-(g) \cap N^-(\ell)$ and $h \in N^+(g) \cap N^+(\ell)$ of the sum are of opposite sign, and that the parts $h \in N^-(g)\cap N^+(\ell)$ and $h \in N^+(g)\cap N^-(\ell)$ are null. So Assumption 1.2.3 is satisfied. One also verifies by using Formula (1.35) that H belongs to $C^\infty(\Phi)$, and that Assumption 1.2.2 holds. It follows that the general results presented before apply.

Now, the operator H' acts as $(H'\varphi)(g) = i\big(\sum_{h>g}\varphi(h) - \sum_{h<g}\varphi(h)\big)$, and it is proved in [68, Sec. 5] that

$$\begin{aligned}\mathcal{H}_{\mathrm{p}}(H) &= \ker(H)\\ &= \ker(H')\\ &= \Big\{\varphi \in \mathcal{H} \mid \sum_{h>g}\varphi(h) = 0 = \sum_{h<g}\varphi(h) \text{ for each } g \in X\Big\}.\end{aligned} \tag{1.36}$$

It is also proved that H is purely absolutely continuous, except at the origin where it may have an eigenvalue with eigenspace given by (1.36). The proof of these statements is based on the method of the weakly conjugate operator [23].

However, in the present generality, it is hardly possible to obtain a simple description of the set $\kappa(H)$ or the operator T_f. We refer then to [68, Sec. 6] for explicit examples of admissible graphs with adjacency operators whose kernels are either trivial or non trivial, and develop one example for which more explicit computations can be performed. This example furnishes an illustration of the discussion in the case 3 of Section 1.6.

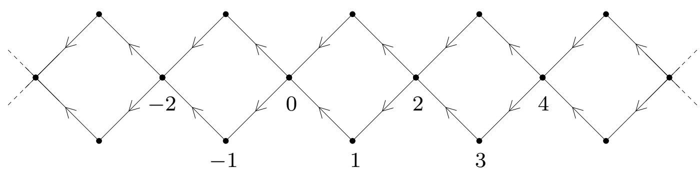

Figure 1.1: Example of an admissible directed graph X

We consider the admissible graph of Figure 1.1, and endow it with the function $\Phi : X \to \mathbb{Z}$ as shown on the picture. The vertices of the graph are denoted by z_- and z_+ when Φ takes an odd value, and by z when Φ takes an even value. More precisely, $\Phi(z) = z$ for z even, and $\Phi(z_-) = \Phi(z_+) = z$ for z odd. By using (1.36), it is easily observed that $\mathcal{K} \equiv \ker\big((H')^2\big)$ is equal to

$$\big\{\varphi \in \mathsf{L}^2(X) \mid \varphi(z) = 0 \text{ for } z \text{ even, and } \varphi(z_-) = -\varphi(z_+) \text{ for } z \text{ odd}\big\}.$$

On the other hand, the orthocomplement $\mathcal{G}$ of $\mathcal{K}$ in $\mathsf{L}^2(X)$ is unitarily equivalent to $\ell^2(\mathbb{Z})$, and the restriction H of H to $\mathcal{G}$ is unitarily equivalent to the operator in $\ell^2(\mathbb{Z})$ defined by

$$\big(\widetilde{\mathsf{H}}\varphi\big)(z) := \sqrt{2}\big\{\varphi(z-1)+\varphi(z+1)\big\}, \qquad \varphi \in \ell^2(\mathbb{Z}).$$

Using the Fourier transformation, one shows that this operator is unitarily equivalent to the multiplication operator M in $\mathsf{L}^2\big((-\pi,\pi]\big)$ given by the function $(-\pi,\pi] \ni \xi \mapsto 2\sqrt{2}\cos(\xi)$.

Now, the operator Φ in $\mathsf{L}^2(X)$ is clearly reduced by the decomposition $\mathcal{K} \oplus \mathcal{G}$. As mentioned in Remark 1.6.2, this implies that the operator T_f is also reduced by this decomposition. By taking Formula (1.33) into account, one obtains that the restriction T_f of T_f to $\mathcal{G}$ is unitarily equivalent to the operator

$$\tfrac{i}{2}\Big\{\tfrac{\mathrm{d}}{\mathrm{d}\xi}\big[-2\sqrt{2}\sin(\xi)\big]^{-1}+\big[-2\sqrt{2}\sin(\xi)\big]^{-1}\tfrac{\mathrm{d}}{\mathrm{d}\xi}\Big\}$$

on $\mathscr{F}\mathscr{D}_1 \subset \mathsf{L}^2\big((-\pi,\pi]\big)$. This implies, as expected, that T_f acts as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H.

1.7.7 Direct integral operators

Let Ω be a measurable subset of $\mathbb{R}^n$ and let us consider a direct integral

$$\mathcal{H} := \int_\Omega^\oplus \mathrm{d}\xi\, \mathcal{H}_\xi,$$

where $\mathrm{d}\xi$ is the usual Lebesgue measure on $\mathbb{R}^n$ and $\mathcal{H}_\xi$ are Hilbert spaces. Take a decomposable self-adjoint operator $H \equiv \int_\Omega^\oplus \mathrm{d}\xi\, H(\xi)$ in $\mathcal{H}$. Assume that there exists a family $\Phi \equiv (\Phi_1,\dots,\Phi_d)$ of operators in $\mathcal{H}$ such that Assumption 1.2.2 is satisfied. Assume also for each $x \in \mathbb{R}^d$ that the operator $H(x)$ defined by (1.9) is decomposable, *i.e.* there exists a family of self-adjoint operators $H(\xi,x)$ in $\mathcal{H}_\xi$ such that $H(x) = \int_\Omega^\oplus \mathrm{d}\xi\, H(\xi,x)$. Finally, assume that the operators $H(\xi)$ and $H(\xi,x)$ commute for each $x \in \mathbb{R}^d$ and *a.e.* $\xi \in \Omega$, so that H and $H(x)$ commute. Then Assumption 1.2.3 holds, and the general theory developed in the preceding sections applies. Moreover, it is easily observed that the fibered structure of the map $x \mapsto H(x)$ implies that the operators H_j' are also decomposable. Therefore, there exists for each $j \in \{1,\dots,d\}$ a family of self-adjoint operators $H_j'(\xi)$ such that $H_j' = \int_\Omega^\oplus \mathrm{d}\xi\, H_j'(\xi)$. In consequence $\lambda \in \mathbb{R}$ is a regular value of H if there exists $\delta > 0$ and $\mathrm{c} < \infty$ such that

$$\lim_{\varepsilon \searrow 0} \big\|\big[\big(H'(\xi)\big)^2+\varepsilon\big]^{-1}E^{H(\xi)}(\lambda;\delta)\big\|_{\mathcal{H}_\xi} < \mathrm{c} \tag{1.37}$$

for *a.e.* $\xi \in \Omega$. We also recall that $\ker\big((H')^2\big) \neq \{0\}$ if and only if there exists a measurable subset $\Omega_0 \subset \Omega$ with positive measure such that $\ker\big(H'(\xi)^2\big) \neq \{0\}$ for each $\xi \in \Omega_0$.

We now give an example of quantum waveguide-type fitting into this setting (see [109] for more details). Let Σ be a bounded open connected set in $\mathbb{R}^m$, and consider in the Hilbert space $\mathsf{L}^2(\Sigma \times \mathbb{R})$ the Dirichlet Laplacian $-\Delta_{\mathrm{D}}$. The partial Fourier transformation along the longitudinal axis sends the initial Hilbert space onto the direct integral $\mathcal{H} := \int_{\mathbb{R}}^\oplus \mathrm{d}\xi\, \mathcal{H}_0$, with $\mathcal{H}_0 := \mathsf{L}^2(\Sigma)$, and it sends $-\Delta_{\mathrm{D}}$ onto the fibered operator $H := \int_{\mathbb{R}}^\oplus \mathrm{d}\xi\, H(\xi)$, with $H(\xi) := \xi^2 - \Delta_{\mathrm{D}}^\Sigma$. Here, $-\Delta_{\mathrm{D}}^\Sigma$ denotes the Dirichlet Laplacian in Σ. By Choosing for Φ

the position operator Q along the longitudinal axis one obtains that $H(x) = \int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi\, H(\xi, x)$ with $H(\xi, x) = (\xi + x)^2 - \Delta_{\mathrm{D}}^{\Sigma}$. Clearly, $H(\xi)$ and $H(\xi, x)$ commute, and so do H and $H(x)$. Furthermore, the operator H is of class $C^\infty(\Phi)$, and H' is the fibered operator given by $H'(\xi) = 2\xi$. It follows that both Assumptions 1.2.2 and 1.2.3 hold, and thus the general theory applies. Now a simple calculation using (1.37) shows that $\kappa(H) = \sigma(-\Delta_{\mathrm{D}}^{\Sigma})$. Furthermore, in the tensorial representation $\mathsf{L}^2(\Sigma) \otimes \mathsf{L}^2(\mathbb{R})$ of $\mathsf{L}^2(\Sigma \times \mathbb{R})$, one obtains that $T_f = T = \frac{1}{4} \otimes (QP^{-1} + P^{-1}Q)$ on the dense set

$$\mathscr{D}_1 = \big\{\varphi \in \mathsf{L}^2(\Sigma) \otimes \mathcal{D}(\langle Q \rangle) \mid \varphi = \eta(-\Delta_{\mathrm{D}})\varphi \text{ for some } \eta \in C_{\mathrm{c}}^\infty\big(\mathbb{R} \setminus \kappa(H)\big)\big\},$$

and T_f is equal to $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of $-\Delta_{\mathrm{D}}$. In [109] it is even shown that the quantum time delay exists and is given by Formula (1.31) for appropriate scattering pairs $\{-\Delta_{\mathrm{D}}, -\Delta_{\mathrm{D}} + V\}$.

Chapter 2

Time delay is a common feature of quantum scattering theory

2.1 Introduction

In quantum scattering theory, there are only few results that are completely model-independent. The simplest one is certainly that the strong limit $\operatorname{s-lim}_{t\to\pm\infty} K\,\mathrm{e}^{-itH}\,P_{\mathrm{ac}}(H)$ vanishes whenever H is a self-adjoint operator in a Hilbert space $\mathcal{H}$, $P_{\mathrm{ac}}(H)$ the projection onto the subspace of absolute continuity of H and K a compact operator in $\mathcal{H}$. Another famous result of this type is RAGE Theorem which establishes propagation estimates for the elements in the continuous subspace of $\mathcal{H}$. At the same level of abstraction, one could also mention the role of H-smooth operators B which lead to estimates of the form $\int_{\mathbb{R}} \mathrm{d}t\,\|B\,\mathrm{e}^{-itH}\,\varphi\|^2 < \infty$ for $\varphi \in \mathcal{H}$.

Our aim in this chapter is to add a new general result to this list. Originally, this result was presented as the existence of global time delay defined in terms of sojourn times and its identity with Eisenbud-Wigner time delay [38, 117]. This identity was proved in different settings by various authors (see [8, 10, 12, 20, 35, 45, 51, 54, 55, 71, 72, 74, 96, 97, 109, 111, 112] and references therein), but a general and abstract statement has never been proposed. Furthermore, it had not been realised until very recently that its proof mainly relies on the general formula relating localisation operators to time operators presented in the previous chapter. Using this formula, we shall prove here that the existence and the identity of the two time delays is in fact a common feature of quantum scattering theory. On the way we shall need to consider a symmetrization procedure [10, 21, 45, 70, 72, 105, 109, 110, 111] which broadly extends the applicability of the theory but which also has the drawback of reducing the physical interpretation of the result.

Quantum scattering theory is mainly a theory of comparison: One fundamental question is whether, given a self-adjoint operator H in a Hilbert space $\mathcal{H}$, one can find a triple $(\mathcal{H}_0, H_0, J)$, with H_0 a self-adjoint operator in an auxiliary Hilbert space $\mathcal{H}_0$ and J a bounded operator from $\mathcal{H}_0$ to $\mathcal{H}$, such that the following strong limits exist

$$W_\pm := \operatorname{s-lim}_{t\to\pm\infty} \mathrm{e}^{itH}\,J\,\mathrm{e}^{-itH_0}\,P_{\mathrm{ac}}(H_0)\ ?$$

Assuming that the operator H_0 is simpler than H, the study of the wave operators $W_\pm$

leads to valuable information on the spectral decomposition of H. Furthermore, if the ranges of both operators $W_\pm$ are equal to $P_{\rm ac}(H)\mathcal{H}$, then the study of the scattering operator $S := W_+^* W_-$ leads to further results on the scattering process. We recall that since S commutes with H_0, S decomposes into a family $\{S(\lambda)\}_{\lambda\in\sigma(H_0)}$ in the spectral representation $\int_{\sigma(H_0)}^{\oplus} \mathrm{d}\lambda\,\mathcal{H}(\lambda)$ of H_0, with $S(\lambda)$ a unitary operator in $\mathcal{H}(\lambda)$ for almost every λ in the spectrum $\sigma(H_0)$ of H_0.

An important additional ingredient when dealing with time delay is a family of position-type operators which permits to define sojourn times, namely, a family of mutually commuting self-adjoint operators $\Phi \equiv (\Phi_1,\dots,\Phi_d)$ in $\mathcal{H}_0$ satisfying two appropriate commutation assumptions with respect to H_0. Roughly speaking, the first one requires that for some $z\in\mathbb{C}\setminus\mathbb{R}$ the map

$$\mathbb{R}^d \ni x \mapsto \mathrm{e}^{-ix\cdot\Phi}(H_0-z)^{-1}\,\mathrm{e}^{ix\cdot\Phi} \in \mathscr{B}(\mathcal{H}_0)$$

is three times strongly differentiable. The second one requires that the family of operators $\mathrm{e}^{-ix\cdot\Phi}\,H_0\,\mathrm{e}^{ix\cdot\Phi}$, $x\in\mathbb{R}^d$, mutually commute. Let also f be any non-negative Schwartz function on $\mathbb{R}^d$ with $f=1$ in a neighbourhood of 0 and $f(-x)=f(x)$ for each $x\in\mathbb{R}^d$. Then, to define the time delay in terms of sojourn times one has to consider for any $r>0$ the expectation values of the localisation operator $f(\Phi/r)$ on the freely evolving state $\mathrm{e}^{-itH_0}\,\varphi$ as well as on the corresponding fully evolving state $\mathrm{e}^{-itH}\,W_-\varphi$. However one immediately faces the problem that the evolution group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ acts in $\mathcal{H}$ whereas $f(\Phi/r)$ is an operator in $\mathcal{H}_0$. As explained in Section 2.4, a general solution for this problem consists in introducing a family $L(t)$ of (identification) operators from $\mathcal{H}$ to $\mathcal{H}_0$ which satisfies some natural requirements (note that in many examples, one can simply take $L(t)=J^*$ for all $t\in\mathbb{R}$). The sojourn time for the evolution group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ is then obtained by considering the expectation value of $f(\Phi/r)$ on the state $L(t)\,\mathrm{e}^{-itH}\,W_-\varphi$. An additional sojourn time naturally appears in this general two Hilbert space setting: the time spent by the scattering state $\mathrm{e}^{-itH}\,W_-\varphi$ inside the time-dependent subset $\big(1-L(t)^*L(t)\big)\mathcal{H}$ of $\mathcal{H}$. Apparently, this sojourn time has never been discussed before in the literature. Finally, the total time delay is defined for fixed r as the integral over the time t of the expectations values involving the fully evolving state $L(t)\,\mathrm{e}^{-itH}\,W_-\varphi$ minus the symmetrized sum of the expectations values involving the freely evolving state $\mathrm{e}^{-itH_0}\,\varphi$ (see Equation (2.8) for a precise definition). Our main result, properly stated in Theorem 2.4.3, is the existence of the limit as $r\to\infty$ of the total time delay and its identity with the Eisenbud-Wigner time delay (see (2.1) below) which we now define in this abstract setting.

Under the mentioned assumptions on Φ and H_0 it has been shown in the previous chapter how a time operator for H_0 can be defined: With the Schwartz function f introduced above, one defines a new function $R_f\in C^\infty\big(\mathbb{R}^d\setminus\{0\}\big)$ and express the time operator in the (oversimplified) form

$$T_f := -\tfrac{1}{2}\big(\Phi\cdot R_f'(H_0')+R_f'(H_0')\cdot\Phi\big),$$

with $R_f' := \nabla R_f$ and $H_0' := \big(i[H_0,\Phi_1],\dots,i[H_0,\Phi_d]\big)$ (see Section 2.3 for details). In suitable situations and in an appropriate sense, the operator T_f acts as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H_0 (for instance, when $H_0=-\Delta$ in $\mathsf{L}^2(\mathbb{R}^d)$, this is verified with Φ the usual family of position operators, see Section 1.7 for details and other examples). Accordingly, it is natural to define in this abstract framework the Eisenbud-Wigner time delay as the expectation value

$$-\langle\varphi, S^*[T_f, S]\varphi\rangle \tag{2.1}$$

for suitable $\varphi \in \mathcal{H}_0$.

The interest of the equality between both definitions of time delay is threefold. It generalises and unifies various results on time delay scattered in the literature. It provides a precise recipe for future investigations on the subject (for instance, for new models in two Hilbert space scattering). And finally, it establishes a relation between the two formulations of scattering theory: Eisenbud-Wigner time delay is a product of the stationary formulation while expressions involving sojourn times are defined using the time dependent formulation. An equality relating these two formulations is always welcome.

In the last section (Section 2.5), we present a sufficient condition for the equality of the symmetrized time delay with the original (unsymmetrized) time delay. The physical interpretation of the latter was, a couple of decades ago, the motivation for the introduction of these concepts.

As a final remark, let us add a comment about the applicability of our abstract result. As already mentioned, most of the existing proofs, if not all, of the existence and the identity of both time delays can be recast in our framework. Furthermore, we are currently working on various new classes of scattering systems for which our approach leads to new results. Among other, we mention the case of scattering theory on manifolds which has recently attracted a lot of attention. Our framework is also general enough for a rigorous approach of time delay in the N-body problem (see [21, 72, 80, 105] for earlier attempts in this direction). However, the verification of our abstract conditions for any non trivial model always require some careful analysis, in particular for the mapping properties of the scattering operator. As a consequence, we prefer to refer to [10, 45, 109, 110, 111] for various incarnations of our approach and to present in this chapter only the abstract framework for the time delay.

2.2 Operators H_0 and Φ

In this section, we recall the framework of the previous chapter on a self-adjoint operator H_0 in a Hilbert space $\mathcal{H}_0$ and its relation with an abstract family $\Phi \equiv (\Phi_1, \dots, \Phi_d)$ of mutually commuting self-adjoint operators in $\mathcal{H}_0$ (we use the term "commute" for operators commuting in the sense of [86, Sec. VIII.5]). In comparison with the notations of the previous chapter, we add an index 0 to all the quantities like the operators, the spaces, *etc.*

In order to express the regularity of H_0 with respect to Φ, we recall from [7] that a self-adjoint operator T with domain $\mathcal{D}(T) \subset \mathcal{H}_0$ is said to be of class $C^1(\Phi)$ if there exists $\omega \in \mathbb{C} \setminus \sigma(T)$ such that the map

$$\mathbb{R}^d \ni x \mapsto \mathrm{e}^{-ix\cdot\Phi}(T-\omega)^{-1}\,\mathrm{e}^{ix\cdot\Phi} \in \mathscr{B}(\mathcal{H}_0)$$

is strongly of class C^1 in $\mathcal{H}_0$. In such a case and for each $j \in \{1, \dots, d\}$, the set $\mathcal{D}(T) \cap \mathcal{D}(\Phi_j)$ is a core for T and the quadratic form $\mathcal{D}(T) \cap \mathcal{D}(\Phi_j) \ni \varphi \mapsto \langle T\varphi, \Phi_j\varphi\rangle - \langle \Phi_j\varphi, T\varphi\rangle$ is continuous in the topology of $\mathcal{D}(T)$. This form extends then uniquely to a continuous quadratic form $[T, \Phi_j]$ on $\mathcal{D}(T)$, which can be identified with a continuous operator from $\mathcal{D}(T)$ to its dual $\mathcal{D}(T)^*$. Finally, the following equality holds:

$$\big[\Phi_j, (T-\omega)^{-1}\big] = (T-\omega)^{-1}[T, \Phi_j](T-\omega)^{-1}.$$

In the sequel, we shall say that $i[T, \Phi_j]$ is essentially self-adjoint on $\mathcal{D}(T)$ if $[T, \Phi_j]\mathcal{D}(T) \subset \mathcal{H}_0$ and if $i[T, \Phi_j]$ is essentially self-adjoint on $\mathcal{D}(T)$ in the usual sense.

Our first main assumption concerns the regularity of H_0 with respect to Φ.

Assumption 2.2.1. *The operator H_0 is of class $C^1(\Phi)$, and for each $j \in \{1, \dots, d\}$, $i[H_0, \Phi_j]$ is essentially self-adjoint on $\mathcal{D}(H_0)$, with its self-adjoint extension denoted by $\partial_j H_0$. The operator $\partial_j H_0$ is of class $C^1(\Phi)$, and for each $k \in \{1, \dots, d\}$, $i[\partial_j H_0, \Phi_k]$ is essentially self-adjoint on $\mathcal{D}(\partial_j H_0)$, with its self-adjoint extension denoted by $\partial_{jk} H_0$. The operator $\partial_{jk} H_0$ is of class $C^1(\Phi)$, and for each $\ell \in \{1, \dots, d\}$, $i[\partial_{jk} H_0, \Phi_\ell]$ is essentially self-adjoint on $\mathcal{D}(\partial_{jk} H_0)$, with its self-adjoint extension denoted by $\partial_{jk\ell} H_0$.*

As shown in Section 1.2, this assumption implies the invariance of $\mathcal{D}(H_0)$ under the action of the unitary group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$. As a consequence, we obtain that each self-adjoint operator

$$H_0(x) := \mathrm{e}^{-ix\cdot\Phi}\, H_0\, \mathrm{e}^{ix\cdot\Phi}$$

has domain $\mathcal{D}[H_0(x)] = \mathcal{D}(H_0)$. Similarly, the domains $\mathcal{D}(\partial_j H_0)$ and $\mathcal{D}(\partial_{jk} H_0)$ are left invariant by the action of the unitary group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$, and the operators $(\partial_j H_0)(x) := \mathrm{e}^{-ix\cdot\Phi}(\partial_j H_0)\,\mathrm{e}^{ix\cdot\Phi}$ and $(\partial_{jk} H_0)(x) := \mathrm{e}^{-ix\cdot\Phi}(\partial_{jk} H_0)\,\mathrm{e}^{ix\cdot\Phi}$ are self-adjoint operators with domains $\mathcal{D}(\partial_j H_0)$ and $\mathcal{D}(\partial_{jk} H_0)$ respectively.

Our second main assumption concerns the family of operators $H_0(x)$.

Assumption 2.2.2. *The operators $H_0(x)$, $x \in \mathbb{R}^d$, mutually commute.*

This assumption is equivalent to the commutativity of each $H_0(x)$ with H_0. As shown in Lemma 1.2.4, Assumptions 2.2.1 and 2.2.2 imply that the operators $H_0(x), (\partial_j H_0)(y)$ and $(\partial_{k\ell} H_0)(z)$ mutually commute for each $j, k, \ell \in \{1, \dots, d\}$ and each $x, y, z \in \mathbb{R}^d$. For simplicity, we write H_0' for the d-tuple $(\partial_1 H_0, \dots, \partial_d H_0)$, and define for each measurable function $g : \mathbb{R}^d \to \mathbb{C}$ the operator $g(H_0')$ by using the d-variables functional calculus. Similarly, we consider the family of operators $\{\partial_{jk} H_0\}$ as the components of a d-dimensional matrix which we denote by H_0''. The symbol $E^{H_0}(\,\cdot\,)$ denotes the spectral measure of H_0, and we use the notation $E^{H_0}(\lambda;\delta)$ for $E^{H_0}\big((\lambda-\delta, \lambda+\delta)\big)$.

We now recall the definition of the critical values of H_0 and state some basic properties which have been established in Lemma 1.2.6.

Definition 2.2.3. *A number $\lambda \in \mathbb{R}$ is called a critical value of H_0 if*

$$\lim_{\varepsilon \searrow 0} \big\| \big(H_0'^2 + \varepsilon\big)^{-1} E^{H_0}(\lambda;\delta) \big\| = +\infty$$

for each $\delta > 0$. We denote by $\kappa(H_0)$ the set of critical values of H_0.

Lemma 2.2.4. *Let H_0 satisfy Assumptions 2.2.1 and 2.2.2. Then the set $\kappa(H_0)$ possesses the following properties:*

(a) $\kappa(H_0)$ *is closed.*

(b) $\kappa(H_0)$ *contains the set of eigenvalues of* H_0.

(c) *The limit* $\lim_{\varepsilon\searrow 0}\big\|\big(H_0'^2+\varepsilon\big)^{-1}E^{H_0}(I)\big\|$ *is finite for each compact set* $I\subset\mathbb{R}\setminus\kappa(H_0)$.

(d) *For each compact set* $I\subset\mathbb{R}\setminus\kappa(H_0)$, *there exists a compact set* $U\subset(0,\infty)$ *such that* $E^{H_0}(I)=E^{|H_0'|}(U)E^{H_0}(I)$.

In Section 1.3 a Mourre estimate is also obtained under Assumptions 2.2.1 and 2.2.2. It implies spectral results for H_0 and the existence of locally H_0-smooth operators. We use the notation $\langle x\rangle:=(1+x^2)^{1/2}$ for any $x\in\mathbb{R}^d$.

Theorem 2.2.5. *Let* H_0 *satisfy Assumptions 2.2.1 and 2.2.2. Then,*

(a) *the spectrum of* H_0 *in* $\sigma(H_0)\setminus\kappa(H_0)$ *is purely absolutely continuous,*

(b) *each operator* $B\in\mathscr{B}\big(\mathcal{D}(\langle\Phi\rangle^{-s}),\mathcal{H}_0\big)$, *with* $s>1/2$, *is locally* H_0*-smooth on* $\mathbb{R}\setminus\kappa(H_0)$.

2.3 Integral formula for H_0

We recall in this section the main result of the previous chapter, which is expressed in terms of a function R_f appearing naturally when dealing with quantum scattering theory. The function R_f is a renormalised average of a function f of localisation around the origin $0\in\mathbb{R}^d$. These functions were already used, in one form or another, in [45, 91, 110, 111]. In these references, part of the results were obtained under the assumption that f belongs to the Schwartz space $\mathscr{S}(\mathbb{R}^d)$. So, for simplicity, we shall assume from the very beginning that $f\in\mathscr{S}(\mathbb{R}^d)$ and also that f is even, *i.e.* $f(x)=f(-x)$ for all $x\in\mathbb{R}^d$. Let us however mention that some of the following results easily extend to the larger class of functions introduced in the previous chapter.

Assumption 2.3.1. *The function* $f\in\mathscr{S}(\mathbb{R}^d)$ *is non-negative, even and equal to* 1 *on a neighbourhood of* $0\in\mathbb{R}^d$.

It is clear that $\text{s-}\lim_{r\to\infty}f(\Phi/r)=1$ if f satisfies Assumption 2.3.1. Furthermore, it also follows from this assumption that the function $R_f:\mathbb{R}^d\setminus\{0\}\to\mathbb{R}$ given by

$$R_f(x):=\int_0^\infty\frac{\mathrm{d}\mu}{\mu}\big(f(\mu x)-\chi_{[0,1]}(\mu)\big)$$

is well-defined. The following properties of R_f are proved in [111, Sec. 2]: The function R_f belongs to $C^\infty(\mathbb{R}^d\setminus\{0\})$ and satisfies

$$R_f'(x)=\int_0^\infty\mathrm{d}\mu\, f'(\mu x)$$

as well as the homogeneity properties $x \cdot R_f'(x) = -1$ and $t^{|\alpha|}(\partial^\alpha R_f)(tx) = (\partial^\alpha R_f)(x)$, where $\alpha \in \mathbb{N}^d$ is a multi-index and $t > 0$. Furthermore, if f is radial, then $R_f'(x) = -x^{-2}x$. We shall also need the function $F_f : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$ defined by

$$F_f(x) := \int_{\mathbb{R}} \mathrm{d}\mu\, f(\mu x). \tag{2.2}$$

The function F_f satisfies several properties as R_f such as $F_f(x) = tF_f(tx)$ for each $t > 0$ and each $x \in \mathbb{R}^d \setminus \{0\}$.

Now, we know from Lemma 2.2.4.(a) that the set $\kappa(H_0)$ is closed. So we can define for each $t \geq 0$ the set

$$\mathscr{D}_t := \big\{\varphi \in \mathcal{D}(\langle\Phi\rangle^t) \mid \varphi = \eta(H_0)\varphi \text{ for some } \eta \in C_{\mathrm{c}}^\infty\big(\mathbb{R} \setminus \kappa(H_0)\big)\big\}.$$

The set $\mathscr{D}_t$ is included in the subspace $\mathcal{H}_{\mathrm{ac}}(H_0)$ of absolute continuity of H_0, due to Theorem 2.2.5.(a), and $\mathscr{D}_{t_1} \subset \mathscr{D}_{t_2}$ if $t_1 \geq t_2$. We refer the reader to Section 1.6 for an account on density properties of the sets $\mathscr{D}_t$.

In the sequel, we sometimes write C^{-1} for an operator C a priori not invertible. In such a case, the operator C^{-1} will always be acting on a set where it is well-defined. Next statement follows from Proposition 1.5.2 and Remark 1.5.4.

Proposition 2.3.2. *Let H_0 satisfy Assumptions 2.2.1 and 2.2.2, and let f satisfy Assumption 2.3.1. Then the map*

$$t_f : \mathscr{D}_1 \to \mathbb{C}, \quad \varphi \mapsto t_f(\varphi) := -\tfrac{1}{2}\sum_j \big\{\big\langle \Phi_j\varphi, (\partial_j R_f)(H_0')\varphi\big\rangle + \big\langle\big(\partial_j R_f\big)(H_0')\varphi, \Phi_j\varphi\big\rangle\big\},$$

is well-defined. Moreover, the linear operator $T_f : \mathscr{D}_1 \to \mathcal{H}_0$ defined by

$$T_f\varphi := -\tfrac{1}{2}\big(\Phi \cdot R_f'(H_0') + R_f'\big(\tfrac{H_0'}{|H_0'|}\big) \cdot \Phi\,|H_0'|^{-1} + iR_f'\big(\tfrac{H_0'}{|H_0'|}\big) \cdot \big(H_0''^{\mathsf{T}} H_0'\big)|H_0'|^{-3}\big)\varphi \tag{2.3}$$

satisfies $t_f(\varphi) = \langle\varphi, T_f\varphi\rangle$ for each $\varphi \in \mathscr{D}_1$. In particular, T_f is a symmetric operator if $\mathscr{D}_1$ is dense in $\mathcal{H}_0$.

Remark 2.3.3. *Formula* (2.3) *is a priori rather complicated and one could be tempted to replace it by the simpler formula $-\frac{1}{2}\big(\Phi \cdot R_f'(H_0') + R_f'(H_0') \cdot \Phi\big)$. Unfortunately, a precise meaning of this expression is not available in general, and its full derivation can only be justified in concrete examples. However, when f is radial, then $(\partial_j R_f)(x) = -x^{-2}x_j$, and T_f is equal on $\mathscr{D}_1$ to*

$$T := \tfrac{1}{2}\big(\Phi \cdot \tfrac{H_0'}{(H_0')^2} + \tfrac{H_0'}{|H_0'|} \cdot \Phi\,|H_0'|^{-1} + \tfrac{iH_0'}{(H_0')^4} \cdot \big(H_0''^{\mathsf{T}} H_0'\big)\big).$$

Next theorem is the main result of the previous chapter; it relates the evolution of the localisation operators $f(\Phi/r)$ to the operator T_f.

Theorem 2.3.4 (Theorem 1.5.5)**.** *Let H_0 satisfy Assumptions 2.2.1 and 2.2.2, and let f satisfy Assumption 2.3.1. Then we have for each $\varphi \in \mathscr{D}_2$*

$$\lim_{r\to\infty} \tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big\langle\varphi, \big(\mathrm{e}^{-itH_0} f(\Phi/r)\,\mathrm{e}^{itH_0} - \mathrm{e}^{itH_0} f(\Phi/r)\,\mathrm{e}^{-itH_0}\big)\varphi\big\rangle = \langle\varphi, T_f\varphi\rangle. \tag{2.4}$$

In particular, when the localisation function f is radial, the operator T_f in the r.h.s. of (2.4) is equal to the operator T, which is independent of f.

2.4 Symmetrized time delay

In this section we prove the existence of symmetrized time delay for a scattering system (H_0, H, J) with free operator H_0, full operator H, and identification operator J. The operator H_0 acts in the Hilbert space $\mathcal{H}_0$ and satisfies the assumptions 2.2.1 and 2.2.2 with respect to the family Φ. The operator H is a self-adjoint operator in a Hilbert space $\mathcal{H}$ satisfying the assumption 2.4.1 below. The operator $J : \mathcal{H}_0 \to \mathcal{H}$ is a bounded operator used to “identify" the Hilbert space $\mathcal{H}_0$ with a subset of $\mathcal{H}$.

The assumption on H concerns the existence, the isometry and the completeness of the generalised wave operators:

Assumption 2.4.1. *The generalised wave operators*

$$W_\pm := \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH} J \,\mathrm{e}^{-itH_0} P_{\rm ac}(H_0)$$

exist, are partial isometries with initial subspaces $\mathcal{H}_0^\pm$ *and final subspaces* $\mathcal{H}_{\rm ac}(H)$.

Sufficient conditions on $JH_0 - HJ$ ensuring the existence and the completeness of $W_\pm$ are given in [118, Chap. 5]. The main consequence of Assumption 2.4.1 is that the scattering operator

$$S := W_+^* W_- : \mathcal{H}_0^- \to \mathcal{H}_0^+$$

is a well-defined unitary operator commuting with H_0.

We now define the sojourn times for the quantum scattering system (H_0, H, J), starting with the sojourn time for the free evolution e^{-itH_0}. So, let $r > 0$ and let f be a non-negative element of $\mathscr{S}(\mathbb{R}^d)$ equal to 1 on a neighbourhood Σ of the origin $0 \in \mathbb{R}^d$. For $\varphi \in \mathscr{D}_0$, we set

$$T_r^0(\varphi) := \int_{\mathbb{R}} \mathrm{d}t \,\big\langle \mathrm{e}^{-itH_0} \varphi, f(\Phi/r)\, \mathrm{e}^{-itH_0} \varphi \big\rangle,$$

where the integral has to be understood as an improper Riemann integral. The operator $f(\Phi/r)$ is approximately the projection onto the subspace $E^\Phi(r\Sigma)\mathcal{H}_0$ of $\mathcal{H}_0$, with $r\Sigma := \{x \in \mathbb{R}^d \mid x/r \in \Sigma\}$. Therefore, if $\|\varphi\| = 1$, then $T_r^0(\varphi)$ can be approximately interpreted as the time spent by the evolving state $\mathrm{e}^{-itH_0} \varphi$ inside $E^\Phi(r\Sigma)\mathcal{H}_0$. Furthermore, the expression $T_r^0(\varphi)$ is finite for each $\varphi \in \mathscr{D}_0$, since we know from Theorem 2.2.5.(b) that each operator $B \in \mathscr{B}\big(\mathcal{D}(\langle\Phi\rangle^{-s}), \mathcal{H}_0\big)$, with $s > \frac{1}{2}$, is locally H_0-smooth on $\mathbb{R} \setminus \kappa(H_0)$.

When defining the sojourn time for the full evolution e^{-itH}, one faces the problem that the localisation operator $f(\Phi/r)$ acts in $\mathcal{H}_0$ while the operator e^{-itH} acts in $\mathcal{H}$. The obvious modification would be to consider the operator $Jf(\Phi/r)J^* \in \mathscr{B}(\mathcal{H})$, but the resulting framework could be not general enough (see Remark 2.4.5 below). Sticking to the basic idea that the freely evolving state $\mathrm{e}^{-itH_0} \varphi$ should approximate, as $t \to \pm\infty$, the corresponding evolving state $\mathrm{e}^{-itH} W_\pm\varphi$, one should look for operators $L(t) : \mathcal{H} \to \mathcal{H}_0$, $t \in \mathbb{R}$, such that

$$\lim_{t\to\pm\infty} \big\|L(t)\, \mathrm{e}^{-itH} W_\pm\varphi - \mathrm{e}^{-itH_0} \varphi\big\| = 0. \tag{2.5}$$

Since we consider vectors $\varphi \in \mathscr{D}_0$, the operators $L(t)$ can be unbounded as long as the products $L(t)E^H(I)$ are bounded for any bounded subset $I \subset \mathbb{R}$. With such a family of operators $L(t)$, it is natural to define the sojourn time for the full evolution e^{-itH} by the expression

$$T_{r,1}(\varphi) := \int_{\mathbb{R}} \mathrm{d}t \left\langle L(t)\,\mathrm{e}^{-itH} W_- \varphi, f(\Phi/r) L(t)\,\mathrm{e}^{-itH} W_- \varphi \right\rangle. \tag{2.6}$$

Another sojourn time appearing naturally in this context is

$$T_2(\varphi) := \int_{\mathbb{R}} \mathrm{d}t \left\langle \mathrm{e}^{-itH} W_- \varphi, \big(1 - L(t)^* L(t)\big)\,\mathrm{e}^{-itH} W_- \varphi \right\rangle_{\mathcal{H}}. \tag{2.7}$$

The finiteness of $T_{r,1}(\varphi)$ and $T_2(\varphi)$ is proved under an additional assumption in Lemma 2.4.2 below. The term $T_{r,1}(\varphi)$ can be approximatively interpreted as the time spent by the scattering state $\mathrm{e}^{-itH} W_- \varphi$, injected in $\mathcal{H}_0$ via $L(t)$, inside $E^{\Phi}(r\Sigma)\mathcal{H}_0$. The term $T_2(\varphi)$ can be seen as the time spent by the scattering state $\mathrm{e}^{-itH} W_- \varphi$ inside the time-dependent subset $\big(1 - L(t)^* L(t)\big)\mathcal{H}$ of $\mathcal{H}$. If $L(t)$ is considered as a time-dependent quasi-inverse for the identification operator J (see [118, Sec. 2.3.2] for the related time-independent notion of quasi-inverse), then the subset $\big(1 - L(t)^* L(t)\big)\mathcal{H}$ can be seen as an approximate complement of $J\mathcal{H}_0$ in $\mathcal{H}$ at time t. When $\mathcal{H}_0 = \mathcal{H}$, one usually sets $L(t) = J^* = 1$, and the term $T_2(\varphi)$ vanishes. Within this general framework, we say that

$$\tau_r(\varphi) := T_r(\varphi) - \tfrac{1}{2}\big\{T_r^0(\varphi) + T_r^0(S\varphi)\big\}, \tag{2.8}$$

with $T_r(\varphi) := T_{r,1}(\varphi) + T_2(\varphi)$, is the symmetrized time delay of the scattering system (H_0, H, J) with incoming state φ. This symmetrized version of the usual time delay

$$\tau_r^{\mathrm{in}}(\varphi) := T_r(\varphi) - T_r^0(\varphi)$$

is known to be the only time delay having a well-defined limit as $r \to \infty$ for complicated scattering systems (see for example [10, 21, 45, 70, 72, 103, 105, 109]).

For the next lemma, we need the auxiliary quantity

$$\tau_r^{\mathrm{free}}(\varphi) := \tfrac{1}{2} \int_0^\infty \mathrm{d}t \left\langle \varphi, S^* \big[\,\mathrm{e}^{itH_0} f(\Phi/r)\,\mathrm{e}^{-itH_0} - \mathrm{e}^{-itH_0} f(\Phi/r)\,\mathrm{e}^{itH_0}, S\big]\varphi \right\rangle, \tag{2.9}$$

which is finite for all $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_0$. We refer the reader to [111, Eq. (4.1)] for a similar definition in the case of dispersive systems, and to [8, Eq. (3)], [55, Eq. (6.2)] and [71, Eq. (5)] for the original definition.

Lemma 2.4.2. *Let H_0, f and H satisfy Assumptions 2.2.1, 2.2.2, 2.3.1 and 2.4.1, and let $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_0$ be such that*

$$\big\|\big(L(t)W_- - 1\big)\,\mathrm{e}^{-itH_0}\varphi\big\| \in \mathsf{L}^1(\mathbb{R}_-, \mathrm{d}t) \quad \text{and} \quad \big\|(L(t)W_+ - 1)\,\mathrm{e}^{-itH_0} S\varphi\big\| \in \mathsf{L}^1(\mathbb{R}_+, \mathrm{d}t). \tag{2.10}$$

Then $T_r(\varphi)$ is finite for each $r > 0$, and

$$\lim_{r\to\infty} \big\{\tau_r(\varphi) - \tau_r^{\mathrm{free}}(\varphi)\big\} = 0. \tag{2.11}$$

Proof. Direct computations with $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_0$ imply that

$$\begin{aligned}
I_r(\varphi) &:= T_{r,1}(\varphi) - \tfrac{1}{2}\big\{T_r^0(\varphi) + T_r^0(S\varphi)\big\} - \tau_r^{\rm free}(\varphi) \\
&= \int_{-\infty}^0 \mathrm{d}t\, \big\{\big\langle L(t)\,\mathrm{e}^{-itH}\,W_-\varphi, f(\Phi/r)L(t)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle \\
&\quad - \big\langle\,\mathrm{e}^{-itH_0}\,\varphi, f(\Phi/r)\,\mathrm{e}^{-itH_0}\,\varphi\big\rangle\big\} \\
&\quad + \int_0^\infty \mathrm{d}t\, \big\{\big\langle L(t)\,\mathrm{e}^{-itH}\,W_-\varphi, f(\Phi/r)L(t)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle \\
&\quad - \big\langle\,\mathrm{e}^{-itH_0}\,S\varphi, f(\Phi/r)\,\mathrm{e}^{-itH_0}\,S\varphi\big\rangle\big\}.
\end{aligned}$$

Using the inequality

$$\big|\|\varphi\|^2 - \|\psi\|^2\big| \le \|\varphi - \psi\| \cdot \big(\|\varphi\| + \|\psi\|\big), \quad \varphi, \psi \in \mathcal{H}_0,$$

the intertwining property of the wave operators and the identity $W_- = W_+S$, one gets the estimates

$$\begin{aligned}
&\big|\big\langle L(t)\,\mathrm{e}^{-itH}\,W_-\varphi, f(\Phi/r)L(t)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle - \big\langle\,\mathrm{e}^{-itH_0}\,\varphi, f(\Phi/r)\,\mathrm{e}^{-itH_0}\,\varphi\big\rangle\big| \\
&\le \mathrm{Const.}\, g_-(t)
\end{aligned}$$

and

$$\begin{aligned}
&\big|\big\langle L(t)\,\mathrm{e}^{-itH}\,W_-\varphi, f(\Phi/r)L(t)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle - \big\langle\,\mathrm{e}^{-itH_0}\,S\varphi, f(\Phi/r)\,\mathrm{e}^{-itH_0}\,S\varphi\big\rangle\big| \\
&\le \mathrm{Const.}\, g_+(t),
\end{aligned}$$

where

$$g_-(t) := \big\|\big(L(t)W_- - 1\big)\,\mathrm{e}^{-itH_0}\,\varphi\big\| \qquad \text{and} \qquad g_+(t) := \big\|\big(L(t)W_+ - 1\big)\,\mathrm{e}^{-itH_0}\,S\varphi\big\|.$$

It follows by (2.10) that $|I_r(\varphi)|$ is bounded by a constant independent of r, and thus $T_{r,1}(\varphi)$ is finite for each $r > 0$. Then, using Lebesgue's dominated convergence theorem, the fact that $\text{s-}\lim_{r\to\infty} f(\Phi/r) = 1$ and the isometry of W_- on $\mathcal{H}_0^-$, one obtains that

$$\begin{aligned}
\lim_{r\to\infty} I_r(\varphi) &= \int_{-\infty}^0 \mathrm{d}t\, \big\{\big\langle L(t)\,\mathrm{e}^{-itH}\,W_-\varphi, L(t)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle - \big\langle\,\mathrm{e}^{-itH_0}\,\varphi, \mathrm{e}^{-itH_0}\,\varphi\big\rangle\big\} \\
&\quad + \int_0^\infty \mathrm{d}t\, \big\{\big\langle L(t)\,\mathrm{e}^{-itH}\,W_-\varphi, L(t)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle - \big\langle\,\mathrm{e}^{-itH_0}\,S\varphi, \mathrm{e}^{-itH_0}\,S\varphi\big\rangle\big\} \\
&= \int_{\mathbb{R}} \mathrm{d}t\, \big\langle\,\mathrm{e}^{-itH}\,W_-\varphi, \big(L(t)^*L(t) - 1\big)\,\mathrm{e}^{-itH}\,W_-\varphi\big\rangle_{\mathcal{H}} \\
&\equiv -T_2(\varphi).
\end{aligned}$$

Thus, $T_2(\varphi)$ is finite, and the equality (2.11) is verified. Since $T_r(\varphi) = T_{r,1}(\varphi) + T_2(\varphi)$, one also infers that $T_r(\varphi)$ is finite for each $r > 0$. □

Next Theorem shows the existence of the symmetrized time delay. It is a direct consequence of Lemma 2.4.2, Definition (2.9) and Theorem 2.3.4. The apparently large number of assumptions reflects nothing more but the need of describing the very general scattering system (H_0, H, J); one needs hypotheses on the relation between H_0 and Φ, conditions on the localisation function f, a compatibility assumption between H_0 and H, and conditions on the state φ on which the calculations are performed.

Theorem 2.4.3. *Let H_0, f and H satisfy Assumptions 2.2.1, 2.2.2, 2.3.1 and 2.4.1, and let $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_2$ satisfy $S\varphi \in \mathscr{D}_2$ and* (2.10)*. Then one has*

$$\lim_{r\to\infty} \tau_r(\varphi) = -\big\langle \varphi, S^*\big[T_f, S\big]\varphi\big\rangle, \tag{2.12}$$

with T_f defined by (2.3)*.*

Remark 2.4.4. *Theorem 2.4.3 is the main result of this chapter. It expresses the identity of the symmetrized time delay (defined in terms of sojourn times) and the Eisenbud-Wigner time delay for general scattering systems (H_0, H, J). The l.h.s. of* (2.12) *is equal to the global symmetrized time delay of the scattering system (H_0, H, J), with incoming state φ, in the dilated regions associated to the localisation operators $f(\Phi/r)$. The r.h.s. of* (2.12) *is the expectation value in φ of the generalised Eisenbud-Wigner time delay operator $-S^*[T_f, S]$. When T_f acts in the spectral representation of H_0 as the differential operator $i\frac{\mathrm{d}}{\mathrm{d}H_0}$, which occurs in most of the situations of interest (see for example Section 1.7), one recovers the usual Eisenbud-Wigner Formula:*

$$\lim_{r\to\infty} \tau_r(\varphi) = -\big\langle \varphi, iS^* \tfrac{\mathrm{d}S}{\mathrm{d}H_0}\,\varphi\big\rangle.$$

Remark 2.4.5. *Equation* (2.5) *is equivalent to the existence of the limits*

$$\widetilde{W}_\pm := \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH_0} L(t)\, \mathrm{e}^{-itH} P_{\mathrm{ac}}(H),$$

together with the equalities $\widetilde{W}_\pm W_\pm = P_0^\pm$, where $P_0^\pm$ are the orthogonal projections on the subspaces $\mathcal{H}_0^\pm$ of $\mathcal{H}_0$. In simple situations, namely, when $\mathcal{H}_0^\pm = \mathcal{H}_{\mathrm{ac}}(H_0)$ and $L(t) \equiv L$ is independent of t and bounded, sufficient conditions implying (2.5) *are given in [118, Thm. 2.3.6]. In more complicated situations, namely, when $\mathcal{H}_0^\pm \neq \mathcal{H}_{\mathrm{ac}}(H_0)$ or $L(t)$ depends on t and is unbounded, the proof of* (2.5) *could be highly non-trivial. This occurs for instance in the case of the N-body systems. In such a situation, the operators $L(t)$ really depend on t and are unbounded (see for instance [36, Sec. 6.7]), and the proof of* (2.5) *is related to the problem of the asymptotic completeness of the N-body systems.*

2.5 Usual time delay

We give in this section conditions under which the symmetrized time delay $\tau_r(\varphi)$ and the usual time delay $\tau_r^{\mathrm{in}}(\varphi)$ are equal in the limit $r \to \infty$. Heuristically, one cannot expect that this equality holds if the scattering is not elastic or is of multichannel type. However, for simple scattering systems, the equality of both time delays presents an interest. At the mathematical level, this equality reduces to giving conditions under which

$$\lim_{r\to\infty} \big\{T_r^0(S\varphi) - T_r^0(\varphi)\big\} = 0. \tag{2.13}$$

Equation (2.13) means that the freely evolving states $\mathrm{e}^{-itH_0}\,\varphi$ and $\mathrm{e}^{-itH_0}\,S\varphi$ tend to spend the same time within the region defined by the localisation function $f(\Phi/r)$ as $r \to \infty$. Formally, the argument goes as follows. Suppose that $F_f(H_0')$, with F_f defined in (2.2), commutes with the scattering operator S. Then, using the change of variables $\mu := t/r$, $\nu := 1/r$, and the symmetry of f, one gets

$$\begin{aligned}
&\lim_{r\to\infty} \big\{T_r^0(S\varphi) - T_r^0(\varphi)\big\} \\
&= \lim_{r\to\infty} \int_{\mathbb{R}} \mathrm{d}t \, \big\langle \varphi, S^*[\mathrm{e}^{itH_0} f(\Phi/r)\,\mathrm{e}^{-itH_0}, S]\varphi\big\rangle - \big\langle \varphi, S^*[F_f(H_0'), S]\varphi\big\rangle \\
&= \lim_{\nu\searrow 0} \int_{\mathbb{R}} \mathrm{d}\mu \, \big\langle \varphi, S^*\big[\tfrac{1}{\nu}\big\{f(\mu H_0' + \nu\Phi) - f(\mu H_0')\big\}, S\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}} \mathrm{d}\mu \, \big\langle \varphi, S^*[\Phi \cdot f'(\mu H_0'), S]\varphi\big\rangle \\
&= 0.
\end{aligned}$$

A rigorous proof of this argument is given in Theorem 2.5.3 below. Before this we introduce an assumption on the behavior of the C_0-group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$ in $\mathcal{D}(H_0)$, and then prove a technical lemma. We use the notation $\mathcal{G}$ for $\mathcal{D}(H_0)$ endowed with the graph topology, and $\mathcal{G}^*$ for its dual space. In the following proofs, we also freely use the notations of [7] for some regularity classes with respect to the group generated by Φ.

Assumption 2.5.1. *The C_0-group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$ is of polynomial growth in $\mathcal{G}$, namely there exists $r > 0$ such that for all $x \in \mathbb{R}^d$*

$$\big\|\mathrm{e}^{ix\cdot\Phi}\big\|_{\mathscr{B}(\mathcal{G},\mathcal{G})} \le \mathrm{Const.}\,\langle x\rangle^r.$$

Lemma 2.5.2. *Let H_0 and Φ satisfy Assumptions 2.2.1, 2.2.2 and 2.5.1, and let $\eta \in C_{\mathrm{c}}^\infty(\mathbb{R})$. Then there exists $\mathrm{c}, s > 0$ such that for all $\mu \in \mathbb{R}$, $x \in \mathbb{R}^d$ and $\nu \in (-1,1)\setminus\{0\}$*

$$\big\|\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x) - H_0]} - \eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\big\| \le \mathrm{c}\,(1+|\mu|)\langle x\rangle^s.$$

Proof. For $x \in \mathbb{R}^d$ and $\mu \in \mathbb{R}$, we define the function

$$g_{x,\mu} : (-1,1)\setminus\{0\} \to \mathscr{B}(\mathcal{H}_0), \quad \nu \mapsto \mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x) - H_0]}\,\eta(H_0).$$

Reproducing the argument of point (ii) of the proof of Theorem 1.5.5, one readily shows that $H_0 \in C_{\mathrm{u}}^1(\Phi; \mathcal{G}, \mathcal{H}_0)$, and then that $g_{x,\mu}$ is continuous with

$$g_{x,\mu}(0) := \lim_{\nu\to 0} g_{x,\mu}(\nu) = \mathrm{e}^{i\mu x\cdot H_0'}\,\eta(H_0).$$

On another hand, since $\eta(H_0)$ belongs to $C_{\mathrm{u}}^1(\Phi)$, one has in $\mathscr{B}(\mathcal{H}_0)$ the equalities

$$\begin{aligned}
\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big) - \eta(H_0)\big\} &= \frac{1}{\nu}\int_0^1 \mathrm{d}t \, \frac{\mathrm{d}}{\mathrm{d}t}\eta\big(H_0(t\nu x)\big) \\
&= i\sum_j x_j \int_0^1 \mathrm{d}t \ \mathrm{e}^{-it\nu x\cdot\Phi}\,\big[\eta(H_0), \Phi_j\big]\,\mathrm{e}^{it\nu x\cdot\Phi}.
\end{aligned}$$

So, combining the two equations, one obtains that

$$\begin{aligned}
&\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]} - \eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\\
&= \tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big) - \eta(H_0)\big\}\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]} + \tfrac{1}{\nu}\big\{g_{x,\mu}(\nu) - g_{x,\mu}(0)\big\}\\
&= i\sum_j x_j\int_0^1 \mathrm{d}t\ \mathrm{e}^{-it\nu x\cdot\Phi}\,\big[\eta(H_0),\Phi_j\big]\,\mathrm{e}^{it\nu x\cdot\Phi}\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]} + \tfrac{1}{\nu}\big\{g_{x,\mu}(\nu) - g_{x,\mu}(0)\big\}.
\end{aligned} \tag{2.14}$$

In order to estimate the difference $g_{x,\mu}(\nu) - g_{x,\mu}(0)$, observe first that one has in $\mathscr{B}(\mathcal{H}_0)$ for any bounded set $I \subset \mathbb{R}$

$$\tfrac{1}{\nu}\big[H_0(\nu x) - H_0\big]E^{H_0}(I) = \tfrac{1}{\nu}\int_0^1 \mathrm{d}t\,\frac{\mathrm{d}}{\mathrm{d}t}H_0(t\nu x)E^{H_0}(I) = \int_0^1 \mathrm{d}t\,x\cdot H_0'(t\nu x)E^{H_0}(I).$$

So, if $\varepsilon \in \mathbb{R}$ is small enough and if the bounded set $I \subset \mathbb{R}$ is chosen such that $\eta(H_0) = E^{H_0}(I)\eta(H_0)$, one obtains in $\mathscr{B}(\mathcal{H}_0)$

$$\begin{aligned}
&g_{x,\mu}(\nu+\varepsilon) - g_{x,\mu}(\nu)\\
&= \big\{\,\mathrm{e}^{i\mu\int_0^1 \mathrm{d}t\,x\cdot H_0'(t(\nu+\varepsilon)x)E^{H_0}(I)} - \mathrm{e}^{i\mu\int_0^1 \mathrm{d}t\,x\cdot H_0'(t\nu x)E^{H_0}(I)}\,\big\}\eta(H_0)\\
&= \mathrm{e}^{i\mu\int_0^1 \mathrm{d}u\,x\cdot H_0'(u\nu x)E^{H_0}(I)}\,\big\{\,\mathrm{e}^{i\mu\int_0^1 \mathrm{d}t\,x\cdot[H_0'(t(\nu+\varepsilon)x)-H_0'(t\nu x)]E^{H_0}(I)} - 1\big\}\eta(H_0)\\
&= \mathrm{e}^{i\mu\int_0^1 \mathrm{d}u\,x\cdot H_0'(u\nu x)E^{H_0}(I)}\,\big\{\,\mathrm{e}^{i\mu\int_0^1 \mathrm{d}t\int_0^1 \mathrm{d}s\,t\varepsilon\sum_{j,k}x_jx_k(\partial_{jk}H_0)(t(\nu+s\varepsilon)x)E^{H_0}(I)} - 1\big\}\eta(H_0).
\end{aligned}$$

Note that the property $\partial_j H_0 \in C^1_{\mathrm{u}}(\Phi;\mathcal{G},\mathcal{H}_0)$ (which follows from Assumption 2.2.1 and [7, Lemma 5.1.2.(b)]) has been taken into account for the last equality. Then, multiplying the above expression by ε^{-1} and taking the limit $\varepsilon \to 0$ in $\mathscr{B}(\mathcal{H}_0)$ leads to

$$g_{x,\mu}'(\nu) = i\mu\,\mathrm{e}^{i\mu\int_0^1 \mathrm{d}u\,x\cdot H_0'(u\nu x)}\int_0^1 \mathrm{d}t\,t\sum_{j,k}x_jx_k(\partial_{jk}H_0)(t\nu x)\,\eta(H_0). \tag{2.15}$$

This formula, together with Equation (2.14) and the mean value theorem, implies that

$$\begin{aligned}
&\big\|\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]} - \eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\big\|\\
&\le \mathrm{Const.}\,|x| + \sup_{\xi\in[0,1]}\big\|g_{x,\mu}'(\xi\nu)\big\|\\
&\le \mathrm{Const.}\,|x| + \mathrm{Const.}\,x^2|\mu|\sup_{\xi\in[0,1]}\sum_{j,k}\big\|(\partial_{jk}H_0)(\xi\nu x)\,\eta(H_0)\big\|.
\end{aligned} \tag{2.16}$$

But one has

$$(\partial_{jk}H_0)(\xi\nu x)\,\eta(H_0) = \mathrm{e}^{-i\xi\nu x\cdot\Phi}(\partial_{jk}H_0)\,\mathrm{e}^{i\xi\nu x\cdot\Phi}\,\eta(H_0)$$

with $\eta(H_0) \in \mathscr{B}(\mathcal{H}_0,\mathcal{G})$ and $(\partial_{jk}H_0) \in \mathscr{B}(\mathcal{G},\mathcal{H}_0)$. So, it follows from Assumption 2.5.1 that there exists $r > 0$ such that

$$\big\|(\partial_{jk}H_0)(\xi\nu x)\,\eta(H_0)\big\| \le \mathrm{Const.}\,\langle\xi\nu x\rangle^r.$$

Hence, one finally gets from (2.16) that for each $\nu \in (-1,1)\setminus\{0\}$

$$\big\|\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]} - \eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\big\| \le \mathrm{Const.}(1+|\mu|)\langle x\rangle^{r+2},$$

which proves the claim with $s := r+2$. □

In the sequel, the symbol $\mathscr{F}$ stands for the Fourier transformation, and the measure $\underline{\mathrm{d}}x$ on $\mathbb{R}^d$ is chosen so that $\mathscr{F}$ extends to a unitary operator in $\mathsf{L}^2(\mathbb{R}^d)$.

Theorem 2.5.3. *Let H_0, f, H and Φ satisfy Assumptions 2.2.1, 2.2.2, 2.3.1, 2.4.1 and 2.5.1, and let $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_2$ satisfy $S\varphi \in \mathscr{D}_2$ and*

$$\big[F_f(H_0'), S\big]\varphi = 0. \tag{2.17}$$

Then the following equality holds:

$$\lim_{r\to\infty} \big\{T_r^0(S\varphi) - T_r^0(\varphi)\big\} = 0.$$

Note that the l.h.s. of (2.17) is well-defined due to the homogeneity property of F_f. Indeed, one has

$$\big[F_f(H_0'), S\big]\varphi = \big[|H_0'|^{-1}\eta(H_0)F_f\big(\tfrac{H_0'}{|H_0'|}\big), S\big]\varphi$$

for some $\eta \in C_c^\infty\big(\mathbb{R}\setminus\kappa(H_0)\big)$, and thus $\big[F_f(H_0'), S\big]\varphi \in \mathcal{H}$ due to Lemma 2.2.4.(d) and the compacity of $F_f(\mathbb{S}^{d-1})$.

Proof. Let $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_2$ satisfies $S\varphi \in \mathscr{D}_2$, take a real $\eta \in C_c^\infty\big(\mathbb{R}\setminus\kappa(H_0)\big)$ such that $\varphi = \eta(H_0)\varphi$, and set $\eta_t(H_0) := \mathrm{e}^{itH_0}\eta(H_0)$. Using (2.17), the definition of F_f and the change of variables $\mu := t/r$, $\nu := 1/r$, one gets

$$\begin{aligned}
&T_{1/\nu}^0(S\varphi) - T_{1/\nu}^0(\varphi)\\
&= \int_{\mathbb{R}} \mathrm{d}\mu\, \big\langle\varphi, S^*\big[\tfrac{1}{\nu}\big\{\eta_{\frac{\mu}{\nu}}(H_0)f(\nu\Phi)\eta_{-\frac{\mu}{\nu}}(H_0) - f(\mu H_0')\big\}, S\big]\varphi\big\rangle\\
&= \int_{\mathbb{R}} \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, (\mathscr{F}f)(x)\big\langle\varphi, S^*\big[\tfrac{1}{\nu}\big\{\mathrm{e}^{i\nu x\cdot\Phi}\,\eta_{\frac{\mu}{\nu}}\big(H_0(\nu x)\big)\eta_{-\frac{\mu}{\nu}}(H_0) - \mathrm{e}^{i\mu x\cdot H_0'}\big\}, S\big]\varphi\big\rangle\\
&= \int_{\mathbb{R}} \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, (\mathscr{F}f)(x)\big\langle\varphi, S^*\big[\tfrac{1}{\nu}(\mathrm{e}^{i\nu x\cdot\Phi} - 1)\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]}, S\big]\varphi\big\rangle \qquad (2.18)\\
&\quad+ \int_{\mathbb{R}} \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, (\mathscr{F}f)(x)\big\langle\varphi, S^*\big[\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]} - \eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}, S\big]\varphi\big\rangle.
\end{aligned}$$

To prove the statement, it is sufficient to show that the limit as $\nu \searrow 0$ of each of these two terms is equal to zero. This is done in points (i) and (ii) below.

(i) For the first term, one can easily adapt the method presented in the proof of Theorem 1.5.5, points (ii) and (iii), in order to apply Lebesgue's dominated convergence theorem to (2.18). So, one gets

$$\begin{aligned}
&\lim_{\nu\searrow 0} \int_{\mathbb{R}} \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, (\mathscr{F}f)(x)\big\langle\varphi, S^*\big[\tfrac{1}{\nu}(\mathrm{e}^{i\nu x\cdot\Phi} - 1)\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]}, S\big]\varphi\big\rangle\\
&= i\int_{\mathbb{R}} \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, (\mathscr{F}f)(x)\big\{\big\langle(x\cdot\Phi)S\varphi, \mathrm{e}^{i\mu x\cdot H_0'}\,S\varphi\big\rangle - \big\langle(x\cdot\Phi)\varphi, \mathrm{e}^{i\mu x\cdot H_0'}\,\varphi\big\rangle\big\},
\end{aligned}$$

and the change of variables $\mu' := -\mu$, $x' := -x$, together with the symmetry of f, implies that this expression is equal to zero.

(ii) For the second term, it is sufficient to prove that

$$\lim_{\nu\searrow 0}\int_{\mathbb{R}}\mathrm{d}\mu\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi,\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]}-\eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\psi\big\rangle \tag{2.19}$$

is equal to zero for any $\psi\in\mathscr{D}_2$ satisfying $\eta(H_0)\psi=\psi$. For the moment, let us assume that we can interchange the limit and the integrals in (2.19) by invoking Lebesgue's dominated convergence theorem. Then, taking Equations (2.14) and (2.15) into account, one obtains

$$\begin{aligned}&\lim_{\nu\searrow 0}\int_{\mathbb{R}}\mathrm{d}\mu\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi,\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]}-\eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\psi\big\rangle\\ &=\int_{\mathbb{R}}\mathrm{d}\mu\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi,\big\{i\big[\eta(H_0),x\cdot\Phi\big]\,\mathrm{e}^{i\mu x\cdot H_0'}\\ &\quad+\tfrac{i\mu}{2}\,\mathrm{e}^{i\mu x\cdot H_0'}\textstyle\sum_{j,k}x_jx_k(\partial_{jk}H_0)\,\eta(H_0)\big\}\psi\big\rangle,\end{aligned}$$

and the change of variables $\mu':=-\mu$, $x':=-x$, together with the symmetry of f, implies that this expression is equal to zero. So, it only remains to show that one can really apply Lebesgue's dominated convergence theorem in order to interchange the limit and the integrals in (2.19). For this, let us set for $\nu\in(-1,1)\setminus\{0\}$ and $\mu\in\mathbb{R}$

$$L(\nu,\mu):=\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi,\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\,\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]}-\eta(H_0)\,\mathrm{e}^{i\mu x\cdot H_0'}\big\}\psi\big\rangle.$$

By using Lemma 2.5.2 and the fact that $\mathscr{F}f\in\mathscr{S}(\mathbb{R}^d)$, one gets that $|L(\nu,\mu)|\le\mathrm{Const.}\,(1+|\mu|)$ with a constant independent of ν. Therefore $|L(\nu,\mu)|$ is bounded uniformly in $\nu\in(-1,1)\setminus\{0\}$ by a function in $\mathsf{L}^1([-1,1],\mathrm{d}\mu)$.

For the case $|\mu|>1$, we first remark that there exists a compact set $I\subset\mathbb{R}\setminus\kappa(H_0)$ such that $\eta(H_0)=E^{H_0}(I)\eta(H_0)$. Due to Lemma 2.2.4.(d), there also exists $\zeta\in C_{\mathrm{c}}^\infty\big((0,\infty)\big)$ such that

$$\eta\big(H_0(\nu x)\big)=\eta\big(H_0(\nu x)\big)\zeta\big(H_0'(\nu x)^2\big)$$

for all $x\in\mathbb{R}^d$ and $\nu\in\mathbb{R}$. So, using the notations

$$A^I_{\nu,\mu}(x):=\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]}\,E^{H_0}(I)\equiv\mathrm{e}^{i\frac{\mu}{\nu}[H_0(\nu x)-H_0]E^{H_0}(I)}\,E^{H_0}(I)$$

and

$$B^I_\mu(x):=\mathrm{e}^{i\mu x\cdot H_0'}\,E^{H_0}(I)\equiv\mathrm{e}^{i\mu x\cdot H_0'E^{H_0}(I)}\,E^{H_0}(I),$$

one can rewrite $L(\nu,\mu)$ as

$$\begin{aligned}&L(\nu,\mu)\\ &=\int_{\mathbb{R}^d}\underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi,\tfrac{1}{\nu}\big\{\eta\big(H_0(\nu x)\big)\zeta\big(H_0'(\nu x)^2\big)A^I_{\nu,\mu}(x)-\eta(H_0)\zeta(H_0'^2)B^I_\mu(x)\big\}\psi\big\rangle.\end{aligned}$$

Now, using the same technics as in the proof of Lemma 2.5.2, one shows that the maps $A^I_{\nu,\mu}:\mathbb{R}^d\to\mathscr{B}(\mathcal{H}_0)$ and $B^I_\mu:\mathbb{R}^d\to\mathscr{B}(\mathcal{H}_0)$ are differentiable, with derivatives

$$\big(\partial_jA^I_{\nu,\mu}\big)(x)=i\mu(\partial_jH_0)(\nu x)\,A^I_{\nu,\mu}(x)\qquad\text{and}\qquad\big(\partial_jB^I_\mu\big)(x)=i\mu(\partial_jH_0)\,B^I_\mu(x).$$

Thus, setting

$$C_j := (H_0')^{-2}\zeta(H_0'^2)(\partial_j H_0)\,\eta(H_0) \in \mathscr{B}(\mathcal{H}_0) \qquad \text{and} \qquad V_x := \mathrm{e}^{-ix\cdot\Phi},$$

one can even rewrite $L(\nu,\mu)$ as

$$L(\nu,\mu) = (i\mu)^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi, \tfrac{1}{\nu}\big\{V_{\nu x}C_jV_{\nu x}^*\big(\partial_j A^I_{\nu,\mu}\big)(x) - C_j\big(\partial_j B^I_\mu\big)(x)\big\}\psi\big\rangle.$$

We shall now use repeatedly the following argument: Let $g \in \mathscr{S}(\mathbb{R}^n)$ and let $X := (X_1,\dots,X_n)$ be a family of self-adjoint and mutually commuting operators in $\mathcal{H}_0$. If all X_j are of class $C^2(\Phi)$, then the operator $g(X)$ belongs to $C^2(\Phi)$, and $\big[[g(X),\Phi_j],\Phi_k\big] \in \mathscr{B}(\mathcal{H}_0)$ for all j,k. Such a statement has been proved in Proposition 1.5.1 in a greater generality. Here, the operator C_j is of the type $g(X)$, since all the operators $H_0, \partial_j H_0, \dots, \partial_d H_0$ are of class $C^2(\Phi)$. Thus, we can perform a first integration by parts (with vanishing boundary contributions) with respect to x_j to obtain

$$\begin{aligned} L(\nu,\mu) = &-(i\mu)^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big[\partial_j(\mathscr{F}f)\big](x)\big\langle\psi, \tfrac{1}{\nu}\big\{V_{\nu x}C_jV_{\nu x}^*A^I_{\nu,\mu}(x) - C_jB^I_\mu(x)\big\}\psi\big\rangle \\ &- \mu^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi, V_{\nu x}[C_j,\Phi_j]V_{\nu x}^*A^I_{\nu,\mu}(x)\psi\big\rangle. \end{aligned}$$

Now, the scalar product in the first term can be written as

$$(i\mu)^{-1}\big\langle\psi, \tfrac{1}{\nu}\big\{V_{\nu x}DV_{\nu x}^*\big(\partial_j A^I_{\nu,\mu}\big)(x) - D\big(\partial_j B^I_\mu\big)(x)\big\}\psi\big\rangle$$

with $D := (H_0')^{-2}\zeta(H_0'^2)\,\eta(H_0) \in \mathscr{B}(\mathcal{H}_0)$. Thus, a further integration by parts leads to

$$L(\nu,\mu) = -\mu^{-2}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big[\partial_j^2(\mathscr{F}f)\big](x)\big\langle\psi, \tfrac{1}{\nu}\big\{V_{\nu x}DV_{\nu x}^*A^I_{\nu,\mu}(x) - DB^I_\mu(x)\big\}\psi\big\rangle \tag{2.20}$$

$$- i\mu^{-2}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big[\partial_j(\mathscr{F}f)\big](x)\big\langle\psi, V_{\nu x}[D,\Phi_j]V_{\nu x}^*A^I_{\nu,\mu}(x)\psi\big\rangle \tag{2.21}$$

$$- \mu^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle\psi, V_{\nu x}[C_j,\Phi_j]V_{\nu x}^*A^I_{\nu,\mu}(x)\psi\big\rangle. \tag{2.22}$$

By setting $E_k := (H_0')^{-4}\zeta(H_0'^2)(\partial_k H_0)\ \eta(H_0) \in \mathscr{B}(\mathcal{H}_0)$ and by performing a further integration by parts, one obtains that (2.20) is equal to

$$\begin{aligned} &i\mu^{-3}\sum_{j,k} \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big[\partial_j^2(\mathscr{F}f)\big](x)\big\langle\psi, \tfrac{1}{\nu}\big\{V_{\nu x}E_kV_{\nu x}^*\big(\partial_k A^I_{\nu,\mu}\big)(x) - E_k\big(\partial_k B^I_\mu\big)(x)\big\}\psi\big\rangle \\ &= -i\mu^{-3}\sum_{j,k} \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big[\partial_k\partial_j^2(\mathscr{F}f)\big](x)\big\langle\psi, \tfrac{1}{\nu}\big\{V_{\nu x}E_kV_{\nu x}^*A^I_{\nu,\mu}(x) - E_kB^I_\mu(x)\big\}\psi\big\rangle \\ &\quad + \mu^{-3}\sum_{j,k} \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,\big[\partial_j^2(\mathscr{F}f)\big](x)\big\langle\psi, V_{\nu x}[E_k,\Phi_k]V_{\nu x}^*A^I_{\nu,\mu}(x)\psi\big\rangle. \end{aligned}$$

By mimicking the proof of Lemma 2.5.2, with $\eta(H_0)$ replaced by E_k, one obtains that there exist $\mathrm{C}, s > 0$ such that for all $|\mu| > 1$, $x \in \mathbb{R}^d$ and $\nu \in (-1,1) \setminus \{0\}$

$$\big\|\tfrac{1}{\nu}\big\{V_{\nu x} E_k V_{\nu x}^* A^I_{\nu,\mu}(x) - E_k B^I_\mu(x)\big\}\big\| \le \mathrm{C}\,(1+|\mu|)\langle x\rangle^s.$$

So, the terms (2.20) and (2.21) can be bounded uniformly in $\nu \in (-1,1)\setminus\{0\}$ by a function in $\mathsf{L}^1\big(\mathbb{R}\setminus[-1,1],\mathrm{d}\mu\big)$. For the term (2.22), a direct calculation shows that it can be written as

$$-i\mu^{-2}\sum_{j,k}\int_{\mathbb{R}} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle V_{\nu x}^*\psi, [C_j,\Phi_j] V_{\nu x}^* C_k V_{\nu x}\big(\partial_k A^I_{\nu,-\mu}\big)(-x) V_{\nu x}^*\psi\big\rangle.$$

So, doing once more an integration by parts with respect to x_k, one also obtains that this term is bounded uniformly in $\nu \in (-1,1)\setminus\{0\}$ by a function in $\mathsf{L}^1\big(\mathbb{R}\setminus[-1,1],\mathrm{d}\mu\big)$.

The last estimates, together with our previous estimate for $|\mu| \le 1$, show that $|L(\nu,\mu)|$ is bounded uniformly in $|\nu| < 1$ by a function in $\mathsf{L}^1(\mathbb{R},\mathrm{d}\mu)$. So, one can interchange the limit $\nu \searrow 0$ and the integration over μ in (2.19). The interchange of the limit $\nu \searrow 0$ and the integration over x in (2.19) is justified by the bound obtained in Lemma 2.5.2. □

The existence of the usual time delay is now a direct consequence of Theorems 2.4.3 and 2.5.3:

Theorem 2.5.4. *Let H_0, f, H and Φ satisfy Assumptions 2.2.1, 2.2.2, 2.3.1, 2.4.1 and 2.5.1. Let $\varphi \in \mathcal{H}_0^- \cap \mathscr{D}_2$ satisfy $S\varphi \in \mathscr{D}_2$,* (2.10) *and* (2.17)*. Then one has*

$$\lim_{r\to\infty}\tau_r^{\mathrm{in}}(\varphi) = \lim_{r\to\infty}\tau_r(\varphi) = -\big\langle\varphi, S^*\big[T_f,S\big]\varphi\big\rangle,$$

with T_f defined by (2.3).

Remark 2.5.5. *In $\mathsf{L}^2(\mathbb{R}^d)$, the position operators Q_j and the momentum operators P_j are related to the free Schrödinger operator by the commutation formula $P_j = i\big[-\frac{1}{2}\Delta, Q_j\big]$. Therefore, if one interprets the collection $\{\Phi_1,\dots,\Phi_d\}$ as a family of position operators, then it is natural (by analogy to the Schrödinger case) to think of the familly*

$$H_0' \equiv \big(i[H_0,\Phi_1],\dots,i[H_0,\Phi_d]\big)$$

as a velocity operator for H_0. As a consequence, one can interpret the commutation assumption (2.17) *as the conservation of (a function of) the velocity operator H_0' by the scattering process, and the meaning of Theorem 2.5.4 reduces to the following: If the scattering process conserves the velocity operator H_0', then the usual and the symmetrized time delays are equal.*

There are several situations where the commutation assumption (2.17) *is satisfied. Here we present three of them:*

(i) Suppose that H_0 is of class $C^1(\Phi)$, and assume that there exists $v \in \mathbb{R}^d\setminus\{0\}$ such that $H_0' = v$. Then the operator $F_f(H_0')$ reduces to the scalar $F_f(v)$, and $\big[F_f(H_0'),S\big] = 0$ in $\mathscr{B}(\mathcal{H}_0)$. This occurs for instance in the case of Friedrichs-type and Stark operators (see Section 1.7.1).

(ii) Suppose that Φ *has only one component and that* $H_0' = H_0$*. Then the operator* $F_f(H_0') \equiv F_f(H_0)$ *is diagonalizable in the spectral representation of* H_0*. We also know that* S *is decomposable in the spectral representation of* H_0*. Thus* (2.17) *is satisfied for each* $\varphi \in \mathscr{D}_0$*, since diagonalizable operators commute with decomposable operators. This occurs in the case of* Φ*-homogeneous operators* H_0 *such as the free Schrödinger operator (see Section 1.7.2 and also [22, Sec. 10 & 11]).*

(iii) More generally, suppose that $F_f(H_0')$ *is diagonalizable in the spectral representation of* H_0*. Then* (2.17) *is once more satisfied for each* $\varphi \in \mathscr{D}_0$*, since diagonalizable operators commute with decomposable operators. For instance, in the case of the Dirac operator and of dispersive systems with a radial symbol, we have neither* $H_0' = v \in \mathbb{R}^d \setminus \{0\}$*, nor* $H_0' = H_0$*. But if we suppose* f *radial, then* $F_f(H_0')$ *is nevertheless diagonalizable in the spectral representation of* H_0 *(see Section 1.7.3 and [111, Rem. 4.9]).*

Chapter 3

Mourre theory in a two-Hilbert spaces setting

3.1 Introduction

It is commonly accepted that Mourre theory is a very powerful tool in spectral and scattering theory for self-adjoint operators. In particular, it naturally leads to limiting absorption principles which are essential when studying the absolutely continuous part of self-adjoint operators. Since the pioneering work of E. Mourre [76], a lot of improvements and extensions have been proposed, and the theory has led to numerous applications. However, in most of the corresponding works, Mourre theory is presented in a one-Hilbert space setting and perturbative arguments are used within this framework. In this work, we propose to extend the theory to a two-Hilbert spaces setting and present some results in that direction. In particular, we show how a Mourre estimate can be deduced for a pair of self-adjoint operators (H, A) in a Hilbert space $\mathcal{H}$ from a similar estimate for a pair of self-adjoint operators (H_0, A_0) in a auxiliary Hilbert space $\mathcal{H}_0$.

The main idea of E. Mourre for obtaining results on the spectrum $\sigma(H)$ of a self-adjoint operator H in a Hilbert space $\mathcal{H}$ is to find an auxiliary self-adjoint operator A in $\mathcal{H}$ such that the commutator $[iH, A]$ is positive when localised in the spectrum of H. Namely, one looks for a subset $I \subset \sigma(H)$, a number $a \equiv a(I) > 0$ and a compact operator $K \equiv K(I)$ in $\mathcal{H}$ such that

$$E^H(I)[iH, A]E^H(I) \geq aE^H(I) + K, \tag{3.1}$$

where $E^H(I)$ is the spectral projection of H on I. Such an estimate is commonly called a Mourre estimate. In general, this positivity condition is obtained via perturbative technics. Typically, H is a perturbation of a simpler operator H_0 in $\mathcal{H}$ for which the commutator $[iH_0, A]$ is easily computable and the positivity condition easily verifiable. In such a case, the commutator of the formal difference $H - H_0$ with A can be considered as a small perturbation of $[iH_0, A]$, and one can still infer the necessary positivity of $[iH, A]$.

In many other situations one faces the problem that H is not the perturbation of any simpler operator H_0 in $\mathcal{H}$. For example, if H is the Laplace-Beltrami operator on a non-compact manifold, there is no candidate for a simpler operator H_0! Alternatively, for multichannel scattering systems, there might exist more than one single candidate for H_0, and one has to take this multiplicity into account. In these situations, it is therefore unclear from the very beginning wether one can find a suitable conjugate operator A for H and how some positivity of $[iH, A]$ can be deduced from a hypothetic similar condition involving a simpler operator H_0. Of course, these interrogations have found positive answers in various situations. Nevertheless, it does not seem to the authors that any general framework has yet been proposed.

The starting point for our investigations is the scattering theory in the two-Hilbert spaces setting. In this setup, one has a self-adjoint operator H in a Hilbert space $\mathcal{H}$, and one looks for a simpler self-adjoint operator H_0 in an auxiliary Hilbert space $\mathcal{H}_0$ and a bounded operator $J : \mathcal{H}_0 \to \mathcal{H}$ such that the strong limits

$$\text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH}\, J\, \mathrm{e}^{-itH_0}\, \varphi$$

exist for suitable vectors $\varphi \in \mathcal{H}_0$. If such limits exist for enough $\varphi \in \mathcal{H}_0$, then some information on the spectral nature of H can be inferred from similar information on the spectrum of H_0. We refer to the books [17] and [118] for general presentations of scattering theory in the two-Hilbert spaces setting. Therefore, the following question naturally arises: If A_0 is a conjugate operator for H_0 such that (3.1) holds with (H_0, A_0) instead of (H, A), can we define a conjugate operator A for H such that (3.1) holds? Under suitable conditions, the answer is "yes", and its justification is the content of this work. In fact, we present a general framework in which a Mourre estimate for a pair (H, A) can be deduced from a similar Mourre estimate for a pair (H_0, A_0). In that framework, we suppose the operators A_0 and A given *a priori*, and then exhibit sufficient conditions on the formal commutators $[iH, A]$ and $[iH_0, A_0]$ guaranteeing the existence of a Mourre estimate for (H, A) if a Mourre estimate for (H_0, A_0) is verified (see the assumptions of Theorem 3.3.1). We also show how a conjugate operator A for H can be constructed from a conjugate operator A_0 for H_0.

Let us finally sketch the organisation of the work. In Section 3.2, we recall a few definitions (borrowed from [7, Chap. 7]) in relation with Mourre theory in the usual one-Hilbert space setting. In Section 3.3, we state our main result, Theorem 3.3.1, on the obtention of a Mourre estimate for (H, A) from a similar estimate for (H_0, A_0). A complementary result on higher order regularity of H with respect to A is also presented. In the second part of Section 3.3, we show how the assumptions of Theorem 3.3.1 can be checked for short-range type and long-range type perturbations (note that the distinction between short-range type and long-range type perturbations is more subtle here, since H_0 and H do not live in the same Hilbert space). We also show how a natural candidate for A can be constructed from A_0. In Section 3.4, we illustrate our results with the simple example of one-dimensional Schrödinger operator with steplike potential. A more challenging application on manifolds will be presented in [94] (many other applications such as curved quantum waveguides, anisotropic Schrödinger operators, spin models, *etc.*, are also conceivable). Finally, in Section 3.5 we prove an auxiliary result on the completeness of the wave operators in the two-Hilbert spaces setting without assuming that the initial sets of the wave operators are equal to the subspace $\mathcal{H}_{\mathrm{ac}}(H_0)$ of absolute continuity of H_0 (in [17] and [118], only that case is presented and this situation is sometimes too restrictive as will be shown for example in [94]).

3.2 Mourre theory in the one-Hilbert space setting

In this section we recall some definitions related to Mourre theory, such as the regularity condition of H with respect to A, providing a precise meaning to the commutators mentioned in the Introduction. We refer to [7, Sec. 7.2] for more information and details.

Let us consider a Hilbert space $\mathcal{H}$ with scalar product $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ and norm $\|\cdot\|_{\mathcal{H}}$. Let also H and A be two self-adjoint operators in $\mathcal{H}$, with domains $\mathcal{D}(H)$ and $\mathcal{D}(A)$. The spectrum of H is denoted by $\sigma(H)$ and its spectral measure by $E^H(\cdot)$. For shortness, we also use the notation $E^H(\lambda;\varepsilon) := E^H\big((\lambda-\varepsilon,\lambda+\varepsilon)\big)$ for all $\lambda\in\mathbb{R}$ and $\varepsilon>0$.

The operator H is said to be of class $C^1(A)$ if there exists $z\in\mathbb{C}\setminus\sigma(H)$ such that the map

$$\mathbb{R}\ni t\mapsto \mathrm{e}^{-itA}(H-z)^{-1}\,\mathrm{e}^{itA}\in\mathscr{B}(\mathcal{H}) \tag{3.2}$$

is strongly of class C^1 in $\mathcal{H}$. In such a case, the set $\mathcal{D}(H)\cap\mathcal{D}(A)$ is a core for H and the quadratic form $\mathcal{D}(H)\cap\mathcal{D}(A)\ni\varphi\mapsto\langle H\varphi,A\varphi\rangle_{\mathcal{H}}-\langle A\varphi,H\varphi\rangle_{\mathcal{H}}$ is continuous in the topology of $\mathcal{D}(H)$. This form extends then uniquely to a continuous quadratic form $[H,A]$ on $\mathcal{D}(H)$, which can be identified with a continuous operator from $\mathcal{D}(H)$ to the adjoint space $\mathcal{D}(H)^*$. Furthermore, the following equality holds:

$$\big[A,(H-z)^{-1}\big]=(H-z)^{-1}[H,A](H-z)^{-1}.$$

This $C^1(A)$-regularity of H with respect to A is the basic ingredient for any investigation in Mourre theory. It is also at the root of the proof of the Virial Theorem (see for example [7, Prop. 7.2.10] or [44]).

Note that if H is of class $C^1(A)$ and if $\eta\in C^\infty_{\mathrm{c}}(\mathbb{R})$ (the set of smooth functions on $\mathbb{R}$ with compact support), then the quadratic form $\mathcal{D}(A)\ni\varphi\mapsto\langle\bar\eta(H)\varphi,A\varphi\rangle_{\mathcal{H}}-\langle A\varphi,\eta(H)\varphi\rangle_{\mathcal{H}}$ also extends uniquely to a continuous quadratic form $[\eta(H)A,]$ on $\mathcal{H}$, identified with a bounded operator on $\mathcal{H}$.

We now recall the definition of two very useful functions in Mourre theory described in [7, Sec. 7.2]. For that purpose, we use the following notations: for two bounded operators S and T in a common Hilbert space we write $S\approx T$ if $S-T$ is compact, and we write $S\lesssim T$ if there exists a compact operator K such that $S\le T+K$. If H is of class $C^1(A)$ and $\lambda\in\mathbb{R}$ we set

$$\varrho^A_H(\lambda):=\sup\big\{a\in\mathbb{R}\mid\exists\varepsilon>0\ \text{s.t.}\ aE^H(\lambda;\varepsilon)\le E^H(\lambda;\varepsilon)[iH,A]E^H(\lambda;\varepsilon)\big\}.$$

A second function, more convenient in applications, is

$$\widetilde\varrho^A_H(\lambda):=\sup\big\{a\in\mathbb{R}\mid\exists\varepsilon>0\ \text{s.t.}\ aE^H(\lambda;\varepsilon)\lesssim E^H(\lambda;\varepsilon)[iH,A]E^H(\lambda;\varepsilon)\big\}.$$

Note that the following equivalent definition is often useful:

$$\widetilde\varrho^A_H(\lambda)=\sup\big\{a\in\mathbb{R}\mid\exists\eta\in C^\infty_{\mathrm{c}}(\mathbb{R})\ \text{real s.t.}\ \eta(\lambda)\neq0,\ a\eta(H)^2\lesssim\eta(H)[iH,A]\eta(H)\big\}. \tag{3.3}$$

It is commonly said that A is conjugate to H at the point $\lambda\in\mathbb{R}$ if $\widetilde\varrho^A_H(\lambda)>0$, and that A is strictly conjugate to H at λ if $\varrho^A_H(\lambda)>0$. Furthermore, the function $\widetilde\varrho^A_H:\mathbb{R}\to(-\infty,\infty]$

is lower semicontinuous and satisfies $\widetilde{\varrho}_H^A(\lambda) < \infty$ if and only if λ belongs to the essential spectrum $\sigma_{\rm ess}(H)$ of H. One also has $\widetilde{\varrho}_H^A(\lambda) \geq \varrho_H^A(\lambda)$ for all $\lambda \in \mathbb{R}$.

Another property of the function $\widetilde{\varrho}$, often used in the one-Hilbert space setting, is its stability under a large class of perturbations: Suppose that H and H' are self-adjoint operators in $\mathcal{H}$ and that both operators H and H' are of class $C^1_{\rm u}(A)$, *i.e.* such that the map (3.2) is C^1 in norm. Assume furthermore that the difference $(H-i)^{-1} - (H'-i)^{-1}$ belongs to $\mathscr{K}(\mathcal{H})$, the algebra of compact operators on $\mathcal{H}$. Then, it is proved in [7, Thm. 7.2.9] that $\widetilde{\varrho}_{H'}^A = \widetilde{\varrho}_H^A$, or in other words that A is conjugate to H' at a point $\lambda \in \mathbb{R}$ if and only if A is conjugate to H at λ.

Our first contribution in this work is to extend such a result to the two-Hilbert spaces setting. But before this, let us recall the importance of the set $\widetilde{\mu}^A(H) \subset \mathbb{R}$ on which $\widetilde{\varrho}_H^A(\,\cdot\,) > 0$: if H is slightly more regular than $C^1(A)$, then H has locally at most a finite number of eigenvalues on $\widetilde{\mu}^A(H)$ (multiplicities counted), and H has no singularly continuous spectrum on $\widetilde{\mu}^A(H)$ (see [7, Thm. 7.4.2] for details).

3.3 Mourre theory in the two-Hilbert spaces setting

From now on, apart from the triple $(\mathcal{H}, H, A)$ of Section 3.2, we consider a second triple $(\mathcal{H}_0, H_0, A_0)$ and an identification operator $J : \mathcal{H}_0 \to \mathcal{H}$. The existence of two such triples is quite standard in scattering theory, at least for the pairs $(\mathcal{H}, H)$ and $(\mathcal{H}_0, H_0)$ (see for instance the books [17, 118]). Part of our goal in what follows is to show that the existence of the conjugate operators A and A_0 is also natural, as was realised in the context of scattering on manifolds [94].

So, let us consider a second Hilbert space $\mathcal{H}_0$ with scalar product $\langle\,\cdot\,,\,\cdot\,\rangle_{\mathcal{H}_0}$ and norm $\|\cdot\|_{\mathcal{H}_0}$. Let also H_0 and A_0 be two self-adjoint operators in $\mathcal{H}_0$, with domains $\mathcal{D}(H_0)$ and $\mathcal{D}(A_0)$. Clearly, the $C^1(A_0)$-regularity of H_0 with respect to A_0 can be defined as before, and if H_0 is of class $C^1(A_0)$ then the definitions of the two functions $\varrho_{H_0}^{A_0}$ and $\widetilde{\varrho}_{H_0}^{A_0}$ hold as well.

In order to compare the two triples, it is natural to require the existence of a map $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ having some special properties (for example, the ones needed for the completeness of the wave operators, see Section 3.5). But for the time being, no additional information on J is necessary. In the one-Hilbert space setting, the operator H is typically a perturbation of the simpler operator H_0. And as mentioned above, the stability of the function $\widetilde{\varrho}_{H_0}^{A_0}$ is an efficient tool to infer information on H from similar information on H_0. In the two-Hilbert spaces setting, we are not aware of any general result allowing the computation of the function $\widetilde{\varrho}_H^A$ in terms of the function $\widetilde{\varrho}_{H_0}^{A_0}$. The obvious reason for this being the impossibility to consider H as a direct perturbation of H_0 since these operators do not live in the same Hilbert space. Nonetheless, the next theorem gives a result in that direction:

Theorem 3.3.1. *Let $(\mathcal{H}, H, A)$ and $(\mathcal{H}_0, H_0, A_0)$ be as above, and assume that*

(i) the operators H_0 and H are of class $C^1(A_0)$ and $C^1(A)$, respectively,

(ii) for any $\eta \in C^\infty_{\rm c}(\mathbb{R})$ the difference of bounded operators $J[iA_0, \eta(H_0)]J^* - [iA, \eta(H)]$ belongs to $\mathscr{K}(\mathcal{H})$,

(iii) for any $\eta \in C_c^\infty(\mathbb{R})$ *the difference* $J\eta(H_0) - \eta(H)J$ *belongs to* $\mathscr{K}(\mathcal{H}_0, \mathcal{H})$*,*

(iv) for any $\eta \in C_c^\infty(\mathbb{R})$ *the operator* $\eta(H)(JJ^* - 1)\eta(H)$ *belongs to* $\mathscr{K}(\mathcal{H})$*.*

Then, one has $\widetilde{\varrho}_H^A \geq \widetilde{\varrho}_{H_0}^{A_0}$*. In particular, if* A_0 *is conjugate to* H_0 *at* $\lambda \in \mathbb{R}$*, then* A *is conjugate to* H *at* λ*.*

Note that with the notations introduced in the previous section, Assumption (ii) reads $J[iA_0, \eta(H_0)]J^* \approx [iA, \eta(H)]$. Furthermore, since the vector space generated by the family of functions $\{(\,\cdot\, - z)^{-1}\}_{z \in \mathbb{C}\setminus\mathbb{R}}$ is dense in $C_0(\mathbb{R})$ and the set $\mathscr{K}(\mathcal{H}_0, \mathcal{H})$ is closed in $\mathscr{B}(\mathcal{H}_0, \mathcal{H})$, the condition $J(H_0 - z)^{-1} - (H - z)^{-1}J \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$ for all $z \in \mathbb{C} \setminus \mathbb{R}$ implies Assumption (iii) (here, $C_0(\mathbb{R})$ denotes the set of continuous functions on $\mathbb{R}$ vanishing at $\pm\infty$).

Proof. Let $\eta \in C_c^\infty(\mathbb{R}; \mathbb{R})$, and define $\eta_1, \eta_2 \in C_c^\infty(\mathbb{R}; \mathbb{R})$ by $\eta_1(x) := x\,\eta(x)$ and $\eta_2(x) := x\,\eta(x)^2$. Under Assumption (i), it is shown in [7, Eq. 7.2.18] that

$$\eta(H)[iA, H]\eta(H) = [iA, \eta_2(H)] - 2\,\mathsf{Re}\big\{[iA, \eta(H)]\eta_1(H)\big\}.$$

Therefore, one infers from Assumptions (ii) and (iii) that

$$\begin{aligned}
&\eta(H)[iA, H]\eta(H) \\
&\approx J[iA_0, \eta_2(H_0)]J^* - 2\,\mathsf{Re}\big\{J[iA_0, \eta(H_0)]J^*\eta_1(H)\big\} \\
&= J[iA_0, \eta_2(H_0)]J^* - 2\,\mathsf{Re}\big\{J[iA_0, \eta(H_0)]\eta_1(H_0)J^*\big\} \\
&\qquad - 2\,\mathsf{Re}\big\{J[iA_0, \eta(H_0)]\big(J^*\eta_1(H) - \eta_1(H_0)J^*\big)\big\} \\
&\approx J[iA_0, \eta_2(H_0)]J^* - 2J\,\mathsf{Re}\big\{[iA_0, \eta(H_0)]\eta_1(H_0)\big\}J^* \\
&= J\eta(H_0)[iA_0, H_0]\eta(H_0)J^*,
\end{aligned}$$

which means that

$$\eta(H)[iA, H]\eta(H) \approx J\eta(H_0)[iA_0, H_0]\eta(H_0)J^*. \tag{3.4}$$

Furthermore, if $a \in \mathbb{R}$ is such that $\eta(H_0)[iA_0, H_0]\eta(H_0) \gtrsim a\eta(H_0)^2$, then Assumptions (iii) and (iv) imply that

$$J\eta(H_0)[iA_0, H_0]\eta(H_0)J^* \gtrsim aJ\eta(H_0)^2J^* \approx a\eta(H)JJ^*\eta(H) \approx a\eta(H)^2. \tag{3.5}$$

Thus, one obtains $\eta(H)[iA, H]\eta(H) \gtrsim a\eta(H)^2$ by combining (3.4) and (3.5). This last estimate, together with the definition (3.3) of the functions $\widetilde{\varrho}_{H_0}^{A_0}$ and $\widetilde{\varrho}_H^A$ in terms of the localisation function η, implies the claim. □

As mentioned in the previous sections, the $C^1(A)$-regularity of H and the Mourre estimate are crucial ingredients for the analysis of the operator H, but they are in general not sufficient. For instance, the nature of the spectrum of H or the existence and the completeness of the wave operators is usually proved under a slightly stronger $C^{1,1}(A)$-regularity condition of H. It would certainly be valuable if this regularity condition could be deduced from a similar information on H_0. Since we have not been able to obtain such a result, we simply refer to [7] for the definition of this class of regularity and present below a coarser result. Namely, we show that the regularity condition "H is of class $C^n(A)$" can be checked by means of explicit computations involving only H and not its resolvent. For simplicity, we present the simplest, non-perturbative version of the result; more refined statements involving perturbations as in Sections 3.3.1 and 3.3.2 could also be proved.

For that purpose, we first recall that H is of class $C^n(A)$ if the map (3.2) is strongly of class C^n. We also introduce the following slightly more general regularity class: Assume that $(\mathcal{G},\mathcal{H})$ is a Friedrichs couple, *i.e.* a pair $(\mathcal{G},\mathcal{H})$ with $\mathcal{G}$ a Hilbert space densely and continuously embedded in $\mathcal{H}$. Assume furthermore that the unitary group $\{\mathrm{e}^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{G}$ invariant. Then, the restriction of this group to $\mathcal{G}$ generates a C_0-group in $\mathcal{G}$, and by duality extends to a C_0-group in $\mathcal{G}^*$ (the adjoint space of $\mathcal{G}$). Without ambiguity, the generators of these groups can be denoted by A (see [7, Sec. 6.3] for details). In such a situation, an operator $T\in\mathscr{B}(\mathcal{G},\mathcal{H})$ is said to belong to $C^n(\mathcal{A};\mathcal{G},\mathcal{H})$ if the map

$$\mathbb{R}\ni t\mapsto \mathrm{e}^{-itA}\,T\,\mathrm{e}^{itA}\in\mathscr{B}(\mathcal{G},\mathcal{H})$$

is strongly of class C^n. Similar definitions hold with T in $\mathscr{B}(\mathcal{H},\mathcal{G})$, $\mathscr{B}(\mathcal{G},\mathcal{G}^*)$ or in $\mathscr{B}(\mathcal{G}^*,\mathcal{H})$, and one clearly has $C^n(A;\mathcal{G},\mathcal{H})\subset C^n(A;\mathcal{G},\mathcal{G}^*)$.

The next proposition (which improves slightly the result of [75, Lemma 1.2]) is an extension of [7, Thm. 6.3.4.(c)] to higher orders of regularity of H with respect to A. We use for it the notation $\mathcal{G}$ for the domain $\mathcal{D}(H)$ of H endowed with its natural Hilbert space structure. We also recall that if H is of class $C^1(A)$, then $[iH,A]$ can be identified with a bounded operator from $\mathcal{G}$ to $\mathcal{G}^*$.

Proposition 3.3.2. *Assume that* $\mathrm{e}^{itA}\,\mathcal{G}\subset\mathcal{G}$ *for all* $t\in\mathbb{R}$ *and suppose that* H *belongs to* $C^{n-1}(A;\mathcal{G},\mathcal{H})\cap C^n(A;\mathcal{G},\mathcal{G}^*)$ *for some integer* $n\geq 1$*. Then,* H *is of class* $C^n(A)$*.*

Proof. We prove the claim by induction on n. For $n=1$, the claim follows from [7, Thm. 6.3.4.(a)].

Now, assume that the statement is true for $n-1\geq 0$, and suppose that H belongs to $C^{n-1}(A;\mathcal{G},\mathcal{H})\cap C^n(A;\mathcal{G},\mathcal{G}^*)$. Since H is of class $C^1(A)$, one has

$$\big[(H-i)^{-1},A\big]=-(H-i)^{-1}[H,A](H-i)^{-1}. \tag{3.6}$$

Furthermore, since $(H\pm i)\in\mathscr{B}(\mathcal{G},\mathcal{H})$ are bijections from $\mathcal{G}$ onto $\mathcal{H}$, one infers from the inclusion $H\in C^{n-1}(A;\mathcal{G},\mathcal{H})$ and from [7, Prop. 5.1.6.(a)] that $(H\pm i)^{-1}\in C^{n-1}(A;\mathcal{H},\mathcal{G})$. One also deduces from [7, Prop. 5.1.7] that $(H\mp i)^{-1}\in C^{n-1}(A;\mathcal{G}^*,\mathcal{H})$. Finally, the inclusion $H\in C^n(A;\mathcal{G},\mathcal{G}^*)$ implies that $[H,A]\in C^{n-1}(A;\mathcal{G},\mathcal{G}^*)$. So, by taking into account account (3.6) and the regularity property for product of operators [7, Prop. 5.1.5], one obtains that $\big[(H-i)^{-1},A\big]\in C^{n-1}(A)$. This implies the inclusion $(H-i)^{-1}\in C^n(A)$, which proves the statement for n. □

Usually, the regularity of H_0 with respect to A_0 is easy to check. On the other hand, the regularity of H with respect to A is in general rather difficult to establish, and various perturbative criteria have been developed for that purpose in the one-Hilbert space setting. Often, a distinction is made between so-called short-range and long-range perturbations.

Roughly speaking, the difference between these types perturbations is that the two terms of the formal commutator $[A, H - H_0] = A(H - H_0) - (H - H_0)A$ are treated separately in the former situation while the commutator $[A, H - H_0]$ is really computed in the latter situation. In the first case, one usually requires more decay and less regularity, while in the second case more regularity but less decay are imposed. Obviously, this distinction cannot be as transparent in the general two-Hilbert spaces setting presented here. Still, a certain distinction remains, and thus we dedicate to it the following two complementary sections.

3.3.1 Short-range type perturbations

We show below how the condition "H is of class $C^1(A)$" and the assumptions (ii) and (iii) of Theorem 3.3.1 can be verified for a class of short-range type perturbations. Our approach is to derive information on H from some equivalent information on H_0, which is usually easier to obtain. Accordingly, our results exhibit some perturbative flavor. The price one has to pay is that a compatibility condition between A_0 and A is necessary. For $z \in \mathbb{C} \setminus \mathbb{R}$, we use the shorter notations $R_0(z) := (H_0 - z)^{-1}$, $R(z) := (H - z)^{-1}$ and

$$B(z) := JR_0(z) - R(z)J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H}). \tag{3.7}$$

Proposition 3.3.3. *Let H_0 be of class $C^1(A_0)$ and assume that $\mathscr{D} \subset \mathcal{H}$ is a core for A such that $J^*\mathscr{D} \subset \mathcal{D}(A_0)$. Suppose furthermore that for any $z \in \mathbb{C} \setminus \mathbb{R}$*

$$\overline{B(z)A_0 \upharpoonright \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H}) \qquad \textit{and} \qquad \overline{R(z)(JA_0J^* - A) \upharpoonright \mathscr{D}} \in \mathscr{B}(\mathcal{H}). \tag{3.8}$$

Then, H is of class $C^1(A)$.

Proof. Take $\psi \in \mathscr{D}$ and $z \in \mathbb{C} \setminus \mathbb{R}$. Then, one gets

$$\begin{aligned}
&\langle R(\bar z)\psi, A\psi\rangle_{\mathcal{H}} - \langle A\psi, R(z)\psi\rangle_{\mathcal{H}} \\
&= \langle R(\bar z)\psi, A\psi\rangle_{\mathcal{H}} - \langle A\psi, R(z)\psi\rangle_{\mathcal{H}} - \langle \psi, J[R_0(z), A_0]J^*\psi\rangle_{\mathcal{H}} \\
&\quad + \langle \psi, J[R_0(z), A_0]J^*\psi\rangle_{\mathcal{H}} \\
&= \langle B(\bar z)A_0J^*\psi, \psi, \rangle_{\mathcal{H}} - \langle \psi, B(z)A_0J^*\psi\rangle_{\mathcal{H}} + \langle \psi, J[R_0(z), A_0]J^*\psi\rangle_{\mathcal{H}} \\
&\quad + \langle R(\bar z)(JA_0J^* - A)\psi, \psi\rangle_{\mathcal{H}} - \langle \psi, R(z)(JA_0J^* - A)\psi\rangle_{\mathcal{H}}.
\end{aligned}$$

Now, one has

$$\big|\langle B(\bar z)A_0J^*\psi, \psi, \rangle_{\mathcal{H}} - \langle \psi, B(z)A_0J^*\psi\rangle_{\mathcal{H}}\big| \le \text{Const.}\, \|\psi\|^2_{\mathcal{H}}$$

due to the first condition in (3.8), and one has

$$\big|\langle R(\bar z)(JA_0J^* - A)\psi, \psi\rangle_{\mathcal{H}} - \langle \psi, R(z)(JA_0J^* - A)\psi\rangle_{\mathcal{H}}\big| \le \text{Const.}\, \|\psi\|^2_{\mathcal{H}}$$

due to the second condition in (3.8). Furthermore, since H_0 is of class $C^1(A_0)$ one also has

$$\big|\langle \psi, J[R_0(z), A_0]J^*\psi\rangle_{\mathcal{H}}\big| \le \text{Const.}\, \|\psi\|^2_{\mathcal{H}}.$$

Since $\mathscr{D}$ is a core for A, the conclusion then follows from [7, Lemma 6.2.9]. □

We now show how the assumption (ii) of Theorem 3.3.1 is verified for a short-range type perturbation. Note that the hypotheses of the following proposition are slightly stronger than the ones of Proposition 3.3.3, and thus H is automatically of class $C^1(A)$.

Proposition 3.3.4. *Let H_0 be of class $C^1(A_0)$ and assume that $\mathscr{D} \subset \mathcal{H}$ is a core for A such that $J^*\mathscr{D} \subset \mathcal{D}(A_0)$. Suppose furthermore that for any $z \in \mathbb{C} \setminus \mathbb{R}$*

$$\overline{B(z)A_0 \restriction \mathcal{D}(A_0)} \in \mathscr{K}(\mathcal{H}_0, \mathcal{H}) \qquad \text{and} \qquad \overline{R(z)(JA_0J^* - A) \restriction \mathscr{D}} \in \mathscr{K}(\mathcal{H}). \tag{3.9}$$

Then, for each $\eta \in C_c^\infty(\mathbb{R})$ the difference of bounded operators $J[A_0, \eta(H_0)]J^* - [A, \eta(H)]$ belongs to $\mathscr{K}(\mathcal{H})$.

Proof. Take $\psi, \psi' \in \mathscr{D}$ and $z \in \mathbb{C} \setminus \mathbb{R}$. Then, one gets from the proof of Proposition 3.3.3 that

$$\begin{aligned}
&\big\langle \psi', J[A_0, R_0(z)]J^*\psi \big\rangle_{\mathcal{H}} - \langle \psi', [A, R(z)]\psi \rangle_{\mathcal{H}} \\
&= \big\langle B(\bar z)A_0J^*\psi', \psi, \big\rangle_{\mathcal{H}} - \big\langle \psi', B(z)A_0J^*\psi \big\rangle_{\mathcal{H}} \\
&\quad + \big\langle R(\bar z)(JA_0J^* - A)\psi', \psi \big\rangle_{\mathcal{H}} - \big\langle \psi', R(z)(JA_0J^* - A)\psi \big\rangle_{\mathcal{H}}.
\end{aligned}$$

By the density of $\mathscr{D}$ in $\mathcal{H}$, one then infers from the hypotheses that $J[A_0, R_0(z)]J^* - [A, R(z)]$ belongs to $\mathscr{K}(\mathcal{H})$.

To show the same result for functions $\eta \in C_c^\infty(\mathbb{R})$ instead of $(\,\cdot - z)^{-1}$, one needs more refined estimates. Taking the first resolvent identity into account one obtains

$$B(z) = \big\{1 + (z - i)R(z)\big\}B(i)\big\{1 + (z - i)R_0(z)\big\}.$$

Thus, one gets on $\mathscr{D}$ the equalities

$$\begin{aligned}
&B(z)A_0J^* \\
&= \big\{1 + (z - i)R(z)\big\}B(i)A_0\big\{1 + (z - i)R_0(z)\big\}J^* + \big\{1 + (z - i)R(z)\big\}\cdot \qquad (3.10)\\
&\quad \cdot B(i)(z - i)[R_0(z), A_0]J^*, \qquad (3.11)
\end{aligned}$$

where

$$[R_0(z), A_0] = \big\{1 + (z - i)R_0(z)\big\}R_0(i)[A_0, H_0]R_0(i)\big\{1 + (z - i)R_0(z)\big\}.$$

Obviously, these equalities extend to all of $\mathcal{H}$ since they involve only bounded operators. Letting $z = \lambda + i\mu$ with $|\mu| \le 1$, one even gets the bound

$$\big\|B(z)A_0J^*\big\|_{\mathscr{B}(\mathcal{H})} \le \text{Const.}\left(1 + \frac{|\lambda + i(\mu - 1)|}{|\mu|}\right)^4.$$

Furthermore, since the first and second terms of (3.10) extend to elements of $\mathscr{K}(\mathcal{H})$, the third term of (3.10) also extends to an element of $\mathscr{K}(\mathcal{H})$. Similarly, the operator on $\mathscr{D}$

$$R(z)(JA_0J^* - A) \equiv \big\{1 + (z - i)R(z)\big\}R(i)(JA_0J^* - A)$$

extends to a compact operator in $\mathcal{H}$, and one has the bound

$$\big\|R(z)(JA_0J^* - A)\big\|_{\mathscr{B}(\mathcal{H})} \le \text{Const.}\left(1 + \frac{|\lambda + i(\mu - 1)|}{|\mu|}\right).$$

Now, observe that for any $\eta \in C_c^\infty(\mathbb{R})$ and any $\psi, \psi' \in \mathscr{D}$ one has

$$\begin{aligned}
&\big\langle \psi', J[A_0, \eta(H_0)]J^*\psi \big\rangle_{\mathcal{H}} - \big\langle \psi', [A, \eta(H)]\psi \big\rangle_{\mathcal{H}} \\
&= \big\langle \big\{J\overline{\eta}(H_0) - \overline{\eta}(H)J\big\}A_0J^*\psi', \psi \big\rangle_{\mathcal{H}} - \big\langle \psi', \big\{J\eta(H_0) - \eta(H)J\big\}A_0J^*\psi \big\rangle_{\mathcal{H}}. \\
&\quad + \big\langle \overline{\eta}(H)(JA_0J^* - A)\psi', \psi \big\rangle_{\mathcal{H}} - \big\langle \psi', \eta(H)(JA_0J^* - A)\psi \big\rangle_{\mathcal{H}}. \qquad (3.12)
\end{aligned}$$

Then, by expressing the operators $\eta(H_0)$ and $\eta(H)$ in terms of their respective resolvents (using for example [7, Eq. 6.1.18]) and by taking the above estimates into account, one obtains that $\big\{J\eta(H_0) - \eta(H)J\big\}A_0J^*$ and $\eta(H)(JA_0J^* - A)$ are equal on $\mathscr{D}$ to a finite sum of norm convergent integrals of compact operators. Since $\mathscr{D}$ is dense in $\mathcal{H}$, these equalities between bounded operators extend continuously to equalities in $\mathscr{B}(\mathcal{H})$, and thus the statement follows by using (3.12). □

Remark 3.3.5. *As mentioned just after Theorem 3.3.1, the requirement $B(z) \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$ for all $z \in \mathbb{C} \setminus \mathbb{R}$ implies the assumption (iii) of Theorem 3.3.1. Since an a priori stronger requirement is imposed in the first condition of* (3.9)*, it is likely that in applications the compactness assumption (iii) will follow from the necessary conditions ensuring the first condition in* (3.9)*.*

Before turning to the long-range case, let us reconsider the above statements in the special situation where $A = JA_0J^*$. This case deserves a particular attention since it represents the most natural choice of conjugate operator for H when A_0 is a conjugate operator for H_0. However, in order to deal with a well-defined self-adjoint operator A, one needs the following assumption:

Assumption 3.3.6. *There exists a set $\mathscr{D} \subset \mathcal{D}(A_0J^*) \subset \mathcal{H}$ such that JA_0J^* is essentially self-adjoint on $\mathscr{D}$, with corresponding self-adjoint extension denoted by A.*

Assumption 3.3.6 might be difficult to check in general, but in concrete situations the choice of the set $\mathscr{D}$ can be quite natural. We now show how the assumptions of the above propositions can easily be checked under Assumption 3.3.6. Recall that the operator $B(z)$ was defined in (3.7).

Corollary 3.3.7. *Let H_0 be of class $C^1(A_0)$, suppose that Assumption 3.3.6 holds for some set $\mathscr{D} \subset \mathcal{H}$, and for any $z \in \mathbb{C} \setminus \mathbb{R}$ assume that*

$$\overline{B(z)A_0 \restriction \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H}).$$

Then, H is of class $C^1(A)$.

Proof. All the assumptions of Proposition 3.3.3 are verified. □

Corollary 3.3.8. *Let H_0 be of class $C^1(A_0)$, suppose that Assumption 3.3.6 holds for some set $\mathscr{D} \subset \mathcal{H}$, and for any $z \in \mathbb{C} \setminus \mathbb{R}$ assume that*

$$\overline{B(z)A_0 \restriction \mathcal{D}(A_0)} \in \mathscr{K}(\mathcal{H}_0, \mathcal{H}). \qquad (3.13)$$

Then, for each $\eta \in C_c^\infty(\mathbb{R})$ the difference of bounded operators $J[A_0, \eta(H_0)]J^* - [A, \eta(H)]$ belongs to $\mathscr{K}(\mathcal{H})$.

Proof. All the assumptions of Proposition 3.3.4 are verified. □

Remark 3.3.9. *As mentioned above the choice $A = JA_0J^*$ is natural when A_0 is a conjugate operator for H_0. With that respect the second conditions in* (3.8) *and* (3.9) *quantify how much one can deviate from this natural choice.*

The most important consequence of Mourre theory is the obtention of a limiting absorption principle for H_0 and H. Rather often, the space defined in terms of A_0 (resp. A) in which holds the limiting absorption principle for H_0 (resp. H) is not adequate for applications. In [7, Prop. 7.4.4] a method is given for expressing the limiting absorption principle for H_0 in terms of an auxiliary operator Φ_0 in $\mathcal{H}_0$ more suitable than A_0. Obviously, this abstract result also applies for three operators H, A and Φ in $\mathcal{H}$, but one crucial condition is that $(H-z)^{-1}\mathcal{D}(\Phi) \subset \mathcal{D}(A)$ for suitable $z \in \mathbb{C}$. In the next lemma, we provide a sufficient condition allowing to infer this information from similar information on the operators H_0, A_0 and Φ_0 in $\mathcal{H}_0$. Note that Φ does not need to be of the form $J\Phi_0J^*$ but that such a situation often appears in applications.

Lemma 3.3.10. *Let $z \in \mathbb{C} \setminus \{\overline{\sigma(H_0) \cup \sigma(H)}\}$. Suppose that Assumption 3.3.6 holds for some set $\mathscr{D} \subset \mathcal{H}$. Assume that $\overline{B(\bar{z})A_0 \upharpoonright \mathcal{D}(A_0)} \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$. Furthermore, let Φ_0 and Φ be self-adjoint operators in $\mathcal{H}_0$ and $\mathcal{H}$ satisfying $(H_0 - z)^{-1}\mathcal{D}(\Phi_0) \subset \mathcal{D}(A_0)$ and*

$$J^*(\Phi - i)^{-1} - (\Phi_0 - i)^{-1}J^* = (\Phi_0 - i)^{-1}B$$

for some $B \in \mathscr{B}(\mathcal{H}, \mathcal{H}_0)$. Then, one has the inclusion $(H-z)^{-1}\mathcal{D}(\Phi) \subset \mathcal{D}(A)$.

Proof. Let $\psi \in \mathscr{D}$ and $\psi' \in \mathcal{H}$. Then, one has

$$\begin{aligned}
&\big\langle A\psi, (H-z)^{-1}(\Phi-i)^{-1}\psi'\big\rangle_{\mathcal{H}} \\
&= \big\langle \big\{(H-\bar{z})^{-1}J - J(H_0-\bar{z})^{-1}\big\}A_0J^*\psi, (\Phi-i)^{-1}\psi'\big\rangle_{\mathcal{H}} \\
&\qquad + \big\langle J(H_0-\bar{z})^{-1}A_0J^*\psi, (\Phi-i)^{-1}\psi'\big\rangle_{\mathcal{H}} \\
&= -\big\langle B(\bar{z})A_0J^*\psi, (\Phi-i)^{-1}\psi'\big\rangle_{\mathcal{H}} + \big\langle (H_0-\bar{z})^{-1}A_0J^*\psi, (\Phi_0-i)^{-1}J^*\psi'\big\rangle_{\mathcal{H}_0} \\
&\qquad + \big\langle (H_0-\bar{z})^{-1}A_0J^*\psi, (\Phi_0-i)^{-1}B\psi'\big\rangle_{\mathcal{H}_0}.
\end{aligned}$$

So, $\big|\big\langle A\psi, (H-z)^{-1}(\Phi-i)^{-1}\psi'\big\rangle_{\mathcal{H}}\big| \leq \text{Const.}\, \|\psi\|_{\mathcal{H}}$, and thus $(H-z)^{-1}(\Phi-i)^{-1}\psi' \in \mathcal{D}(A)$, since A is essentially self-adjoint on $\mathscr{D}$. □

3.3.2 Long-range type perturbations

In the case of a long-range type perturbation, the situation is slightly less satisfactory than in the short-range case. One reason comes from the fact that one really has to compute the commutator $[A, H - H_0]$ instead of treating the terms $A(H - H_0)$ and $(H - H_0)A$ separately. However, a rather efficient method for checking that "H is of class $C^1(A)$" has been put into evidence in [47, Lemma. A.2]. We start by recalling this result and then we propose a perturbative type argument for checking the assumption (ii) of Theorem 3.3.1. Note that there is a missprint in the hypothesis 1 of [47, Lemma A.2]; the meaningless condition $\sup_n \|\chi_n\|_{\mathcal{D}(H)} < \infty$ has to be replaced by $\sup_n \|\chi_n\|_{\mathscr{B}(\mathcal{D}(H))} < \infty$.

Lemma 3.3.11 (Lemma A.2 of [47])**.** *Let $\mathscr{D} \subset \mathcal{H}$ be a core for A such that $\mathscr{D} \subset \mathcal{D}(H)$ and $H\mathscr{D} \subset \mathscr{D}$. Let $\{\chi_n\}_{n\in\mathbb{N}}$ be a family of bounded operators on $\mathcal{H}$ such that*

(i) $\chi_n\mathscr{D} \subset \mathscr{D}$ *for each* $n \in \mathbb{N}$, $\operatorname{s-lim}_{n\to\infty} \chi_n = 1$ *and* $\sup_n \|\chi_n\|_{\mathscr{B}(\mathcal{D}(H))} < \infty$,

(ii) for all $\psi \in \mathscr{D}$, *one has* $\operatorname{s-lim}_{n\to\infty} A\chi_n\psi = A\psi$,

(iii) there exists $z \in \mathbb{C} \setminus \sigma(H)$ *such that* $\chi_n R(z)\mathscr{D} \subset \mathscr{D}$ *and* $\chi_n R(\bar{z})\mathscr{D} \subset \mathscr{D}$ *for each* $n \in \mathbb{N}$,

(iv) one has $\operatorname{s-lim}_{n\to\infty} A[H, \chi_n]R(z)\psi = 0$ *and* $\operatorname{s-lim}_{n\to\infty} A[H, \chi_n]R(\bar{z})\psi = 0$ *for all* $\psi \in \mathscr{D}$.

Finally, assume that for all $\psi \in \mathscr{D}$

$$\big|\langle A\psi, H\psi\rangle_{\mathcal{H}} - \langle H\psi, A\psi\rangle_{\mathcal{H}}\big| \le \text{Const.}\big(\|H\psi\|^2_{\mathcal{H}} + \|\psi\|^2_{\mathcal{H}}\big).$$

Then, H is of class $C^1(A)$.

In the next statement we provide conditions under which the assumption (ii) of Theorem 3.3.1 is verified for a long-range type perturbation. One condition is that for each $z \in \mathbb{C} \setminus \mathbb{R}$ the operator $B(z)$ belongs to $\mathscr{K}(\mathcal{H}_0, \mathcal{H})$, which means that the hypothesis (iii) of Theorem 3.3.1 is also automatically satisfied. We stress that no direct relation between A_0 and A is imposed; the single relation linking A_0 and A only involves the commutators $[H_0, A_0]$ and $[H, A]$. On the other hand, the condition on H_0 is slightly stronger than just the $C^1(A_0)$-regularity.

Proposition 3.3.12. *Let H_0 be of class $C^1(A_0)$ with $[H_0, A_0] \in \mathscr{B}\big(\mathcal{D}(H_0), \mathcal{H}_0\big)$ and let H be of class $C^1(A)$. Assume that the operator $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ extends to an element of $\mathscr{B}\big(\mathcal{D}(H_0)^*, \mathcal{D}(H)^*\big)$, and suppose that for each $z \in \mathbb{C} \setminus \mathbb{R}$ the operator $B(z)$ belongs to $\mathscr{K}(\mathcal{H}_0, \mathcal{H})$ and that the difference $J[H_0, A_0]J^* - [H, A]$ belongs to $\mathscr{K}\big(\mathcal{D}(H), \mathcal{D}(H)^*\big)$. Then, for each $\eta \in C^\infty_c(\mathbb{R})$ the difference of bounded operators*

$$J[A_0, \eta(H_0)]J^* - [A, \eta(H)]$$

belongs to $\mathscr{K}(\mathcal{H})$.

Proof. By taking the various hypotheses into account one gets for any $z \in \mathbb{C} \setminus \mathbb{R}$ that

$$\begin{aligned}
&J[A_0, R_0(z)]J^* - [A, R(z)] \\
&= JR_0(z)[H_0, A_0]R_0(z)J^* - R(z)[H, A]R(z) \\
&= \big\{JR_0(z) - R(z)J\big\}[H_0, A_0]R_0(z)J^* + R(z)J[H_0, A_0]\big\{R_0(z)J^* - J^*R(z)\big\} \\
&\qquad + R(z)\big\{J[H_0, A_0]J^* - [H, A]\big\}R(z) \\
&= B(z)[H_0, A_0]R_0(z)J^* + R(z)J[H_0, A_0]B(\bar{z})^* + R(z)\big\{J[H_0, A_0]J^* - [H, A]\big\}R(z),
\end{aligned}$$

with each term on the last line in $\mathscr{K}(\mathcal{H})$. Now, by taking the first resolvent identity into account, one obtains

$$\begin{aligned}
&B(z)[H_0, A_0]R_0(z)J^* \\
&= \big\{1 + (z - i)R(z)\big\}B(i)\big\{1 + (z - i)R_0(z)\big\}[H_0, A_0]R_0(i)\big\{1 + (z - i)R_0(z)\big\}J^*
\end{aligned}$$

and

$$\begin{aligned}&R(z)J[H_0,A_0]B(\bar z)^*\\&\quad=\big\{1+(z-i)R(z)\big\}R(i)J[H_0,A_0]\big\{1+(z-i)R_0(z)\big\}B(-i)^*\big\{1+(z-i)R(z)\big\}\end{aligned}$$

as well as

$$\begin{aligned}&R(z)\big\{J[H_0,A_0]J^*-[H,A]\big\}R(z)\\&\quad=\big\{1+(z-i)R(z)\big\}R(i)\big\{J[H_0,A_0]J^*-[H,A]\big\}R(i)\big\{1+(z-i)R(z)\big\}.\end{aligned}$$

Thus, by letting $z=\lambda+i\mu$ with $|\mu|\leq 1$, one gets the bound

$$\big\|J[A_0,R_0(z)]J^*-[A,R(z)]\big\|_{\mathscr{B}(\mathcal{H})}\leq \text{Const.}\left(1+\frac{|\lambda+i(\mu-1)|}{|\mu|}\right)^3.$$

One concludes as in the proof of Proposition 3.3.4 by expressing $J[A_0,\eta(H_0)]J^*-[A,\eta(H)]$ in terms of $J[A_0,R_0(z)]J^*-[A,R(z)]$ (using for example [7, Eq. 6.2.16]), and then by dealing with a finite number of norm convergent integrals of compact operators. □

As mentioned before the statement, no direct relation between A_0 and A has been imposed, and thus considering the special case $A=JA_0J^*$ is not really relevant. However, it is not difficult to check how the quantity $J[H_0,A_0]J^*-[H,A]$ looks like in that special case, and in applications such an approach could be of interest. However, since the resulting formulas are rather involved in general, we do not further investigate in that direction.

3.4 One illustrative example

To illustrate our approach, we present below a simple example for which all the computations can be made by hand (more involved examples will be presented elsewhere, like in [94], where part of the results of the present work is used). In this model, usually called one-dimensional Schrödinger operator with steplike potential, the choice of a conjugate operator is rather natural, whereas the computation of the ϱ-functions is not completely trivial due to the anisotropy of the potential. We refer to [4, 10, 28, 29, 46] for earlier works on that model and to [88] for a n-dimensional generalisation.

So, we consider in the Hilbert space $\mathcal{H}:=\mathsf{L}^2(\mathbb{R})$ the Schrödinger operator $H:=-\Delta+V$, where V is the operator of multiplication by a function $v\in C(\mathbb{R};\mathbb{R})$ with finite limits $v_\pm$ at infinity, *i.e.* $v_\pm:=\lim_{x\to\pm\infty}v(x)\in\mathbb{R}$. The operator H is self-adjoint on $\mathcal{H}^2(\mathbb{R})$, since V is bounded. As a second operator, we consider in the auxiliary Hilbert space $\mathcal{H}_0:=\mathsf{L}^2(\mathbb{R})\oplus\mathsf{L}^2(\mathbb{R})$ the operator

$$H_0:=(-\Delta+v_-)\oplus(-\Delta+v_+),$$

which is also self-adjoint on its natural domain $\mathcal{H}^2(\mathbb{R})\oplus\mathcal{H}^2(\mathbb{R})$. Then, we take a function $j_+\in C^\infty(\mathbb{R};[0,1])$ with $j_+(x)=0$ if $x\leq 1$ and $j_+(x)=1$ if $x\geq 2$, we set $j_-(x):=j_+(-x)$ for each $x\in\mathbb{R}$, and we define the identification operator $J\in\mathscr{B}(\mathcal{H}_0,\mathcal{H})$ by the formula

$$J(\varphi_-,\varphi_+):=j_-\varphi_-+j_+\varphi_+,\quad(\varphi_-,\varphi_+)\in\mathcal{H}_0.$$

Clearly, the adjoint operator $J^* \in \mathscr{B}(\mathcal{H}, \mathcal{H}_0)$ is given by $J^*\psi = (j_-\psi, j_+\psi)$ for any $\psi \in \mathcal{H}$, and the operator $JJ^* \in \mathscr{B}(\mathcal{H})$ is equal to the operator of multiplication by $j_-^2 + j_+^2$.

Let us now come to the choice of the conjugate operators. For H_0, the most natural choice consists in two copies of the generator of dilations on $\mathbb{R}$, that is, $A_0 := (D, D)$ with D the generator of the group

$$\big(\mathrm{e}^{itD}\,\psi\big)(x) := \mathrm{e}^{t/2}\,\psi(\mathrm{e}^t\,x), \quad \psi \in \mathscr{S}(\mathbb{R}),\ t, x \in \mathbb{R},$$

where $\mathscr{S}(\mathbb{R})$ denotes the Schwartz space on $\mathbb{R}$. In such a case, the map (3.2) with (H, A) replaced by (H_0, A_0) is strongly of class C^∞ in $\mathcal{H}_0$. Moreover, the ϱ-functions can be computed explicitly (see [7, Sec. 8.3.5] for a similar calculation in an abstract setting):

$$\widetilde{\varrho}_{H_0}^{A_0}(\lambda) = \varrho_{H_0}^{A_0}(\lambda) = \begin{cases} +\infty & \text{if } \lambda < \min\{v_-, v_+\} \\ 2\big(\lambda - \min\{v_-, v_+\}\big) & \text{if } \min\{v_-, v_+\} \le \lambda < \max\{v_-, v_+\} \\ 2\big(\lambda - \max\{v_-, v_+\}\big) & \text{if } \lambda \ge \max\{v_-, v_+\}. \end{cases}$$

For the conjugate operator for H, two natural choices exist: either one can use again the generator D of dilations in $\mathcal{H}$, or one can use the (formal) operator JA_0J^* which appears naturally in our framework. Since the latter choice illustrates better the general case, we opt here for this choice and just note that the former choice would also be suitable and would lead to similar results. So, we set $\mathscr{D} := \mathscr{S}(\mathbb{R})$ and $j := j_- + j_+$, and then observe that JA_0J^* is well-defined and equal to

$$JA_0J^* = jDj \tag{3.14}$$

on $\mathscr{D}$. This equality, the fact that j is of class $C^1(D)$, and [7, Lemma 7.2.15], imply that JA_0J^* is essentially self-adjoint on $\mathscr{D}$. We denote by A the corresponding self-adjoint extension.

We are now in a position for applying results of the previous sections such as Theorem 3.3.1. First, recall that H_0 is of class $C^1(A_0)$ and observe that the assumption (iv) of Theorem 3.3.1 is satisfied with the operator J introduced above. Similarly, one easily shows that the assumption (iii) of Theorem 3.3.1 also holds. Indeed, as mentioned after the statement of Theorem 3.3.1, the assumption (iii) holds if one shows that $B(z) \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$ for each $z \in \mathbb{C} \setminus \mathbb{R}$. But, for any $(\varphi_-, \varphi_+) \in \mathcal{H}_0$, a direct calculation shows that $B(z)(\varphi_-, \varphi_+) = B_-(z)\varphi_- + B_+(z)\varphi_+$, with

$$B_\pm(z) := (H - z)^{-1}\big\{[-\Delta, j_\pm] + j_\pm(V - v_\pm)\big\}(-\Delta + v_\pm - z)^{-1} \in \mathscr{K}(\mathcal{H}).$$

So, one readily concludes that $B(z) \in \mathscr{K}(\mathcal{H}_0, \mathcal{H})$.

Thus, one is only left with showing the assumption (ii) of Theorem 3.3.1 and the $C^1(A)$-regularity of H. We first consider a short-range type perturbation. In such a case, with A defined as above, we know it is enough to check the condition (3.13) of Corollary 3.3.8. For that purpose, we assume the following stronger condition on v :

$$\lim_{|x|\to\infty} |x|\big(v(x) - v_\pm\big) = 0, \tag{3.15}$$

and observe that for each $(\varphi_-,\varphi_+) \in \mathscr{S}(\mathbb{R}) \oplus \mathscr{S}(\mathbb{R})$ and $z \in \mathbb{C} \setminus \mathbb{R}$ we have the equality

$$B(z)A_0(\varphi_-,\varphi_+) = B_-(z)D\varphi_- + B_+(z)D\varphi_+.$$

Then, taking into account the expressions for $B_-(z)$ and $B_+(z)$ as well as the above assumption on v, one proves easily that $\overline{B_\pm(z)D \upharpoonright \mathcal{D}(D)} \in \mathscr{K}(\mathcal{H})$, which implies (3.13). Collecting our results, we end up with:

Lemma 3.4.1 (Short-range case)**.** *Assume that $v \in C(\mathbb{R};\mathbb{R})$ satisfies* (3.15)*, then the operator H is of class $C^1(A)$ and one has $\widetilde{\varrho}_H^A \geq \widetilde{\varrho}_{H_0}^{A_0}$. In particular, A is conjugate to H on $\mathbb{R} \setminus \{v_-,v_+\}$.*

We now consider a long-range type perturbation and thus show that the assumptions of Proposition 3.3.12 hold with A defined as above. For that purpose, we assume that $v \in C^1(\mathbb{R};\mathbb{R})$ and that

$$\lim_{|x|\to\infty} |x|\, v'(x) = 0. \tag{3.16}$$

Then, a standard computation taking the inclusion $(H-z)^{-1}\mathscr{D} \subset \mathcal{D}(A)$ into account shows that H is of class $C^1(A)$ with

$$[A,H] = \big[j(-i\nabla)\,\mathrm{id}_{\mathbb{R}}\, j, -\Delta\big] - ij^2\,\mathrm{id}_{\mathbb{R}}\, v' + \frac{i}{2}\big[j^2,-\Delta\big], \tag{3.17}$$

where $\mathrm{id}_{\mathbb{R}}$ is the function $\mathbb{R} \ni x \mapsto x \in \mathbb{R}$. Then, using (3.16) and (3.17), one infers that $J[H_0,A_0]J^* - [H,A]$ belongs to $\mathscr{K}\big(\mathcal{D}(H),\mathcal{D}(H)^*\big)$. Furthermore, simple considerations show that J extends to an element of $\mathscr{B}\big(\mathcal{D}(H_0)^*,\mathcal{D}(H)^*\big)$. These results, together with the ones already obtained, permit to apply Proposition 3.3.12, and thus to get:

Lemma 3.4.2 (Long-range case)**.** *Assume that $v \in C^1(\mathbb{R};\mathbb{R})$ satisfies* (3.16)*, then the operator H is of class $C^1(A)$ and one has $\widetilde{\varrho}_H^A \geq \widetilde{\varrho}_{H_0}^{A_0}$. In particular, A is conjugate to H on $\mathbb{R} \setminus \{v_-,v_+\}$.*

3.5 Completeness of the wave operators

One of the main goal in scattering theory is the proof of the completeness of the wave operators. In our setting, this amounts to show that the strong limits

$$W_\pm(H,H_0,J) := \operatorname{s-lim}_{t\to\pm\infty} \mathrm{e}^{itH}\, J\, \mathrm{e}^{-itH_0}\, P_{\mathrm{ac}}(H_0) \tag{3.18}$$

exist and have ranges equal to $\mathcal{H}_{\mathrm{ac}}(H)$. If the wave operators $W_\pm(H,H_0,J)$ are partial isometries with initial sets $\mathcal{H}_0^\pm$, this implies in particular that the scattering operator

$$S := W_+(H,H_0,J)^*\, W_-(H,H_0,J)$$

is well-defined and unitary from $\mathcal{H}_0^-$ to $\mathcal{H}_0^+$.

When defining the completeness of the wave operators, one usually requires that $\mathcal{H}_0^\pm = \mathcal{H}_{\mathrm{ac}}(H_0)$ (see for example [17, Def. III.9.24] or [118, Def. 2.3.1]). However, in applications it may happen that the ranges of $W_\pm(H,H_0,J)$ are equal to $\mathcal{H}_{\mathrm{ac}}(H)$ but that $\mathcal{H}_0^\pm \neq$

$\mathcal{H}_{\rm ac}(H_0)$. Typically, this happens for multichannel type scattering processes. In such situations, the usual criteria for completeness, as [17, Prop. III.9.40] or [118, Thm. 2.3.6], cannot be applied. So, we present below a result about the completeness of the wave operators without assuming that $\mathcal{H}_0^\pm = \mathcal{H}_{\rm ac}(H_0)$. Its proof is inspired by [118, Thm. 2.3.6].

Proposition 3.5.1. *Suppose that the wave operators defined in* (3.18) *exist and are partial isometries with initial set projections $P_0^\pm$. If there exists $\widetilde{J} \in \mathscr{B}(\mathcal{H}, \mathcal{H}_0)$ such that*

$$W_\pm\big(H_0, H, \widetilde{J}\big) := \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH_0}\, \widetilde{J}\, \mathrm{e}^{-itH}\, P_{\rm ac}(H) \tag{3.19}$$

exist and such that

$$\text{s-}\lim_{t\to\pm\infty} \big(J\widetilde{J} - 1\big)\, \mathrm{e}^{-itH}\, P_{\rm ac}(H) = 0, \tag{3.20}$$

then the equalities $\mathsf{Ran}\,\big(W_\pm(H, H_0, J)\big) = \mathcal{H}_{\rm ac}(H)$ *hold. Conversely, if one assumes that* $\mathsf{Ran}\,\big(W_\pm(H, H_0, J)\big) = \mathcal{H}_{\rm ac}(H)$ *and if there exists $\widetilde{J} \in \mathscr{B}(\mathcal{H}, \mathcal{H}_0)$ such that*

$$\text{s-}\lim_{t\to\pm\infty} \big(\widetilde{J}J - 1\big)\, \mathrm{e}^{-itH_0}\, P_0^\pm = 0, \tag{3.21}$$

then $W_\pm\big(H_0, H, \widetilde{J}\big)$ exist and (3.20) *holds.*

Proof. (i) By using the chain rule for wave operators [118, Thm. 2.1.7], we deduce from the definitions (3.18)-(3.19) that the limits

$$W_\pm\big(H, H, J\widetilde{J}\big) := \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH}\, J\widetilde{J}\, \mathrm{e}^{-itH}\, P_{\rm ac}(H)$$

exist and satisfy

$$W_\pm\big(H, H, J\widetilde{J}\big) = W_\pm(H, H_0, J) W_\pm\big(H_0, H, \widetilde{J}\big). \tag{3.22}$$

In consequence, the equality

$$\text{s-}\lim_{t\to\pm\infty} \big(\mathrm{e}^{itH}\, J\widetilde{J}\, \mathrm{e}^{-itH}\, P_{\rm ac}(H) - P_{\rm ac}(H)\big) = 0,$$

which follow from (3.20), implies that $W_\pm\big(H, H, J\widetilde{J}\big)P_{\rm ac}(H) = P_{\rm ac}(H)$. This, together with (3.22) and the equality $W_\pm\big(H_0, H, \widetilde{J}\big) = W_\pm\big(H_0, H, \widetilde{J}\big)P_{\rm ac}(H)$, gives

$$W_\pm(H, H_0, J)W_\pm\big(H_0, H, \widetilde{J}\big) = W_\pm\big(H, H, J\widetilde{J}\big)P_{\rm ac}(H) = P_{\rm ac}(H),$$

which is equivalent to

$$W_\pm\big(H_0, H, \widetilde{J}\big)^* W_\pm(H, H_0, J)^* = P_{\rm ac}(H).$$

This gives the inclusion $\mathsf{Ker}\,\big(W_\pm(H, H_0, J)^*\big) \subset \mathcal{H}_{\rm ac}(H)^\perp$, which together with the fact that the range of a partial isometry is closed imply that

$$\mathcal{H} = \mathsf{Ran}\,\big(W_\pm(H, H_0, J)\big) \oplus \mathsf{Ker}\,\big(W_\pm(H, H_0, J)^*\big) \subset \mathcal{H}_{\rm ac}(H) \oplus \mathcal{H}_{\rm ac}(H)^\perp = \mathcal{H}.$$

So, one must have $\mathsf{Ran}\,\big(W_\pm(H, H_0, J)\big) = \mathcal{H}_{\rm ac}(H)$, and the first claim is proved.

(ii) Conversely, assume that $\mathsf{Ran}\,\big(W_\pm(H,H_0,J)\big)=\mathcal{H}_{\rm ac}(H)$ and consider $\psi\in\mathcal{H}_{\rm ac}(H)$. Then, by hypothesis there exist $\psi_\pm\in P_0^\pm\mathcal{H}_0$ such that

$$\lim_{t\to\pm\infty}\big\|\,\mathrm{e}^{-itH}\,\psi-J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big\|_{\mathcal{H}}=0. \tag{3.23}$$

Together with (3.21), this implies that the norm

$$\begin{aligned}
&\big\|\,\mathrm{e}^{itH_0}\,\widetilde{J}\,\mathrm{e}^{-itH}\,\psi-P_0^\pm\psi_\pm\big\|_{\mathcal{H}_0}\\
&\le\big\|\,\mathrm{e}^{itH_0}\,\widetilde{J}\big(\,\mathrm{e}^{-itH}\,\psi-J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big)\big\|_{\mathcal{H}_0}+\big\|\,\mathrm{e}^{itH_0}\,\widetilde{J}J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm-P_0^\pm\psi_\pm\big\|_{\mathcal{H}_0}\\
&\le\mathrm{Const.}\big\|\,\mathrm{e}^{-itH}\,\psi-J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big\|_{\mathcal{H}}+\big\|\big(\widetilde{J}J-1\big)\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big\|_{\mathcal{H}_0}
\end{aligned}$$

converges to 0 as $t\to\pm\infty$, showing that the wave operators (3.19) exist.

For the relation (3.20), observe first that (3.21) gives

$$\mathrm{s}\text{-}\lim_{t\to\pm\infty}\big(J\widetilde{J}-1\big)J\,\mathrm{e}^{-itH_0}\,P_0^\pm=\mathrm{s}\text{-}\lim_{t\to\pm\infty}J\big(\widetilde{J}J-1\big)\,\mathrm{e}^{-itH_0}\,P_0^\pm=0.$$

Together with (3.23), this implies that the norm

$$\begin{aligned}
&\big\|\big(J\widetilde{J}-1\big)\,\mathrm{e}^{-itH}\,\psi\big\|_{\mathcal{H}}\\
&\le\big\|\big(J\widetilde{J}-1\big)\big(J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm-\mathrm{e}^{-itH}\,\psi\big)\big\|_{\mathcal{H}}+\big\|\big(J\widetilde{J}-1\big)J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big\|_{\mathcal{H}}\\
&\le\mathrm{Const.}\big\|\,\mathrm{e}^{-itH}\,\psi-J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big\|_{\mathcal{H}}+\big\|\big(J\widetilde{J}-1\big)J\,\mathrm{e}^{-itH_0}\,P_0^\pm\psi_\pm\big\|_{\mathcal{H}}
\end{aligned}$$

converges to 0 as $t\to\pm\infty$, showing that (3.20) also holds. □

Chapter 4

Spectral and scattering theory for the Aharonov-Bohm operators

4.1 Introduction

The Aharonov-Bohm (A-B) model describing the motion of a charged particle in a magnetic field concentrated at a single point is one of the few systems in mathematical physics for which the spectral and the scattering properties can be completely computed. It has been introduced in [3] and the first rigorous treatment appeared in [100]. A more general class of models involving boundary conditions at the singularity point has then been developed in [2, 32] and further extensions or refinements appeared since these simultaneous works. Being unable to list all these subsequent papers, let us simply mention few of them : [107] in which it is proved that the A-B models can be obtained as limits in a suitable sense of systems with less singular magnetic fields, [106] in which it is shown that the low energy behavior of the scattering amplitude for two dimensional magnetic Schrödinger operators is similar to the scattering amplitude of the A-B models, and the series [15, 16, 115] in which, among other results, high energy estimates are obtained for the scattering operator. Concerning the extensions we mention the papers [40] which considers the A-B operators with an additional uniform magnetic field and [67] which studies the A-B operators on the hyperbolic plane.

The aim of the present work is to provide the spectral and the scattering analysis of the A-B operators on $\mathbb{R}^2$ for all possible values of the parameters (boundary conditions). The work is motivated by the recent result of one of the authors [89] showing that the A-B wave operators can be rewritten in terms of explicit functions of the generator of dilations and of the Laplacian. However, the proof of this result used certain complicated expressions for the scattering operator borrowed from [2] and we have in the meanwhile found a simpler approach. For those reasons, we have decided to start again the analysis from scratch using the modern operator-theoretical machinery. For example, in contrast to [2] and [32] our computations do not involve an explicit parametrization of $U(2)$. Simultaneously, we recast this analysis in the up-to-date theory of self-adjoint extensions [27] and derive rigorously the expressions for the wave operators and the scattering operator from the stationary approach of scattering theory as presented in [118].

So let us now describe the content of this review work. In Section 4.2 we introduce the operator H_α which corresponds to a Schrödinger operator in $\mathbb{R}^2$ with a δ-type magnetic field at the origin. The index α corresponds to the total flux of the magnetic field, and on a natural domain this operator has deficiency indices $(2,2)$. The description of this natural domain is recalled and some of its properties are exhibited.

Section 4.3 is devoted to the description of all self-adjoint extensions of the operator H_α. More precisely, a boundary triple for the operator H_α is constructed in Proposition 4.3.1. It essentially consists in the definition of two linear maps Γ_1, Γ_2 from the domain $\mathcal{D}(H_\alpha^*)$ of the adjoint of H_α to $\mathbb{C}^2$ which have some specific properties with respect to H_α, as recalled at the beginning of this section. Once these maps are exhibited, all self-adjoint extensions of H_α can be labeled by two 2×2-matrices C and D satisfying two simple conditions presented in (4.7). These self-adjoint extensions are denoted by H_α^{CD}. The γ-field and the Weyl function corresponding to the boundary triple are then constructed. By taking advantage of some general results related to the boundary triple's approach, they allow us to explicit the spectral properties of H_α^{CD} in very simple terms. At the end of the section we add some comments about the role of the parameters C and D and discuss some of their properties.

The short Section 4.4 contains formulae on the Fourier transform and on the dilation group that are going to be used subsequently. Section 4.5 is the main section on scattering theory. It contains the time dependent approach as well as the stationary approach of the scattering theory for the A-B models. Some calculations involving Bessel functions or hypergeometric ${}_2F_1$-functions look rather tricky but they are necessary for a rigorous derivation of the stationary expressions. Fortunately, the final expressions are much more easily understandable. For example, it is proved in Proposition 4.5.4 that the channel wave operators for the original A-B operator H_α^{AB} are equal to very explicit functions of the generator of dilation. These functions are continuous on $[-\infty,\infty]$ and take values in the set of complex number of modulus 1. Theorem 4.5.5 contains a similar explicit description of the wave operators for the general operator H_α^{CD}.

In Section 4.6 we study the scattering operator and in particular its asymptotics at small and large energies. These properties highly depend on the parameters C and D but also on the flux α of the singular magnetic field. All the various possibilities are explicitly analysed. The statement looks rather messy, but this simply reflects the richness of the model.

The parametrization of the self-adjoint extensions of H_α with the pair (C,D) is highly non unique. For convenience, we introduce in the last section a one-to-one parametrization of all self-adjoint extensions and explicit some of the previous results in this framework. For further investigations in the structure of the set of all self-adjoint extensions, this unique parametrization has many advantages.

Finally, let us mention that this work is essentially self-contained. Furthermore, despite the rather long and rich history of the Aharonov-Bohm model most of the our results are new or exhibited in the present form for the first time.

Remark 4.1.1. *After the completion of this work, the authors were informed about the closely related work [25]. In this paper, the differential expression* $-\partial_x^2 + (m^2 - 1/4)x^{-2}$ *on* $\mathbb{R}_+$ *is considered and a holomorphic family of extensions for* $\Re(m) > -1$ *is studied. Formulae for the wave operators similar to our formula* (4.14) *were independently obtained by its authors.*

Remark 4.1.2. *In December 2009, a two-day meeting celebrated the 50 anniversary of the Aharonov-Bohm effect, and 25 anniversary since the discovery of the related geometric, or Berry phase. It was pointed out to us by the referee that an interesting discussion took place in the physics literature on this occasion. We refer to the letter [18] for more information on the subject and thank the referee for drawing our attention to this reference.*

4.2 General setting

Let $\mathcal{H}$ denote the Hilbert space $\mathsf{L}^2(\mathbb{R}^2)$ with its scalar product $\langle\cdot,\cdot\rangle$ and its norm $\|\cdot\|$. For any $\alpha\in\mathbb{R}$, we set $A_\alpha:\mathbb{R}^2\setminus\{0\}\to\mathbb{R}^2$ by

$$A_\alpha(x,y)=-\alpha\Big(\frac{-y}{x^2+y^2},\frac{x}{x^2+y^2}\Big),$$

corresponding formally to the magnetic field $B=\alpha\delta$ (δ is the Dirac delta function), and consider the operator

$$H_\alpha:=(-i\nabla-A_\alpha)^2,\qquad \mathcal{D}(H_\alpha)=C_c^\infty\big(\mathbb{R}^2\setminus\{0\}\big)\ .$$

Here $C_c^\infty(\Xi)$ denotes the set of smooth functions on Ξ with compact support. The closure of this operator in $\mathcal{H}$, which is denoted by the same symbol, is symmetric and has deficiency indices $(2,2)$ [2, 32]. For further investigation we need some more information on this closure.

So let us first decompose the Hilbert space $\mathcal{H}$ with respect to polar coordinates: For any $m\in\mathbb{Z}$, let ϕ_m be the complex function defined by $[0,2\pi)\ni\theta\mapsto\phi_m(\theta):=\frac{e^{im\theta}}{\sqrt{2\pi}}$. Then, by taking the completeness of the family $\{\phi_m\}_{m\in\mathbb{Z}}$ in $\mathsf{L}^2(\mathbb{S}^1)$ into account, one has the canonical isomorphism

$$\mathcal{H}\cong\bigoplus_{m\in\mathbb{Z}}\mathcal{H}_r\otimes[\phi_m]\ , \tag{4.1}$$

where $\mathcal{H}_r:=\mathsf{L}^2(\mathbb{R}_+,r\,\mathrm{d}r)$ and $[\phi_m]$ denotes the one dimensional space spanned by ϕ_m. For shortness, we write $\mathcal{H}_m$ for $\mathcal{H}_r\otimes[\phi_m]$, and often consider it as a subspace of $\mathcal{H}$. Clearly, the Hilbert space $\mathcal{H}_m$ is isomorphic to $\mathcal{H}_r$, for any m

In this representation the operator H_α is equal to [32, Sec. 2]

$$\bigoplus_{m\in\mathbb{Z}}H_{\alpha,m}\otimes 1, \tag{4.2}$$

with

$$H_{\alpha,m}=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{(m+\alpha)^2}{r^2},$$

and with a domain which depends on $m+\alpha$. It clearly follows from this representation that replacing α by $\alpha+n$, $n\in\mathbb{Z}$, corresponds to a unitary transformation of H_α. In particular, the case $\alpha\in\mathbb{Z}$ is equivalent to the magnetic field-free case $\alpha=0$, *i.e.* the Laplacian and its zero-range perturbations, see [5, Chapt. 1.5]. Hence throughout the work we restrict our attention to the values $\alpha\in(0,1)$.

So, for $\alpha \in (0,1)$ and $m \notin \{0,-1\}$, the domain $\mathcal{D}(H_{\alpha,m})$ is given by

$$\Big\{f \in \mathcal{H}_r \cap \mathcal{H}^{2,2}_{loc}(\mathbb{R}_+) \mid -f'' - r^{-1}f' + (m+\alpha)^2 r^{-2} f \in \mathcal{H}_r\Big\}\ .$$

For $m \in \{0,-1\}$, let $H^{(1)}_\nu$ denote the Hankel function of the first kind and of order ν, and for $f,h \in \mathcal{H}^{2,2}_{loc}$ let $W(g,h)$ stand for the Wronskian

$$W(f,h) := \overline{f}h' - \overline{f'}h\ .$$

One then has

$$\begin{aligned}\mathcal{D}(H_{\alpha,m}) = \Big\{&f \in \mathcal{H}_r \cap \mathcal{H}^{2,2}_{loc}(\mathbb{R}_+) \mid \\ &- f'' - r^{-1}f' + (m+\alpha)^2 r^{-2} f \in \mathcal{H}_r \text{ and } \lim_{r\searrow 0} r\big[W(f,h_{\pm i,m})\big](r) = 0\Big\},\end{aligned}$$

where $h_{+i,m}(r) = H^{(1)}_{|m+\alpha|}(e^{i\pi/4}r)$ and $h_{-i,m}(r) = H^{(1)}_{|m+\alpha|}(e^{i3\pi/4}r)$. It is known that the operator $H_{\alpha,m}$ for $m \notin \{0,-1\}$ are self-adjoint on the mentioned domain, while $H_{\alpha,0}$ and $H_{\alpha,-1}$ have deficiency indices $(1,1)$. This explains the deficiency indices $(2,2)$ for the operator H_α.

The problem of the description of all self-adjoint extensions of the operator H_α can be approached by two methods. On the one hand, there exists the classical description of von Neumann based on unitary operators between the deficiency subspaces. On the other hand, there exists the theory of boundary triples which has been widely developed for the last twenty years [27, 37]. Since our construction is based only on the latter approach, we shall recall it briefly in the sequel.

Before stating a simple result on $\mathcal{D}(H_{\alpha,m})$ for $m \in \{0,-1\}$ let us set some conventions. For a complex number $z \in \mathbb{C} \setminus \mathbb{R}_+$, the branch of the square root $z \mapsto \sqrt{z}$ is fixed by the condition $\Im\sqrt{z} > 0$. In other words, for $z = re^{i\varphi}$ with $r > 0$ and $\varphi \in (0,2\pi)$ one has $\sqrt{z} = \sqrt{r}e^{i\varphi/2}$. On the other hand, for $\beta \in \mathbb{R}$ we always take the principal branch of the power $z \mapsto\rightarrow z^\beta$ by taking the principal branch of the argument $\arg z \in (-\pi,\pi)$. This means that for $z = re^{i\varphi}$ with $r > 0$ and $\varphi \in (-\pi,\pi)$ we have $z^\beta = r^\beta e^{i\beta\varphi}$. Let us also recall the asymptotic behavior of $H^{(1)}_\nu(w)$ as $w \to 0$ in $\mathbb{C} \setminus \mathbb{R}_-$ and for $\nu \notin \mathbb{Z}$:

$$H^{(1)}_\nu(w) = -\frac{2^\nu i}{\sin(\pi\nu)\Gamma(1-\nu)}\, w^{-\nu} + \frac{2^{-\nu} i e^{-i\pi\nu}}{\sin(\pi\nu)\Gamma(1+\nu)}\, w^{\nu} + O(w^{2-\nu}). \tag{4.3}$$

Proposition 4.2.1. *For any $f \in \mathcal{D}(H_{\alpha,m})$ with $m \in \{0,-1\}$, the following asymptotic behavior holds:*

$$\lim_{r\searrow 0} \frac{f(r)}{r^{|m+\alpha|}} = 0.$$

Proof. Let us set $\nu := |m+\alpha| \in (0,1)$, and recall that $f \in \mathcal{D}(H_{\alpha,m})$ implies $f \in C^1\big((0,+\infty)\big)$ and that the Hankel function satisfies $\big(H^{(1)}_\nu(z)\big)' = H^{(1)}_{\nu-1}(z) - \frac{\nu}{z}H^{(1)}_\nu(z)$. By taking this and (4.3) into account, the condition $\lim_{r\searrow 0} r[W(h_{\pm i,m},f)](r) = 0$ implies that

$$\lim_{r\searrow 0}\big\{r^{\nu+1}f'(r) - \nu r^\nu f(r)\big\} = 0 \tag{4.4}$$

and that

$$\lim_{r\searrow 0}\big\{r^{1-\nu}f'(r)+\nu r^{-\nu}f(r)\big\}=0\ . \tag{4.5}$$

Multiplying both terms of (4.5) by $r^{2\nu}$ and subtracting it from (4.4) one obtains that

$$\lim_{r\searrow 0} r^{\nu}f(r)=0. \tag{4.6}$$

On the other hand, considering (4.5) as a linear differential equation for f: $r^{1-\nu}f'(r)+\nu r^{-\nu}f(r)=b(r)$, and using the variation of constant one gets for some $C\in\mathbb{C}$:

$$f(r)=\frac{C}{r^{\nu}}+\frac{1}{r^{\nu}}\int_0^r t^{2\nu-1}b(t)\,\mathrm{d}t\ .$$

Now Eq. (4.6) implies that $C=0$, and by using l'Hôpital's rule, one finally obtains:

$$\lim_{r\searrow 0}\frac{f(r)}{r^{\nu}}=\lim_{r\searrow 0}\frac{\int_0^r t^{2\nu-1}b(t)\,\mathrm{d}t}{r^{2\nu}}=\lim_{r\searrow 0}\frac{r^{2\nu-1}b(r)}{2\,\nu\,r^{2\nu-1}}=\frac{1}{2\,\nu}\lim_{r\searrow 0}b(r)=0. \qquad \square$$

4.3 Boundary conditions and spectral theory

In this section, we explicitly construct a boundary triple for the operator H_α and we briefly exhibit some spectral results in that setting. Clearly, our construction is very close to the one in [32], but this paper does not contain any reference to the boundary triple machinery. Our aim is thus to recast the construction in an up-to-date theory. The following presentation is strictly adapted to our setting, and as a general rule we omit to write the dependence on α on each of the objects. We refer to [27, 37] for more information on boundary triples.

Let H_α be the densely defined closed and symmetric operator in $\mathcal{H}$ previously introduced. The adjoint of H_α is denoted by H_α^* and is defined on the domain

$$\mathcal{D}(H_\alpha^*)=\Big\{\mathfrak{f}\in\mathcal{H}\cap H^{2,2}_{loc}\big(\mathbb{R}^2\setminus\{0\}\big)\mid H_\alpha\mathfrak{f}\in\mathcal{H}\Big\}.$$

Let Γ_1,Γ_2 be two linear maps from $\mathcal{D}(H_\alpha^*)$ to $\mathbb{C}^2$. The triple $(\mathbb{C}^2,\Gamma_1,\Gamma_2)$ is called a *boundary triple for* H_α if the following two conditions are satisfied:

(1) $\langle\mathfrak{f},H_\alpha^*\,\mathfrak{g}\rangle-\langle H_\alpha^*\,\mathfrak{f},\mathfrak{g}\rangle=\langle\Gamma_1\,\mathfrak{f},\Gamma_2\,\mathfrak{g}\rangle-\langle\Gamma_2\,\mathfrak{f},\Gamma_1\,\mathfrak{g}\rangle$ for any $\mathfrak{f},\mathfrak{g}\in\mathcal{D}(H_\alpha^*)$,

(2) the map $(\Gamma_1,\Gamma_2):\mathcal{D}(H_\alpha^*)\to\mathbb{C}^2\oplus\mathbb{C}^2$ is surjective.

It is proved in the reference mentioned above that such a boundary triple exists, and that all self-adjoint extensions of H_α can be described in this framework. More precisely, let $C,D\in M_2(\mathbb{C})$ be 2×2 matrices, and let us denote by H_α^{CD} the restriction of H_α^* on the domain

$$\mathcal{D}(H_\alpha^{CD}):=\{\mathfrak{f}\in\mathcal{D}(H_\alpha^*)\mid C\Gamma_1\mathfrak{f}=D\Gamma_2\mathfrak{f}\}\ .$$

Then, the operator H_α^{CD} is self-adjoint if and only if the matrices C and D satisfy the following conditions:

$$\text{(i) } CD^* \text{ is self-adjoint,}\qquad \text{(ii) } \det(CC^*+DD^*)\neq 0. \tag{4.7}$$

Moreover, any self-adjoint extension of H_α in $\mathcal{H}$ is equal to one of the operator H_α^{CD}.

We shall now construct explicitly a boundary triple for the operator H_α. For that purpose, let us consider $z \in \mathbb{C} \setminus \mathbb{R}_+$ and choose $k = \sqrt{z}$ with $\Im(k) > 0$. It is easily proved that the following two functions $\mathfrak{f}_{z,0}$ and $\mathfrak{f}_{z,-1}$ define an orthonormal basis in $\ker(H_\alpha^* - z)$, namely in polar coordinates:

$$\mathfrak{f}_{z,0}(r,\theta) = N_{z,0}\, H_\alpha^{(1)}(kr)\,\phi_0(\theta), \quad \mathfrak{f}_{z,-1}(r,\theta) = N_{z,-1}\, H_{1-\alpha}^{(1)}(kr)\,\phi_{-1}(\theta),$$

where $N_{z,m}$ is the normalization such that $\|f_{z,0}\| = \|f_{z,-1}\| = 1$. In particular, by making use of the equality

$$\int_0^\infty r\big|H_\nu^{(1)}(kr)\big|^2 \mathrm{d}r = \big(\pi\cos(\pi\nu/2)\big)^{-1}$$

valid for $k \in \{e^{i\pi/4}, e^{i3\pi/4}\}$, one has

$$N_{\pm i,0} = \big(\pi\cos(\pi\alpha/2)\big)^{1/2} \quad \text{and} \quad N_{\pm i,-1} = \big(\pi\cos(\pi(1-\alpha)/2)\big)^{1/2} = \big(\pi\sin(\pi\alpha/2)\big)^{1/2}.$$

Let us also introduce the averaging operator $\mathcal{P}$ with respect to the polar angle acting on any $\mathfrak{f} \in \mathcal{H}$ and for almost every $r > 0$ by

$$[\mathcal{P}(\mathfrak{f})](r) = \int_0^{2\pi} \mathfrak{f}(r,\theta)\,\mathrm{d}\theta.$$

Following [32, Sec. 3] we can then define the following four linear functionals on suitable $\mathfrak{f}$:

$$\begin{aligned}
\Phi_0(\mathfrak{f}) &= \lim_{r\searrow 0} r^{\alpha}[\mathcal{P}(\mathfrak{f}\overline{\phi_0})](r), & \Psi_0(\mathfrak{f}) &= \lim_{r\searrow 0} r^{-\alpha}\big([\mathcal{P}(\mathfrak{f}\overline{\phi_0})](r) - r^{-\alpha}\Phi_0(\mathfrak{f})\big),\\
\Phi_{-1}(\mathfrak{f}) &= \lim_{r\searrow 0} r^{1-\alpha}[\mathcal{P}(\mathfrak{f}\overline{\phi_{-1}})](r), & \Psi_{-1}(\mathfrak{f}) &= \lim_{r\searrow 0} r^{\alpha-1}\big([\mathcal{P}(\mathfrak{f}\overline{\phi_{-1}})](r) - r^{\alpha-1}\Phi_{-1}(\mathfrak{f})\big).
\end{aligned}$$

For example, by taking the asymptotic behavior (4.3) into account one obtains

$$\begin{aligned}
\Phi_0(\mathfrak{f}_{z,0}) &= N_{z,0}\, a_\alpha(z), & \Phi_{-1}(\mathfrak{f}_{z,0}) &= 0,\\
\Psi_0(\mathfrak{f}_{z,0}) &= N_{z,0}\, b_\alpha(z), & \Psi_{-1}(\mathfrak{f}_{z,0}) &= 0,\\
\Phi_{-1}(\mathfrak{f}_{z,-1}) &= N_{z,-1}\, a_{1-\alpha}(z), & \Phi_0(\mathfrak{f}_{z,-1}) &= 0,\\
\Psi_{-1}(\mathfrak{f}_{z,-1}) &= N_{z,-1}\, b_{1-\alpha}(z), & \Psi_0(\mathfrak{f}_{z,-1}) &= 0,
\end{aligned} \tag{4.8}$$

with

$$a_\nu(z) = -\frac{2^\nu i}{\sin(\pi\nu)\Gamma(1-\nu)}\,k^{-\nu}, \quad b_\nu(z) = \frac{2^{-\nu} i e^{-i\pi\nu}}{\sin(\pi\nu)\Gamma(1+\nu)}\,k^{\nu}. \tag{4.9}$$

The main result of this section is:

Proposition 4.3.1. *The triple* $(\mathbb{C}^2, \Gamma_1, \Gamma_2)$*, with* Γ_1, Γ_2 *defined on* $\mathfrak{f} \in \mathcal{D}(H_\alpha^*)$ *by*

$$\Gamma_1\mathfrak{f} := \begin{pmatrix} \Phi_0(\mathfrak{f}) \\ \Phi_{-1}(\mathfrak{f}) \end{pmatrix}, \quad \Gamma_2\mathfrak{f} := 2\begin{pmatrix} \alpha\,\Psi_0(\mathfrak{f}) \\ (1-\alpha)\,\Psi_{-1}(\mathfrak{f}) \end{pmatrix},$$

is a boundary triple for H_α.

Proof. We use the schema from [26, Lem. 5]. For any $\mathfrak{f}, \mathfrak{g} \in \mathcal{D}(H_\alpha^*)$ let us define the sesquilinear forms

$$B_1(\mathfrak{f}, \mathfrak{g}) := \langle \mathfrak{f}, H_\alpha^* \mathfrak{g}\rangle - \langle H_\alpha^* \mathfrak{f}, \mathfrak{g}\rangle$$

and

$$B_2(\mathfrak{f}, \mathfrak{g}) := \langle \Gamma_1 \mathfrak{f}, \Gamma_2 \mathfrak{g}\rangle - \langle \Gamma_2 \mathfrak{f}, \Gamma_1 \mathfrak{g}\rangle.$$

We are going to show that these expressions are well defined and that $B_1 = B_2$.

i) Clearly, B_1 is well defined. For B_2, let us first recall that $\mathcal{D}(H_\alpha^*) = \mathcal{D}(H_\alpha) + \ker(H_\alpha^* - i) + \ker(H_\alpha^* + i)$. It has already been proved above that the four maps $\Phi_0, \Phi_{-1}, \Psi_0$ and Ψ_{-1} are well defined on the elements of $\ker(H_\alpha^* - i)$ and $\ker(H_\alpha^* + i)$. We shall now prove that $\Gamma_1 \mathfrak{f} = \Gamma_2 \mathfrak{f} = 0$ for $\mathfrak{f} \in \mathcal{D}(H_\alpha)$, which shows that B_2 is also well defined on $\mathcal{D}(H_\alpha^*)$. In view of the decomposition (4.2) it is sufficient to consider functions $\mathfrak{f}$ of the form $\mathfrak{f}(r,\theta) = f_m(r)\phi_m(\theta)$ for any $m \in \mathbb{Z}$ and with $f_m \in \mathcal{D}(H_{\alpha,m})$. Obviously, for such a function $\mathfrak{f}$ with $m \notin \{0,-1\}$ one has $[P(\mathfrak{f})](r) = 0$ for almost every r, and thus $\Gamma_1 \mathfrak{f} = \Gamma_2 \mathfrak{f} = 0$. For $m \in \{0, 1\}$ the equalities $\Gamma_1 \mathfrak{f} = \Gamma_2 \mathfrak{f} = 0$ follow directly from Proposition 4.2.1.

ii) Now, since $\Gamma_1 \mathfrak{f} = \Gamma_2 \mathfrak{g} = 0$ for all $\mathfrak{f}, \mathfrak{g} \in \mathcal{D}(H_\alpha)$, the only non trivial contributions to the sesquilinear form B_2 come from $\mathfrak{f}, \mathfrak{g} \in \ker(H_\alpha^* - i) + \ker(H_\alpha^* + i)$. On the other hand one also has $B_1(\mathfrak{f}, \mathfrak{g}) = 0$ for $\mathfrak{f}, \mathfrak{g} \in \mathcal{D}(H_\alpha)$. Thus, we are reduced in proving the equalities

$$B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',n}) = B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',n})$$

for any $z, z' \in \{-i, i\}$ and $m, n \in \{0, -1\}$.

Observe first that for $z \neq z'$ and arbitrary m, n one has

$$B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',n}) = \langle \mathfrak{f}_{z,m}, z'\mathfrak{f}_{z',n}\rangle - \langle z\mathfrak{f}_{z,m}, \mathfrak{f}_{z',n}\rangle = 0$$

since $z' = \overline{z}$. Now, for $m \neq n$ one has $\Gamma_1 \mathfrak{f}_{z,m} \perp \Gamma_2 \mathfrak{f}_{z',n}$, and hence $B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',n}) = 0 = B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',n})$. For $m = n$ one easily calculate with $\nu := |m - \alpha|$ that

$$B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',m}) = 2\nu \overline{N_{z,m}} N_{z',m} \big(\overline{a_\nu(z)}\, b_\nu(z') - \overline{b_\nu(z)}\, a_\nu(z')\big) = 0\ ,$$

and then $B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',m}) = 0 = B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z',m})$.

We now consider $z = z'$ and $m \neq n$. One has

$$B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,n}) = \langle \mathfrak{f}_{z,m}, z\mathfrak{f}_{z,n}\rangle - \langle z\mathfrak{f}_{z,m}, \mathfrak{f}_{z,n}\rangle = 2z\langle \mathfrak{f}_{z,m}, \mathfrak{f}_{z,n}\rangle = 0$$

and again $\Gamma_1 \mathfrak{f}_{z,m} \perp \Gamma_2 \mathfrak{f}_{z,n}$. It then follows that $B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,n}) = 0 = B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,n})$.

So it only remains to show that $B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}) = B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m})$. For that purpose, observe first that

$$B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}) = 2z\langle \mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}\rangle = 2z.$$

On the other hand, one has

$$B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}) = 2i\Im\big(\langle \Gamma_1 \mathfrak{f}_{z,m}, \Gamma_2 \mathfrak{f}_{z,m}\big) = 2i\Im\Big(2\nu |N_{z,m}|^2\, \overline{a_\nu(z)}\, b_\nu(z)\Big)$$

with $\nu = |m - \alpha|$. By inserting (4.9) into this expression, one obtains (with $k = \sqrt{z}$ and $\Im(k) > 0$)

$$\begin{aligned} B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}) &= 4i\nu |N_{z,m}|^2 \Im\Big(\frac{-(k^\nu)^2 e^{-i\pi\nu}}{\sin^2(\pi\nu)\,\Gamma(1-\nu)\,\Gamma(1+\nu)} \Big) \\ &= 4z\nu |N_{z,m}|^2 \frac{\sin(\pi\nu/2)}{\sin^2(\pi\nu)\,\Gamma(1-\nu)\,\Gamma(1+\nu)} \ . \end{aligned}$$

Finally, by taking the equality

$$\Gamma(1-\nu)\Gamma(1+\nu) = \frac{\pi\nu}{\sin(\pi\nu)}$$

into account, one obtains

$$B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}) = 4z|N_{z,m}|^2 \frac{\sin(\pi\nu/2)}{\sin(\pi\nu)\,\pi} = 4z\pi\, \cos(\pi\nu/2) \frac{\sin(\pi\nu/2)}{\sin(\pi\nu)\,\pi} = 2z \ ,$$

which implies $B_2(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m}) = 2z = B_1(\mathfrak{f}_{z,m}, \mathfrak{f}_{z,m})$.

iii) The surjectivity of the map $(\Gamma_1, \Gamma_2) : \mathcal{D}(H_\alpha^*) \to \mathbb{C}^2 \oplus \mathbb{C}^2$ follows from the equalities (4.8). □

Let us now construct *the Weyl function* corresponding to the above boundary triple. The presentation is again adapted to our setting, and we refer to [27] for general definitions.

As already mentioned, all self-adjoint extensions of H_α can be characterized by the 2×2 matrices C and D satisfying two simple conditions, and these extensions are denoted by H_α^{CD}. In the special case $(C, D) = (1, 0)$, then H_α^{10} is equal to the original Aharonov-Bohm operator H_α^{AB}. Recall that this operator corresponds to the Friedrichs extension of H_α and that its spectrum is equal to $\mathbb{R}_+$. This operator is going to play a special role in the sequel.

Let us consider $\xi = (\xi_0, \xi_{-1}) \in \mathbb{C}^2$ and $z \in \mathbb{C} \setminus \mathbb{R}_+$. It is proved in [27] that there exists a unique $\mathfrak{f} \in \ker(H_\alpha^* - z)$ with $\Gamma_1 \mathfrak{f} = \xi$. This solution is explicitly given by the formula: $\mathfrak{f} := \gamma(z)\xi$ with

$$\gamma(z)\xi = \frac{\xi_0}{N_{z,0}\, a_\alpha(z)}\, \mathfrak{f}_{z,0} + \frac{\xi_{-1}}{N_{z,-1} a_{1-\alpha}(z)} \mathfrak{f}_{z,-1}$$

The Weyl function $M(z)$ is then defined by the relation $M(z) := \Gamma_2\, \gamma(z)$. In view of the previous calculations one has

$$\begin{aligned} M(z) &= 2 \begin{pmatrix} \alpha\, b_\alpha(z)/a_\alpha(z) & 0 \\ 0 & (1-\alpha)\, b_{1-\alpha}(z)/a_{1-\alpha}(z) \end{pmatrix} \\ &= -\frac{2}{\pi} \sin(\pi\alpha) \begin{pmatrix} \frac{\Gamma(1-\alpha)^2 e^{-i\pi\alpha}}{4^\alpha} (k^\alpha)^2 & 0 \\ 0 & \frac{\Gamma(\alpha)^2 e^{-i\pi(1-\alpha)}}{4^{1-\alpha}} (k^{1-\alpha})^2 \end{pmatrix} . \end{aligned}$$

In particular, one observes that for $z \in \mathbb{C} \setminus \mathbb{R}_+$ one has $M(0) := \lim_{z\to 0} M(z) = 0$.

In terms of the Weyl function and of the γ-*field* γ the Krein resolvent formula has the simple form:

$$\begin{aligned} (H_\alpha^{CD} - z)^{-1} - (H_\alpha^{AB} - z)^{-1} &= -\gamma(z)\big(DM(z) - C\big)^{-1} D\gamma(\bar{z})^* \\ &= -\gamma(z)D^*\big(M(z)D^* - C^*\big)^{-1}\gamma(\bar{z})^* \quad (4.10) \end{aligned}$$

for $z \in \rho(H_\alpha^{AB}) \cap \rho(H_\alpha^{CD})$. The following result is also derived within this formalism, see [6] for i), [37, Thm. 5] and the matrix reformulation [48, Thm. 3] for ii). In the statement, the equality $M(0) = 0$ has already been taken into account.

Lemma 4.3.2. *i) The value $z \in \mathbb{R}_-$ is an eigenvalue of H_α^{CD} if and only if $\det\big(DM(z) - C\big) = 0$, and in that case one has*

$$\ker(H_\alpha^{CD} - z) = \gamma(z) \ker\big(DM(z) - C\big)\,.$$

ii) The number of negative eigenvalues of H_α^{CD} coincides with the number of negative eigenvalues of the matrix CD^*.

We stress that the number of eigenvalues does not depend on $\alpha \in (0,1)$, but only on the choice of C and D.

Let us now add some comments about the role of the parameters C and D and discuss some of their properties. Two pairs of matrices (C, D) and (C', D') satisfying (4.7) define the same boundary condition (*i.e.* the same self-adjoint extension) if and only if there exists some invertible matrix $L \in M_2(\mathbb{C})$ such that $C' = LC$ and $D' = LD$ [81, Prop. 3]. In particular, if (C, D) satisfies (4.7) and if $\det(D) \neq 0$, then the pair $(D^{-1}C, 1)$ defines the same boundary condition (and $D^{-1}C$ is self-adjoint). Hence there is an arbitrariness in the choice of these parameters. This can avoided in several ways.

First, one can establish a bijection between all boundary conditions and the set $U(2)$ of the unitary 2×2 matrices U by setting

$$C = C(U) := \frac{1}{2}(1 - U) \quad \text{and} \quad D = D(U) = \frac{i}{2}(1 + U)\,, \tag{4.11}$$

see a detailed discussion in [52]. We shall comment more on this in the last section.

Another possibility is as follows (*cf.* [84] for details): There is a bijection between the set of all boundary conditions and the set of triples $(\mathcal{L}, I, L)$, where $\mathcal{L} \in \big\{\{0\}, \mathbb{C}, \mathbb{C}^2\big\}$, $I : \mathcal{L} \to \mathbb{C}^2$ is an identification map (identification of $\mathcal{L}$ as a linear subspace of $\mathbb{C}^2$) and L is a self-adjoint operator in $\mathcal{L}$. For example, given such a triple $(\mathcal{L}, I, L)$ the corresponding boundary condition is obtained by setting

$$C = C(\mathcal{L}, I, L) := L \oplus 1 \quad \text{and} \quad D = D(\mathcal{L}, I, L) := 1 \oplus 0$$

with respect to the decomposition $\mathbb{C}^2 = [I\mathcal{L}] \oplus [I\mathcal{L}]^\perp$. On the other hand, for a pair (C, D) satisfying (4.7), one can set $\mathcal{L} := \mathbb{C}^d$ with $d := 2 - \dim[\ker(D)]$, $I : \mathcal{L} \to \mathbb{C}^2$ is the identification map of $\mathcal{L}$ with $\ker(D)^\perp$ and $L := (DI)^{-1}CI$. In this framework, one can check by a direct calculation that for any $K \in M_2(\mathbb{C})$ such that $DK - C$ is invertible, one has

$$\big(DK - C\big)^{-1} D = I(PKI - L)^{-1} P, \tag{4.12}$$

where $P : \mathbb{C}^2 \to \mathcal{L}$ is the adjoint of I, *i.e.* the composition of the orthogonal projection onto $I\mathcal{L}$ together with the identification of $I\mathcal{L}$ with $\mathcal{L}$.

Let us finally note that the conditions (4.7) imply some specific properties related to commutativity and adjointness. We shall need in particular:

Lemma 4.3.3. *Let* (C, D) *satisfies* (4.7) *and* $K \in M_2(\mathbb{C})$ *with* $\Im K > 0$. *Then*

i) The matrices $DK - C$ *and* $DK^* - C$ *are invertible,*

ii) The equality $\big[(DK - C)^{-1}D\big]^* = (DK^* - C)^{-1}D$ *holds.*

Proof. i) By contraposition, let us assume that $\det(DK - C) = 0$. Passing to the adjoint, one also has $\det(K^*D^* - C^*) = 0$, *i.e.* there exists $f \in \mathbb{C}^2$ such that $K^*D^*f = C^*f$. By taking the scalar product with D^*f one obtains that $\langle D^*f, KD^*f\rangle = \langle f, CD^*f\rangle$. The right-hand side is real due to (i) in (4.7). But since $\Im K > 0$, the equality is possible if and only if $D^*f = 0$. It then follows that $C^*f = K^*D^*f = 0$, which contradicts (ii) in (4.7). The invertibility of $DK^* - C$ can be proved similarly.

ii) If $\det(D) \neq 0$, then the matrix $A := D^{-1}C$ is self-adjoint and it follows that

$$\big[(DK - C)^{-1}D\big]^* = \big[(K - A)^{-1}\big]^* = (K^* - A)^{-1} = (DK^* - C)^{-1}D\ .$$

If $D = 0$, then the equality is trivially satisfied. Finally, if $\det(D) = 0$ but $D \neq 0$ one has $\mathcal{L} := \mathbb{C}$. Furthermore, let us define $I : \mathbb{C} \to \mathbb{C}^2$ by $I\mathcal{L} := \ker(D)^\perp$ and let $P : \mathbb{C}^2 \to \mathbb{C}$ be its adjoint map. Then, by the above construction there exists $\ell \in \mathbb{R}$ such that $(DK - C)^{-1}D = I(PKI - \ell)^{-1}P$. It is also easily observed that PKI is just the multiplication by some $k \in \mathbb{C}$ with $\Im k > 0$, and hence $(DK - C)^{-1}D = I(k - \ell)^{-1}P$. Similarly one has $(DK^* - C)^{-1}D = I(\bar{k} - \ell)^{-1}P$. Taking the adjoint of the first expression leads directly to the expected equality. □

4.4 Fourier transform and the dilation group

Before starting with the scattering theory, we recall some properties of the Fourier transform and of the dilation group in relation with the decomposition (4.1). Let $\mathcal{F}$ be the usual Fourier transform, explicitly given on any $\mathfrak{f} \in \mathcal{H}$ and $y \in \mathbb{R}^2$ by

$$[\mathcal{F}\mathfrak{f}](y) = \frac{1}{2\pi}\,\mathrm{l.i.m.}\int_{\mathbb{R}^2} \mathfrak{f}(x)\, e^{-ix\cdot y}\,\mathrm{d}x$$

where $\mathrm{l.i.m.}$ denotes the convergence in the mean. Its inverse is denoted by $\mathcal{F}^*$. Since the Fourier transform maps the subspace $\mathcal{H}_m$ of $\mathcal{H}$ onto itself, we naturally set $\mathcal{F}_m : \mathcal{H}_r \to \mathcal{H}_r$ by the relation $\mathcal{F}(f\phi_m) = \mathcal{F}_m(f)\phi_m$ for any $f \in \mathcal{H}_r$. More explicitly, the application $\mathcal{F}_m$ is the unitary map from $\mathcal{H}_r$ to $\mathcal{H}_r$ given on any $f \in \mathcal{H}_r$ and almost every $\kappa \in \mathbb{R}_+$ by

$$\hat{f}(\kappa) := [\mathcal{F}_m f](\kappa) = (-i)^{|m|}\,\mathrm{l.i.m.}\int_{\mathbb{R}_+} r\, J_{|m|}(r\,\kappa)\, f(r)\,\mathrm{d}r\ ,$$

where $J_{|m|}$ denotes the Bessel function of the first kind and of order $|m|$. The inverse Fourier transform $\mathcal{F}_m^*$ is given by the same formula, with $(-i)^{|m|}$ replaced by $i^{|m|}$.

Now, let us recall that the unitary dilation group $\{U_\tau\}_{\tau\in\mathbb{R}}$ is defined on any $\mathfrak{f} \in \mathcal{H}$ and $x \in \mathbb{R}^2$ by

$$[U_\tau\mathfrak{f}](x) = e^\tau\mathfrak{f}(e^\tau x)\ .$$

Its self-adjoint generator A is formally given by $\frac{1}{2}(X \cdot (-i\nabla) + (-i\nabla) \cdot X)$, where X is the position operator and $-i\nabla$ is its conjugate operator. All these operators are essentially self-adjoint on the Schwartz space on $\mathbb{R}^2$.

An important property of the operator A is that it leaves each subspace $\mathcal{H}_m$ invariant. For simplicity, we shall keep the same notation for the restriction of A to each subspace $\mathcal{H}_m$. So, for any $m \in \mathbb{Z}$, let φ_m be an essentially bounded function on $\mathbb{R}$. Assume furthermore that the family $\{\varphi_m\}_{m\in\mathbb{Z}}$ is bounded. Then the operator $\varphi(A) : \mathcal{H} \to \mathcal{H}$ defined on $\mathcal{H}_m$ by $\varphi_m(A)$ is a bounded operator in $\mathcal{H}$.

Let us finally recall a general formula about the Mellin transform.

Lemma 4.4.1. *Let φ be an essentially bounded function on $\mathbb{R}$ such that its inverse Fourier transform is a distribution on $\mathbb{R}$. Then, for any $\mathfrak{f} \in C_c^\infty\big(\mathbb{R}^2 \setminus \{0\}\big)$ one has*

$$[\varphi(A)\mathfrak{f}](r,\theta) = (2\pi)^{-1/2} \int_0^\infty \check{\varphi}\big(-\ln(s/r)\big)\, \mathfrak{f}(s,\theta)\, \frac{\mathrm{d}s}{r}\ ,$$

where the r.h.s. has to be understood in the sense of distributions.

Proof. The proof is a simple application for $n = 2$ of the general formulae developed in [55, p. 439]. Let us however mention that the convention of this reference on the minus sign for the operator A in its spectral representation has not been adopted. □

As already mentioned $\varphi(A)$ leaves $\mathcal{H}_m$ invariant. More precisely, if $\mathfrak{f} = f\phi_m$ for some $f \in C_c^\infty(\mathbb{R}_+)$, then $\varphi(A)\mathfrak{f} = [\varphi(A)f]\phi_m$ with

$$[\varphi(A)f](r) = (2\pi)^{-1/2} \int_0^\infty \check{\varphi}\big(-\ln(s/r)\big)\, f(s)\, \frac{\mathrm{d}s}{r}\ , \tag{4.13}$$

where the r.h.s. has again to be understood in the sense of distributions

4.5 Scattering theory

In this section we briefly recall the main definitions of the scattering theory, and then give explicit formulae for the wave operators. The scattering operator will be studied in the following section.

Let H_1, H_2 be two self-adjoint operators in $\mathcal{H}$, and assume that the operator H_1 is purely absolutely continuous. Then the (time dependent) *wave operators* are defined by the strong limits

$$W_\pm(H_2, H_1) := s - \lim_{t\to\pm\infty} e^{itH_2}\, e^{-itH_1}$$

whenever these limits exist. In this case, these operators are isometries, and they are said *complete* if their ranges are equal to the absolutely continuous subspace $\mathcal{H}_{ac}(H_2)$ of $\mathcal{H}$ with respect to H_2. In such a situation, the (time dependent) *scattering operator* for the system (H_2, H_1) is defined by the product

$$S(H_2, H_1) := W_+^*(H_2, H_1)\, W_-(H_2, H_1)$$

and is a unitary operator in $\mathcal{H}$. Furthermore, it commutes with the operator H_1, and thus is unitarily equivalent to a family of unitary operators in the spectral representation of H_1.

We shall now prove that the wave operators exist for our model and that they are complete. For that purpose, let us denote by $H_0 := -\Delta$ the Laplace operator on $\mathbb{R}^2$.

Lemma 4.5.1. *For any self-adjoint extension H_α^{CD}, the wave operators $W_\pm(H_\alpha^{CD}, H_0)$ exist and are complete.*

Proof. On the one hand, the existence and the completeness of the operators $W_\pm(H_\alpha^{AB}, H_0)$ has been proved in [100]. On another hand, the existence and the completeness of the operator $W_\pm(H_\alpha^{CD}, H_\alpha^{AB})$ is well known since the difference of the resolvents is a finite rank operator, see for example [57, Sec. X.4.4]. The statement of the lemma follows then by taking the chain rule [118, Thm. 2.1.7] and the Theorem 2.3.3 of [118] on completeness into account. ☐

The derivation of the explicit formulae for the wave operators is based on the stationary approach, as presented in Sections 2.7 and 5.2 of [118]. For simplicity, we shall consider only $W_-^{CD} := W_-(H_\alpha^{CD}, H_0)$. For that purpose, let $\lambda \in \mathbb{R}_+$ and $\varepsilon > 0$. We first study the expression

$$\frac{\varepsilon}{\pi}\left\langle (H_0 - \lambda + i\varepsilon)^{-1}\mathfrak{f}, (H_\alpha^{CD} - \lambda + i\varepsilon)^{-1}\mathfrak{g}\right\rangle$$

and its limit as $\varepsilon \searrow 0$ for suitable $\mathfrak{f}, \mathfrak{g} \in \mathcal{H}$ specified later on. By taking Krein resolvent formula into account, one can consider separately the two expressions:

$$\frac{\varepsilon}{\pi}\left\langle (H_0 - \lambda + i\varepsilon)^{-1}\mathfrak{f}, (H_\alpha^{AB} - \lambda + i\varepsilon)^{-1}\mathfrak{g}\right\rangle$$

and

$$-\frac{\varepsilon}{\pi}\Big\langle (H_0 - \lambda + i\varepsilon)^{-1}\mathfrak{f}, \gamma(\lambda - i\varepsilon)\big(DM(\lambda - i\varepsilon) - C\big)^{-1} D\gamma(\lambda + i\varepsilon)^*\mathfrak{g}\Big\rangle .$$

The first term will lead to the wave operator for the original Aharonov-Bohm system, as shown below. So let us now concentrate on the second expression.

For simplicity, we set $z = \lambda + i\varepsilon$ and observe that

$$\begin{aligned} & -\frac{\varepsilon}{\pi}\left\langle (H_0 - \bar z)^{-1}\mathfrak{f}, \gamma(\bar z)\big(DM(\bar z) - C\big)^{-1} D\gamma(z)^*\mathfrak{g}\right\rangle \\ = \; & -\frac{\varepsilon}{\pi}\left\langle \gamma(z)\big[\big(DM(\bar z) - C\big)^{-1} D\big]^*\gamma(\bar z)^*(H_0 - \bar z)^{-1}\mathfrak{f}, \mathfrak{g}\right\rangle . \end{aligned}$$

Then, for every $r \in \mathbb{R}_+$ and $\theta \in [0, 2\pi)$ one has

$$\begin{aligned} & -\frac{\varepsilon}{\pi}\Big[\gamma(z)\big[\big(DM(\bar z) - C\big)^{-1} D\big]^*\gamma(\bar z)^*(H_0 - \bar z)^{-1}\mathfrak{f}\Big](r, \theta) \\ = \; & -\frac{\varepsilon}{\pi}\begin{pmatrix} H_\alpha^{(1)}(\sqrt{z}r)\phi_0(\theta) \\ H_{1-\alpha}^{(1)}(\sqrt{z}r)\phi_{-1}(\theta)\end{pmatrix}^T \cdot A(z)\big[\big(DM(\bar z) - C\big)^{-1} D\big]^* A(\bar z)^* \begin{pmatrix}\xi_0(z,\mathfrak{f}) \\ \xi_{-1}(z,\mathfrak{f})\end{pmatrix} \end{aligned}$$

with

$$A(z) := \begin{pmatrix} a_\alpha(z)^{-1} & 0 \\ 0 & a_{1-\alpha}(z)^{-1}\end{pmatrix}$$

and

$$\begin{aligned}
\begin{pmatrix} \xi_0(z,\mathfrak{f}) \\ \xi_{-1}(z,\mathfrak{f}) \end{pmatrix} &= \begin{pmatrix} \big\langle H^{(1)}_{\alpha}(\sqrt{\bar z}\cdot)\phi_0, (H_0-\bar z)^{-1}\mathfrak{f}\big\rangle \\ \big\langle H^{(1)}_{1-\alpha}(\sqrt{\bar z}\cdot)\phi_{-1}, (H_0-\bar z)^{-1}\mathfrak{f}\big\rangle \end{pmatrix} \\
&= \begin{pmatrix} \big\langle \mathcal{F}(H_0-z)^{-1}H^{(1)}_{\alpha}(\sqrt{\bar z}\cdot)\phi_0, \hat{\mathfrak{f}}\big\rangle \\ \big\langle \mathcal{F}(H_0-z)^{-1}H^{(1)}_{1-\alpha}(\sqrt{\bar z}\cdot)\phi_{-1}, \hat{\mathfrak{f}}\big\rangle \end{pmatrix} \\
&= \begin{pmatrix} \big\langle \mathcal{F}_0(H_0-z)^{-1}H^{(1)}_{\alpha}(\sqrt{\bar z}\cdot), \hat f_0\big\rangle_{\mathbb{R}_+} \\ \big\langle \mathcal{F}_{-1}(H_0-z)^{-1}H^{(1)}_{1-\alpha}(\sqrt{\bar z}\cdot), \hat f_{-1}\big\rangle_{\mathbb{R}_+} \end{pmatrix} \\
&= \begin{pmatrix} \big\langle (X^2-z)^{-1}\mathcal{F}_0H^{(1)}_{\alpha}(\sqrt{\bar z}\cdot), \hat f_0\big\rangle_{\mathbb{R}_+} \\ \big\langle (X^2-z)^{-1}\mathcal{F}_{-1}H^{(1)}_{1-\alpha}(\sqrt{\bar z}\cdot), \hat f_{-1}\big\rangle_{\mathbb{R}_+} \end{pmatrix}
\end{aligned}$$

where $\langle\cdot,\cdot\rangle_{\mathbb{R}_+}$ denotes the scalar product in $\mathsf{L}^2(\mathbb{R}_+, r\,\mathrm{d}r)$.

We shall now calculate separately the limit as $\varepsilon \to 0$ of the different terms. We recall the convention that for $z \in \mathbb{C}\setminus\mathbb{R}_+$ on choose $k=\sqrt{z}$ with $\Im(z)>0$. For $\lambda\in\mathbb{R}_+$ one sets $\lim_{\varepsilon\searrow 0}\sqrt{\lambda+i\varepsilon} =: \kappa$ with $\kappa\in\mathbb{R}_+$. We first observe that for $\nu\in(0,1)$ one has

$$a_\nu(\lambda_+) := \lim_{\varepsilon\searrow 0} a_\nu(\lambda+i\varepsilon) = -\frac{2^\nu i}{\sin(\pi\nu)\Gamma(1-\nu)}\,\kappa^{-\nu}$$

but

$$a_\nu(\lambda_-) := \lim_{\varepsilon\searrow 0} a_\nu(\lambda-i\varepsilon) = -\frac{2^\nu i e^{-i\pi\nu}}{\sin(\pi\nu)\Gamma(1-\nu)}\,\kappa^{-\nu}\ .$$

Similarly, one observes that

$$M(\lambda_\pm) := \lim_{\varepsilon\searrow 0} M(\lambda\pm i\varepsilon) = -\frac{2}{\pi}\sin(\pi\alpha)\begin{pmatrix} \frac{\Gamma(1-\alpha)^2 e^{\mp i\pi\alpha}}{4^\alpha}\kappa^{2\alpha} & 0 \\ 0 & \frac{\Gamma(\alpha)^2 e^{\mp i\pi(1-\alpha)}}{4^{1-\alpha}}\kappa^{2(1-\alpha)} \end{pmatrix}.$$

Note that $M(\lambda_+) = M(\lambda_-)^*$. Finally, the most elaborated limit is calculated in the next lemma.

Lemma 4.5.2. *For $m\in\mathbb{Z}$, $\nu\in(0,1)$ and $f\in C_c^\infty(\mathbb{R}_+)$ one has*

$$\lim_{\varepsilon\searrow 0}\varepsilon\big\langle (X^2-z)^{-1}\mathcal{F}_m H^{(1)}_\nu(\sqrt{\bar z}\cdot), f\big\rangle_{\mathbb{R}_+} = ie^{i\pi\nu/2}(-1)^{|m|}f(\kappa)\ .$$

Proof. Let us start by recalling that for $w\in\mathbb{C}$ satisfying $-\frac{\pi}{2} < \arg(w) \le \pi$ one has [1, eq. 9.6.4] :

$$H^{(1)}_\nu(w) = \frac{2}{i\pi}\,e^{-i\pi\nu/2}\,K_\nu(-iw)\ ,$$

where K_ν is the modified Bessel function of the second kind and of order ν. Then, for

$r \in \mathbb{R}_+$ it follows that (by using [114, Sec. 13.45] for the last equality)

$$\begin{aligned}
&[\mathcal{F}_m H_\nu^{(1)}(\sqrt{\bar{z}}\cdot)](r) \\
= \;& (-i)^{|m|}\text{l.i.m.}\int_{\mathbb{R}_+} \rho J_{|m|}(r\rho) H_\nu^{(1)}\big(\sqrt{\bar{z}}\rho\big)\mathrm{d}\rho \\
= \;& (-i)^{|m|}\frac{2}{i\pi}\, e^{-i\pi\nu/2}\text{l.i.m.}\int_{\mathbb{R}_+} \rho J_{|m|}(r\rho) K_\nu\big(-i\sqrt{\bar{z}}\rho\big)\mathrm{d}\rho \\
= \;& (-i)^{|m|}\frac{2}{i\pi}\, e^{-i\pi\nu/2}\frac{1}{r^2}\text{l.i.m.}\int_{\mathbb{R}_+} \rho J_{|m|}(\rho) K_\nu\Big(-i\frac{\sqrt{\bar{z}}}{r}\rho\Big)\mathrm{d}\rho \\
= \;& c\frac{1}{r^2}\Big(-i\frac{\sqrt{\bar{z}}}{r}\Big)^{-2-|m|}{}_2F_1\Big(\frac{|m|+\nu}{2}+1, \frac{|m|-\nu}{2}+1; |m|+1; -\Big(-i\frac{\sqrt{\bar{z}}}{r}\Big)^{-2}\Big)
\end{aligned}$$

where ${}_2F_1$ is the Gauss hypergeometric function [1, Chap. 15] and c is given by

$$c := (-i)^{|m|}\frac{2}{i\pi}\, e^{-i\pi\nu/2}\frac{\Gamma\big(\frac{|m|+\nu}{2}+1\big)\,\Gamma\big(\frac{|m|-\nu}{2}+1\big)}{\Gamma(|m|+1)}\ .$$

Now, observe that $\Big(-i\frac{\sqrt{\bar{z}}}{r}\Big)^{-2-|m|} = -(-i)^{-|m|}\Big(\frac{\sqrt{\bar{z}}}{r}\Big)^{-2-|m|}$ and $-\Big(-i\frac{\sqrt{\bar{z}}}{r}\Big)^{-2} = \frac{r^2}{\bar{z}}$. Thus, one has obtained

$$[\mathcal{F}_m H_\nu^{(1)}(\sqrt{\bar{z}}\cdot)](r) = d\frac{1}{r^2}\Big(\frac{\sqrt{\bar{z}}}{r}\Big)^{-2-|m|}{}_2F_1\Big(\frac{|m|+\nu}{2}+1, \frac{|m|-\nu}{2}+1; |m|+1; \frac{r^2}{\bar{z}}\Big)$$

with

$$d = -\frac{2}{i\pi}\, e^{-i\pi\nu/2}\frac{\Gamma\big(\frac{|m|+\nu}{2}+1\big)\,\Gamma\big(\frac{|m|-\nu}{2}+1\big)}{\Gamma(|m|+1)}\ .$$

By taking into account Equality 15.3.3 of [1] one can isolate from the ${}_2F_1$-function a factor which is singular when the variable goes to 1:

$$\begin{aligned}
&{}_2F_1\Big(\frac{|m|+\nu}{2}+1, \frac{|m|-\nu}{2}+1; |m|+1; \frac{r^2}{\bar{z}}\Big) \\
= \;& \frac{1}{1-r^2\bar{z}^{-1}}\;{}_2F_1\Big(\frac{|m|+\nu}{2}, \frac{|m|-\nu}{2}; |m|+1; \frac{r^2}{\bar{z}}\Big) \\
= \;& -\frac{\bar{z}}{r^2-\bar{z}}\;{}_2F_1\Big(\frac{|m|+\nu}{2}, \frac{|m|-\nu}{2}; |m|+1; \frac{r^2}{\bar{z}}\Big)\ .
\end{aligned}$$

Altogether, one has thus obtained:

$$\begin{aligned}
&\varepsilon\big[(X^2-z)^{-1}\mathcal{F}_m H_\nu^{(1)}(\sqrt{\bar{z}}\cdot)\big](r) \\
= \;& -d\frac{\varepsilon}{(r^2-\bar{z})(r^2-z)}\frac{\bar{z}}{r^2}\Big(\frac{\sqrt{\bar{z}}}{r}\Big)^{-2-|m|}{}_2F_1\Big(\frac{|m|+\nu}{2}, \frac{|m|-\nu}{2}; |m|+1; \frac{r^2}{\bar{z}}\Big)\ .
\end{aligned}$$

Now, observe that

$$\frac{\varepsilon}{(r^2-\bar{z})(r^2-z)} = \frac{\varepsilon}{(r^2-\lambda+i\varepsilon)(r^2-\lambda-i\varepsilon)} = \frac{\varepsilon}{(r^2-\lambda)^2+\varepsilon^2} =: \pi\delta_\varepsilon(r^2-\lambda)$$

which converges to $\pi\delta(r^2-\lambda)$ in the sense of distributions on $\mathbb{R}$ as ε goes to 0. Furthermore, the map

$$\mathbb{R}_+ \ni r \mapsto {}_2F_1\Big(\frac{|m|+\nu}{2}, \frac{|m|-\nu}{2}; |m|+1; \frac{r^2}{\lambda - i\varepsilon}\Big) \in \mathbb{C}$$

is locally uniformly convergent as $\varepsilon \to 0$ to a continuous function which is equal for $r = \kappa = \sqrt{\lambda}$ to $\Gamma(|m|+1)\big[\Gamma\big(\frac{|m|+\nu}{2}+1\big)\,\Gamma\big(\frac{|m|-\nu}{2}+1\big)\big]^{-1}$. By considering trivial extensions on $\mathbb{R}$, it follows that

$$\begin{aligned}
&\lim_{\varepsilon \searrow 0} \varepsilon \big\langle (X^2-z)^{-1}\mathcal{F}_m H_\nu^{(1)}(\sqrt{z}\cdot), f\big\rangle_{\mathbb{R}_+} \\
&= -\bar{d}\pi \lim_{\varepsilon \searrow 0} \int_{\mathbb{R}_+} r\delta_\varepsilon(r^2-\lambda)\overline{\frac{z}{r^2}\Big(\frac{\sqrt{z}}{r}\Big)^{-2-|m|}{}_2F_1\Big(\frac{|m|+\nu}{2}, \frac{|m|-\nu}{2}; |m|+1; \frac{r^2}{\bar{z}}\Big)} f(r)\mathrm{d}r \\
&= -\frac{\bar{d}\pi}{2\kappa}\kappa(-1)^{-|m|}\frac{\Gamma(|m|+1)}{\Gamma\big(\frac{|m|+\nu}{2}+1\big)\Gamma\big(\frac{|m|-\nu}{2}+1\big)} f(\kappa) \\
&= ie^{i\pi\nu/2}(-1)^{|m|} f(\kappa)\ .
\end{aligned}$$

□

By adding these different results and by taking Lemma 4.3.3 into account, one has thus proved:

Lemma 4.5.3. *For any $\mathfrak{f}$ of the form $\sum_{m\in\mathbb{Z}} f_m\phi_m$ with $f_m = 0$ except for a finite number of m for which $\hat{f}_m \in C_c^\infty(\mathbb{R}_+)$ and for any $\mathfrak{g} \in C_c^\infty(\mathbb{R}^2 \setminus \{0\})$, one has*

$$\begin{aligned}
&\lim_{\varepsilon \searrow 0} -\frac{\varepsilon}{\pi}\Big\langle (H_0-\lambda+i\varepsilon)^{-1}\mathfrak{f}, \gamma(\lambda-i\varepsilon)\big(DM(\lambda-i\varepsilon)-C\big)^{-1}D\gamma(\lambda+i\varepsilon)^*\mathfrak{g}\Big\rangle \\
&= -\frac{1}{\pi}\Big\langle \begin{pmatrix} H_\alpha^{(1)}(\kappa\cdot)\phi_0 \\ H_{1-\alpha}^{(1)}(\kappa\cdot)\phi_{-1}\end{pmatrix}^T \cdot A(\lambda_+)\big(DM(\lambda_+)-C\big)^{-1}DA(\lambda_-)^*\begin{pmatrix} ie^{i\pi\alpha/2}\hat{f}_0(\kappa) \\ -ie^{i\pi(1-\alpha)/2}\hat{f}_{-1}(\kappa)\end{pmatrix}, \mathfrak{g}\Big\rangle
\end{aligned}$$

Before stating the main result on W_-^{CD}, let us first present the explicit form of the stationary wave operator $\widetilde{W}_-^{AB}$. Note that for this operator the equality between the time dependent approach and the stationary approach is known [2, 32, 100], and that a preliminary version of the following result has been given in [89]. So, let us observe that since the operator H_α^{AB} leaves each subspace $\mathcal{H}_m$ invariant [100], it gives rise to a sequence of channel operators $H_{\alpha,m}^{AB}$ acting on $\mathcal{H}_m$. The usual operator H_0 admitting a similar decomposition, the stationary wave operators $\widetilde{W}_\pm^{AB}$ can be defined in each channel, *i.e.* separately for each $m \in \mathbb{Z}$. Let us immediately observe that the angular part does not play any role for defining such operators. Therefore, we shall omit it as long as it does not lead to any confusion, and consider the channel wave operators $\widetilde{W}_{\pm,m}^{AB}$ from $\mathcal{H}_r$ to $\mathcal{H}_r$.

The following notation will be useful: $\mathbb{T} := \{z \in \mathbb{C} \mid |z| = 1\}$ and

$$\delta_m^\alpha = \tfrac{1}{2}\pi\big(|m| - |m+\alpha|\big) = \begin{cases} -\tfrac{1}{2}\pi\alpha & \text{if } m \geq 0 \\ \tfrac{1}{2}\pi\alpha & \text{if } m < 0 \end{cases}.$$

Proposition 4.5.4. *For each $m \in \mathbb{Z}$, one has*

$$W_{\pm,m}^{AB} = \widetilde{W}_{\pm,m}^{AB} = \varphi_m^\pm(A)\ ,$$

with $\varphi_m^\pm \in C\big([-\infty,+\infty],\mathbb{T}\big)$ *given explicitly by*

$$\varphi_m^\pm(x) := e^{\mp i\delta_m^\alpha}\,\frac{\Gamma\big(\frac{1}{2}(|m|+1+ix)\big)}{\Gamma\big(\frac{1}{2}(|m|+1-ix)\big)}\,\frac{\Gamma\big(\frac{1}{2}(|m+\alpha|+1-ix)\big)}{\Gamma\big(\frac{1}{2}(|m+\alpha|+1+ix)\big)} \tag{4.14}$$

and satisfying $\varphi_m^\pm(\pm\infty)=1$ *and* $\varphi_m^\pm(\mp\infty)=e^{\mp 2i\delta_m^\alpha}$.

Proof. As already mentioned, the first equality in proved in [100]. Furthermore it is also proved there that for any $f\in\mathcal{H}_r$ and $r\in\mathbb{R}_+$ one has

$$[W_{\pm,m}^{AB}f](r) = i^{|m|}\ \text{l.i.m.}\int_{\mathbb{R}_+}\kappa\,J_{|m+\alpha|}(\kappa r)\,e^{\mp i\delta_m^\alpha}\,[\mathcal{F}_m f](\kappa)\,\mathrm{d}\kappa\,.$$

In particular, if $f\in C_c^\infty(\mathbb{R}_+)$, this expression can be rewritten as

$$\begin{aligned}
& s-\lim_{N\to\infty} e^{\mp i\delta_m^\alpha}\int_0^N \kappa\,J_{|m+\alpha|}(\kappa r)\Big[\int_0^\infty s\,J_{|m|}(s\kappa)\,f(s)\,\mathrm{d}s\Big]\mathrm{d}\kappa\\
= \;& s-\lim_{N\to\infty} e^{\mp i\delta_m^\alpha}\int_0^\infty s\,f(s)\Big[\int_0^N \kappa\,J_{|m|}(s\kappa)\,J_{|m+\alpha|}(\kappa r)\,\mathrm{d}\kappa\Big]\mathrm{d}s\\
= \;& s-\lim_{N\to\infty} e^{\mp i\delta_m^\alpha}\int_0^\infty \frac{s}{r}\,f(s)\Big[\int_0^{Nr} \kappa\,J_{|m|}(\tfrac{s}{r}\kappa)\,J_{|m+\alpha|}(\kappa)\,\mathrm{d}\kappa\Big]\frac{\mathrm{d}s}{r}\\
= \;& e^{\mp i\delta_m^\alpha}\int_0^\infty \frac{s}{r}\Big[\int_0^\infty \kappa\,J_{|m|}(\tfrac{s}{r}\kappa)\,J_{|m+\alpha|}(\kappa)\,\mathrm{d}\kappa\Big]f(s)\,\frac{\mathrm{d}s}{r}\,,
\end{aligned} \tag{4.15}$$

where the last term has to be understood in the sense of distributions on $\mathbb{R}_+$. The distribution between square brackets has been computed in [63, Prop. 2] but we shall not use here its explicit form.

Now, by comparing (4.15) with (4.13), one observes that the channel wave operator $W_{\pm,m}^{AB}$ is equal on a dense set in $\mathcal{H}_r$ to $\varphi_m^\pm(A)$ for a function $\varphi_m^\pm$ whose inverse Fourier transform is the distribution which satisfies for $y\in\mathbb{R}$:

$$\check{\varphi}_m^\pm(y) = \sqrt{2\pi}\,e^{\mp i\delta_m^\alpha}\,e^{-y}\,\Big[\int_0^\infty \kappa\,J_{|m|}(e^{-y}\kappa)\,J_{|m+\alpha|}(\kappa)\,\mathrm{d}\kappa\Big]\,.$$

The Fourier transform of this distribution can be computed. Explicitly one has (in the sense of distributions) :

$$\begin{aligned}
\varphi_m^\pm(x) &= e^{\mp i\delta_m^\alpha}\int_{\mathbb{R}} e^{-ixy}\,e^{-y}\Big[\int_{\mathbb{R}_+}\kappa\,J_{|m|}(e^{-y}\kappa)\,J_{|m+\alpha|}(\kappa)\,\mathrm{d}\kappa\Big]\mathrm{d}y\\
&= e^{\mp i\delta_m^\alpha}\int_{\mathbb{R}_+}\kappa^{(1-ix)-1}\,J_{|m+\alpha|}(\kappa)\,\mathrm{d}\kappa\int_{\mathbb{R}_+} s^{(1+ix)-1}\,J_{|m|}(s)\,\mathrm{d}s
\end{aligned}$$

which is the product of two Mellin transforms. The explicit form of these transforms are presented in [79, Eq. 10.1] and a straightforward computation leads directly to the expression (4.14). The second equality of the statement follows then by a density argument.

The additional properties of $\varphi_m^\pm$ can easily be obtained by taking into account the equality $\Gamma(\overline{z})=\overline{\Gamma(z)}$ valid for any $z\in\mathbb{C}$ as well as the asymptotic development of the function Γ as presented in [1, Eq. 6.1.39]. □

Since the wave operators $W_\pm^{AB}$ admit a decomposition into channel wave operators, so does the scattering operator. The channel scattering operator $S_m^{AB} := (W_{+,m}^{AB})^* \, W_{-,m}^{AB}$, acting from $\mathcal{H}_r$ to $\mathcal{H}_r$, is simply given by

$$S_m^{AB} = \overline{\varphi_m^+}(A)\,\varphi_m^-(A) = e^{2i\delta_m^\alpha}\,.$$

Now, let us set $\mathcal{H}_{\text{int}} := \mathcal{H}_0 \oplus \mathcal{H}_{-1}$ which is clearly isomorphic to $\mathcal{H}_r \otimes \mathbb{C}^2$, and consider the decomposition $\mathcal{H} = \mathcal{H}_{\text{int}} \oplus \mathcal{H}_{\text{int}}^\perp$. It follows from the considerations of Section 4.2 that for any pair (C, D) the operator $\widetilde{W}_\pm^{CD}$ is reduced by this decomposition and that $\widetilde{W}_-^{CD}|_{\mathcal{H}_{\text{int}}^\perp} = W_-^{CD}|_{\mathcal{H}_{\text{int}}^\perp} = W_-^{AB}|_{\mathcal{H}_{\text{int}}^\perp}$. Since the form of W_-^{AB} has been exposed above, we shall concentrate only of the restriction of $\widetilde{W}_-^{CD}$ to $\mathcal{H}_{\text{int}}$. For that purpose, let us define a matrix valued function which is closely related to the scattering operator. For $\kappa \in \mathbb{R}_+$ we set

$$\begin{aligned}\widetilde{S}_\alpha^{CD}(\kappa) := 2i\sin(\pi\alpha) &\begin{pmatrix} \frac{\Gamma(1-\alpha)\,e^{-i\pi\alpha/2}}{2^\alpha}\,\kappa^\alpha & 0 \\ 0 & \frac{\Gamma(\alpha)\,e^{-i\pi(1-\alpha)/2}}{2^{1-\alpha}}\,\kappa^{(1-\alpha)} \end{pmatrix} \\ &\cdot \left(D \begin{pmatrix} \frac{\Gamma(1-\alpha)^2\,e^{-i\pi\alpha}}{4^\alpha}\,\kappa^{2\alpha} & 0 \\ 0 & \frac{\Gamma(\alpha)^2\,e^{-i\pi(1-\alpha)}}{4^{1-\alpha}}\,\kappa^{2(1-\alpha)} \end{pmatrix} + \frac{\pi}{2\sin(\pi\alpha)} C \right)^{-1} D \\ &\cdot \begin{pmatrix} \frac{\Gamma(1-\alpha)\,e^{-i\pi\alpha/2}}{2^\alpha}\,\kappa^\alpha & 0 \\ 0 & -\frac{\Gamma(\alpha)\,e^{-i\pi(1-\alpha)/2}}{2^{1-\alpha}}\,\kappa^{(1-\alpha)} \end{pmatrix}.\end{aligned} \tag{4.16}$$

Theorem 4.5.5. *For any pair (C, D) satisfying* (4.7)*, the restriction of the wave operator W_-^{CD} to $\mathcal{H}_{\text{int}}$ satisfies the equality*

$$W_-^{CD}|_{\mathcal{H}_{\text{int}}} = \widetilde{W}_-^{CD}|_{\mathcal{H}_{\text{int}}} = \begin{pmatrix} \varphi_0^-(A) & 0 \\ 0 & \varphi_{-1}^-(A) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(A) & 0 \\ 0 & \tilde{\varphi}_{-1}(A) \end{pmatrix} \widetilde{S}_\alpha^{CD}(\sqrt{H_0}), \tag{4.17}$$

where $\tilde{\varphi}_m \in C\big([-\infty, +\infty], \mathbb{C}\big)$ for $m \in \{0, -1\}$. Explicitly, for every $x \in \mathbb{R}$, $\tilde{\varphi}_m(x)$ is given by

$$\frac{1}{2\pi}\, e^{-i\pi|m|/2}\, e^{\pi x/2}\, \frac{\Gamma\big(\frac{1}{2}(|m|+1+ix)\big)}{\Gamma\big(\frac{1}{2}(|m|+1-ix)\big)} \Gamma\Big(\frac{1}{2}(1+|m+\alpha|-ix)\Big)\,\Gamma\Big(\frac{1}{2}(1-|m+\alpha|-ix)\Big)$$

and satisfies $\tilde{\varphi}_m(-\infty) = 0$ and $\tilde{\varphi}_m(+\infty) = 1$.

Proof. a) The stationary representation $\widetilde{W}_-^{CD}$ is defined by the formula [118, Def. 2.7.2]:

$$\big\langle \widetilde{W}_-^{CD}\mathfrak{f}, \mathfrak{g} \big\rangle = \int_0^\infty \lim_{\varepsilon \searrow 0} \frac{\varepsilon}{\pi} \big\langle (H_0 - \lambda + i\varepsilon)^{-1}\mathfrak{f}, (H_\alpha^{CD} - \lambda + i\varepsilon)^{-1}\mathfrak{g} \big\rangle \,\mathrm{d}\lambda$$

for any $\mathfrak{f}$ of the form $\sum_{m\in\mathbb{Z}} f_m\phi_m$ with $f_m = 0$ except for a finite number of m for which $\hat{f}_m \in C_c^\infty(\mathbb{R}_+)$ and $\mathfrak{g} \in C_c^\infty(\mathbb{R}^2 \setminus \{0\})$. By taking Krein resolvent formula into account, we can first consider the expression

$$\int_0^\infty \lim_{\varepsilon \searrow 0} \frac{\varepsilon}{\pi} \big\langle (H_0 - \lambda + i\varepsilon)^{-1}\mathfrak{f}, (H_\alpha^{AB} - \lambda + i\varepsilon)^{-1}\mathfrak{g} \big\rangle \,\mathrm{d}\lambda$$

which converges to [2, 32, 100]:

$$\int_0^\infty \Big\langle \sum_{m\in\mathbb{Z}} i^{|m|}\, e^{i\delta_m^\alpha} J_{|m+\alpha|}(\kappa\cdot)\, \hat{f}_m(\kappa)\, \phi_m, \mathfrak{g}\Big\rangle\, \kappa\, \mathrm{d}\kappa\,.$$

This expression was the starting point for the formulae derived in Proposition 4.5.4. This leads to the first term in the r.h.s. of (4.17).

b) The second term to analyze is

$$-\int_0^\infty \lim_{\varepsilon\searrow 0}\frac{\varepsilon}{\pi}\Big\langle (H_0-\lambda+i\varepsilon)^{-1}\mathfrak{f}, \gamma(\lambda-i\varepsilon)\big(DM(\lambda-i\varepsilon)-C\big)^{-1}D\gamma(\lambda+i\varepsilon)^*\mathfrak{g}\Big\rangle\, \mathrm{d}\lambda\,. \quad (4.18)$$

By using then Lemma 4.5.3 and by performing some simple calculations, one obtains that (4.18) is equal to

$$\int_0^\infty \Big\langle \begin{pmatrix} \frac{1}{2} i^\alpha H_\alpha^{(1)}(\kappa\cdot)\phi_0 \\ \frac{1}{2} i^{1-\alpha} H_{1-\alpha}^{(1)}(\kappa\cdot)\phi_{-1}\end{pmatrix}^T \widetilde{S}_\alpha^{CD}(\kappa) \begin{pmatrix}\hat{f}_0(\kappa)\\ \hat{f}_{-1}(\kappa)\end{pmatrix}, \mathfrak{g}\Big\rangle \kappa\, \mathrm{d}\kappa\,.$$

Now, it is proved below that the operator T_m defined for $m\in\{0,-1\}$ on $\mathcal{F}^*[C_c^\infty(\mathbb{R}_+)]$ by

$$[T_m f](r) := \frac{1}{2} i^{|m+\alpha|}\int_0^\infty H_{|m+\alpha|}^{(1)}(\kappa r)\,[\mathcal{F}_m f](\kappa)\,\kappa\,\mathrm{d}\kappa \quad (4.19)$$

satisfies the equality $T_m=\tilde{\varphi}_m(A)$ with $\tilde{\varphi}_m$ given in the above statement. The stationary expression is then obtained by observing that $\mathcal{F}^*\widetilde{S}_\alpha^{CD}(\mathrm{K})\mathcal{F}=\widetilde{S}_\alpha^{CD}(\sqrt{H_0})$, where $\widetilde{S}_\alpha^{CD}(\mathrm{K})$ is the operator of multiplication by the function $\widetilde{S}_\alpha^{CD}(\cdot)$. Finally, the equality between the time dependent wave operator and the stationary wave operator is a consequence of Lemma 4.5.1 and of [118, Thm. 5.2.4].

c) By comparing (4.19) with (4.13), one observes that the operator T_m is equal on a dense set in $\mathcal{H}_r$ to $\tilde{\varphi}_m(A)$ for a function $\tilde{\varphi}_m$ whose inverse Fourier transform is the distribution which satisfies for $y\in\mathbb{R}$:

$$\check{\tilde{\varphi}}_m(y)=\frac{1}{2}\sqrt{2\pi}\, e^{-i\delta_m^\alpha}\, e^y \int_{\mathbb{R}_+}\kappa\, H_{|m+\alpha|}^{(1)}(e^y\kappa)\, J_{|m|}(\kappa)\,\mathrm{d}\kappa\,.$$

As before, the Fourier transform of this distribution can be computed. Explicitly one has (in the sense of distributions) :

$$\begin{aligned}\tilde{\varphi}_m(x) &= \frac{1}{2} e^{-i\delta_m^\alpha}\int_{\mathbb{R}} e^{-ixy}\, e^y\Big[\int_{\mathbb{R}_+}\kappa\, H_{|m+\alpha|}^{(1)}(e^y\kappa)\, J_{|m|}(\kappa)\,\mathrm{d}\kappa\Big]\mathrm{d}y\\ &= \frac{1}{2} e^{-i\delta_m^\alpha}\int_{\mathbb{R}_+}\kappa^{(1+ix)-1}\, J_{|m|}(\kappa)\,\mathrm{d}\kappa \int_{\mathbb{R}_+} s^{(1-ix)-1}\, H_{|m+\alpha|}^{(1)}(s)\,\mathrm{d}s\\ &= \frac{1}{2\pi}\, e^{-i\pi|m|/2}\,(-i)^{ix}\,\frac{\Gamma\big(\frac{1}{2}(|m|+1+ix)\big)}{\Gamma\big(\frac{1}{2}(|m|+1-ix)\big)}\\ &\quad\cdot\Gamma\Big(\frac{1}{2}(1+|m+\alpha|-ix)\Big)\,\Gamma\Big(\frac{1}{2}(1-|m+\alpha|-ix)\Big)\,.\end{aligned}$$

The last equality is obtained by taking into account the relation between the Hankel function $H_\nu^{(1)}$ and the Bessel function K_ν of the second kind as well as the Mellin transform of the functions J_ν and the function K_ν as presented in [79, Eq. 10.1 & 11.1].

The additional properties of $\tilde{\varphi}_m$ can easily be obtained by using the asymptotic development of the function Γ as presented in [1, Eq. 6.1.39]. □

4.6 Scattering operator

In this section, we concentrate on the scattering operator and on its asymptotic values for large and small energies.

Proposition 4.6.1. *The restriction of the scattering operator $S(H_\alpha^{CD}, H_0)$ to $\mathcal{H}_{\rm int}$ is explicitly given by*

$$S(H_\alpha^{CD}, H_0)\big|_{\mathcal{H}_{\rm int}} = S_\alpha^{CD}(\sqrt{H_0}) \quad \textit{with} \quad S_\alpha^{CD}(\kappa) := \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix} + \widetilde{S}_\alpha^{CD}(\kappa)\ .$$

Proof. Let us first recall that the scattering operator can be obtained from W_-^{CD} by the formula [11, Prop. 4.2]:

$$s-\lim_{t\to+\infty} e^{itH_0}\, e^{-itH} W_-^{CD} = S(H_\alpha^{CD}, H_0).$$

We stress that the completeness has been taken into account for this equality. Now, let us set $U(t) := e^{-it\ln(H_0)/2}$, where $\ln(H_0)$ is the self-adjoint operator obtained by functional calculus. By the intertwining property of the wave operators and by the invariance principle, one also has

$$s-\lim_{t\to+\infty} U(-t)\, W_-^{CD}\, U(t) = S(H_\alpha^{CD}, H_0).$$

On the other hand, the operator $\ln(H_0)/2$ is the generator of translations in the spectrum of A, *i.e.* $U(-t)\,\varphi(A)\,U(t) = \varphi(A+t)$ for any $\varphi : \mathbb{R} \to \mathbb{C}$. Since $\{U(t)\}_{t\in\mathbb{R}}$ is also reduced by the decomposition (4.1), it follows that

$$\begin{aligned} & s-\lim_{t\to+\infty} U(-t)\,\Big[W_-^{CD}\big|_{\mathcal{H}_{\rm int}}\Big]\,U(t) \\ = \;& s-\lim_{t\to+\infty} U(-t)\Big[\begin{pmatrix} \varphi_0^-(A) & 0 \\ 0 & \varphi_{-1}^-(A) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(A) & 0 \\ 0 & \tilde{\varphi}_{-1}(A) \end{pmatrix}\widetilde{S}_\alpha^{CD}(\sqrt{H_0})\Big]\,U(t) \\ = \;& \begin{pmatrix} \varphi_0^-(+\infty) & 0 \\ 0 & \varphi_{-1}^-(+\infty) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(+\infty) & 0 \\ 0 & \tilde{\varphi}_{-1}(+\infty) \end{pmatrix}\widetilde{S}_\alpha^{CD}(\sqrt{H_0}). \end{aligned}$$

The initial statement is then obtained by taking the asymptotic values mentioned in Proposition 4.5.4 and Theorem 4.5.5 into account. □

Even if the unitarity of the scattering operator follows from the general theory we give below a direct verification in order to better understand its structure. In the next statement, we only provide the value of the scattering matrix at energy 0 and energy equal to $+\infty$. However, more explicit expressions for $S_\alpha^{CD}(\kappa)$ are exhibited in the proof.

Proposition 4.6.2. *The map*

$$\mathbb{R}_+ \ni \kappa \mapsto S_\alpha^{CD}(\kappa) \in M_2(\mathbb{C}) \tag{4.20}$$

is continuous, takes values in the set $U(2)$ and has explicit asymptotic values for $\kappa = 0$ and $\kappa = +\infty$. More explicitly, depending on C, D or α one has:

i) If $D = 0$, then $S_\alpha^{CD}(\kappa) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$, *ii) If* $\det(D) \neq 0$*, then* $S_\alpha^{CD}(+\infty) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

iii) If $\dim[\ker(D)] = 1$ *and* $\alpha = 1/2$*, then* $S_\alpha^{CD}(+\infty) = (2\mathrm{P} - 1) \left(\begin{smallmatrix} i & 0 \\ 0 & -i \end{smallmatrix}\right)$*, where* P *is the orthogonal projection onto* $\ker(D)^\perp$,

iv) If $\ker(D) = \left(\begin{smallmatrix} \mathbb{C} \\ 0 \end{smallmatrix}\right)$ *or if* $\dim[\ker(D)] = 1$, $\alpha < 1/2$ *and* $\ker(D) \neq \left(\begin{smallmatrix} 0 \\ \mathbb{C} \end{smallmatrix}\right)$*, then* $S_\alpha^{CD}(+\infty) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

v) If $\ker(D) = \left(\begin{smallmatrix} 0 \\ \mathbb{C} \end{smallmatrix}\right)$ *or if* $\dim[\ker(D)] = 1$, $\alpha > 1/2$ *and* $\ker(D) \neq \left(\begin{smallmatrix} \mathbb{C} \\ 0 \end{smallmatrix}\right)$*, then* $S_\alpha^{CD}(+\infty) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$.

Furthermore,

a) If $C = 0$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

b) If $\det(C) \neq 0$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$,

c) If $\dim[\ker(C)] = 1$ *and* $\alpha = 1/2$*, then* $S_\alpha^{CD}(0) = (1 - 2\Pi) \left(\begin{smallmatrix} i & 0 \\ 0 & -i \end{smallmatrix}\right)$*, where* Π *is the orthogonal projection on* $\ker(C)^\perp$.

d) If $\ker(C) = \left(\begin{smallmatrix} 0 \\ \mathbb{C} \end{smallmatrix}\right)$ *or if* $\dim[\ker(C)] = 1$, $\alpha > 1/2$ *and* $\ker(C) \neq \left(\begin{smallmatrix} \mathbb{C} \\ 0 \end{smallmatrix}\right)$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

e) If $\ker(C) = \left(\begin{smallmatrix} \mathbb{C} \\ 0 \end{smallmatrix}\right)$ *or if* $\dim[\ker(C)] = 1$, $\alpha < 1/2$ *and* $\ker(C) \neq \left(\begin{smallmatrix} 0 \\ \mathbb{C} \end{smallmatrix}\right)$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$.

Proof. Let us fix $\kappa > 0$ and set $S := S_\alpha^{CD}(\kappa)$. For shortness, we also set $L := \frac{\pi}{2\sin(\pi\alpha)}\, C$ and

$$B = B(\kappa) := \begin{pmatrix} \frac{\Gamma(1-\alpha)}{2^\alpha}\,\kappa^\alpha & 0 \\ 0 & \frac{\Gamma(\alpha)}{2^{1-\alpha}}\,\kappa^{(1-\alpha)} \end{pmatrix}, \quad \Phi := \begin{pmatrix} e^{-i\pi\alpha/2} & 0 \\ 0 & e^{-i\pi(1-\alpha)/2} \end{pmatrix}, \quad J := \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right).$$

Note that the matrices B, Φ and J commute with each other, that the matrix B is self-adjoint and invertible, and that J and Φ are unitary.

I) It is trivially checked that if $D = 0$ the statement i) is satisfied.

II) Let us assume $\det(D) \neq 0$, *i.e.* D is invertible. Without loss of generality and as explained at the end of Section 4.3, we assume than that $D = 1$ and that the matrix C is self-adjoint. Then one has

$$\begin{aligned} S &= \Phi^2 J + 2i\sin(\pi\alpha)\, B\,\Phi (B^2\Phi^2 + L)^{-1} B\,\Phi\, J \\ &= B\,\Phi\,(B^2\Phi^2 + L)^{-1}\big[B\left(\Phi^2 + 2i\sin(\pi\alpha)\right) + L\,B^{-1}\big]\Phi\, J. \end{aligned}$$

By taking the equality $\Phi^2 + 2i\sin(\pi\alpha) = \Phi^{-2}$ into account, it follows that

$$\begin{aligned} S &= B\,\Phi\,(B^2\Phi^2 + L)^{-1}\big(B\,\Phi^{-2} + L\,B^{-1}\big)\Phi\, J \\ &= \Phi\left(\Phi^2 + B^{-1}L\,B^{-1}\right)^{-1}\big(\Phi^{-2} + B^{-1}L\,B^{-1}\big)\Phi\, J \\ &= \Phi\big(B^{-1}L\,B^{-1} + \cos(\pi\alpha)J - i\sin(\pi\alpha)\big)^{-1}\big(B^{-1}L\,B^{-1} + \cos(\pi\alpha)J + i\sin(\pi\alpha)\big)\Phi\, J\,. \end{aligned}$$

Since the matrix $B^{-1}LB^{-1} + \cos(\pi\alpha)J$ is self-adjoint, the above expression can be rewritten as

$$S = \Phi\,\frac{B^{-1}LB^{-1} + \cos(\pi\alpha)J + i\sin(\pi\alpha)}{B^{-1}LB^{-1} + \cos(\pi\alpha)J - i\sin(\pi\alpha)}\,\Phi\,J \tag{4.21}$$

which is clearly a unitary operator. The only dependence on κ in the terms B is continuous and one has

$$\lim_{\kappa\to+\infty} S^{CD}_\alpha(\kappa) = \Phi\,\frac{\cos(\pi\alpha)J + i\sin(\pi\alpha)}{\cos(\pi\alpha)J - i\sin(\pi\alpha)}\,\Phi\,J = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha}\end{pmatrix}$$

which proves the statement ii)

III) We shall now consider the situation $\det(D) = 0$ but $D \neq 0$. Obviously, $\ker(D)$ is of dimension 1. So let $p = (p_1, p_2)$ be a vector in $\ker(D)$ with $\|p\| = 1$. By (4.12) and by using the notation introduced in that section one has

$$S = \Phi^2\,J + 2i\sin(\pi\alpha)\,B\,\Phi\,I\,(P\,B^2\,\Phi^2\,I + \ell)^{-1}P\,B\,\Phi\,J. \tag{4.22}$$

Note that the matrix of $\mathrm{P} := IP : \mathbb{C}^2 \to \mathbb{C}^2$, *i.e.* the orthogonal projection onto $p^\perp$, is given by

$$\mathrm{P} = \begin{pmatrix} |p_2|^2 & -p_1\bar{p}_2 \\ -\bar{p}_1 p_2 & |p_1|^2 \end{pmatrix}$$

and that $PB^2\Phi^2 I$ is just the multiplication by the number

$$c(\kappa) = b_1^2(\kappa)\,|p_2|^2\,e^{-i\pi\alpha} - b_2^2(\kappa)\,|p_1|^2\,e^{i\pi\alpha}, \tag{4.23}$$

with $b_1(\kappa) = \frac{\Gamma(1-\alpha)}{2^\alpha}\,\kappa^\alpha$ and $b_2(\kappa) = \frac{\Gamma(\alpha)}{2^{1-\alpha}}\,\kappa^{(1-\alpha)}$.

In the special case $\alpha = 1/2$, the matrices B and Φ have the special form $B = \sqrt{\frac{\pi}{2}}\,\kappa^{1/2}$ and $\phi = e^{-i\pi/4}$. Clearly, one also has $b_1 = b_2 = \sqrt{\frac{\pi}{2}}\,\kappa^{1/2} := b$ and $c(\kappa) = -i\,b^2$. In that case, the expression (4.22) can be rewritten as

$$S = i\left[\frac{\pi\,\kappa/2 - i\,\ell}{\pi\,\kappa/2 + i\,\ell}\,\mathrm{P} + (\mathrm{P} - 1)\right] J \tag{4.24}$$

which is the product of unitary operators and thus is unitary. Furthermore, the dependence in κ is continuous and the asymptotic value is easily determined. This proves statement iii)

If $\alpha \neq 1/2$, let us rewrite S as

$$S = \Phi\,\big(c(\kappa) + \ell\big)^{-1}\big[2\,i\,\sin(\pi\alpha)\,B\,\mathrm{P}\,B + c(\kappa) + \ell\big]\,\Phi\,J\,. \tag{4.25}$$

Furthermore, by setting $X_- := \big(b_1^2\,|p_2|^2 - b_2^2\,|p_1|^2\big)$ and $X_+ := \big(b_1^2\,|p_2|^2 + b_2^2\,|p_1|^2\big)$ one has

$$c(\kappa) + \ell = \cos(\pi\alpha)\,X_- + \ell - i\sin(\pi\alpha)\,X_+$$

and

$$M := 2\,i\,\sin(\pi\alpha)\,B\,\mathrm{P}\,B + c(\kappa) + \ell = \begin{pmatrix} e^{i\pi\alpha}\,X_- + \ell & -2\,i\,\sin(\pi\alpha)\,b_1\,b_2\,p_1\,\bar{p}_2 \\ -2\,i\,\sin(\pi\alpha)\,b_1\,b_2\,\bar{p}_1\,p_2 & e^{-i\pi\alpha}\,X_- + \ell \end{pmatrix}.$$

With these notations, the unitary of S easily follows from the equality $\det(M) = |c(\kappa)+\ell|^2$. The continuity in κ of all the expressions also implies the expected continuity of the map (4.20). Finally, by taking (4.23) and the explicit form of M into account, the asymptotic values of $S_\alpha^{CD}(\kappa)$ for the cases iv) and v) can readily be obtained.

IV) Let us now consider the behavior of the scattering matrix near the zero energy. If $C = 0$, then $\det(D) \neq 0$ and one can use (4.21) with $L = 0$. The statement a) follows easily.

V) Assume that $\det(C) \neq 0$. In this case, it directly follows from (4.16) that $\widetilde{S}_\alpha^{CD}(0) = 0$, and then $S(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$ which proves b).

VI) We now assume that $\dim[\ker(C)] = 1$ and consider two cases.

Firstly, if $\det(D) \neq 0$ we can assume as in II) that C is self-adjoint and use again (4.21). Introducing the entries of L,

$$L = \begin{pmatrix} l_{11} & l_{12} \\ \overline{l_{12}} & l_{22} \end{pmatrix}$$

one obtains

$$\frac{B^{-1}LB^{-1} + \cos(\pi\alpha)J + i\sin(\pi\alpha)}{B^{-1}LB^{-1} + \cos(\pi\alpha)J - i\sin(\pi\alpha)} = \frac{1}{b_1^2\, l_{22}\, e^{-i\pi\alpha} - b_2^2\, l_{11}\, e^{i\pi\alpha} - b_1^2 b_2^2}$$
$$\cdot \begin{pmatrix} b_1^2\, l_{22}\, e^{i\pi\alpha} - b_2^2\, l_{11}\, e^{i\pi\alpha} - b_1^2 b_2^2\, e^{2i\pi\alpha} & b_1\, b_2\, l_{12}\,(e^{-i\pi\alpha} - e^{i\pi\alpha}) \\ b_1\, b_2\, \overline{l_{12}}\,(e^{-i\pi\alpha} - e^{i\pi\alpha}) & b_1^2\, l_{22}\, e^{-i\pi\alpha} - b_2^2\, l_{11}\, e^{-i\pi\alpha} - b_1^2 b_2^2\, e^{-2i\pi\alpha} \end{pmatrix}.$$

For $\alpha \neq 1/2$ one easily obtains the result stated in d) and e). For $\alpha = 1/2$, it follows that

$$\lim_{\kappa \searrow 0} \frac{B^{-1}LB^{-1} + \cos(\pi\alpha)J + i\sin(\pi\alpha)}{B^{-1}LB^{-1} + \cos(\pi\alpha)J - i\sin(\pi\alpha)} = \frac{2}{\mathrm{tr}(L)}\, L - 1,$$

and it only remains to observe that $L = \mathrm{tr}(L)\,\Pi$, where Π is the orthogonal projection on $\ker(L)^\perp = \ker(C)^\perp$. This proves c).

Secondly, let us assume that $\dim[\ker(D)] = 1$. By (4.11) there exists $U \in U(2)$ such that $\ker(C) = \ker(1-U)$ and $\ker(D) = \ker(1+U)$. As a consequence, one has $\ker(C) = \ker(D)^\perp$ and then $\mathrm{P} = 1 - \Pi$. On the other hand, we can use the expressions for the scattering operator obtained in III). However, observe that $CI = C\big|_{\ker(D)^\perp} = C\big|_{\ker(C)} = 0$ so we only have to consider these expressions in the special case $\ell = 0$. The asymptotic at 0 energy are then easily deduced from these expressions.

By summing the results obtained for $\det(D) \neq 0$ and for $\dim[\ker(D)] = 1$, and since $D = 0$ is not allowed if $\det(C) = 0$, one proves the cases c), d) and e). □

Remark 4.6.3. *As can be seen from the proof, the scattering matrix is independent of the energy in the following cases only:*

- $D = 0$, *then* $S_\alpha^{CD}(\kappa) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$,
- $C = 0$, *then* $S_\alpha^{CD}(\kappa) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$, *see* (4.21),
- $\ker(C) = \ker(D)^\perp = \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$, *then* $S_\alpha^{CD}(\kappa) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$, *see* (4.25),

- $\ker(C) = \ker(D)^\perp = \left(\begin{smallmatrix} 0 \\ \mathbb{C} \end{smallmatrix}\right)$, *then* $S_\alpha^{CD}(\kappa) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$, *see* (4.25),
- $\alpha = 1/2$ *and* $\det(C) = \det(D) = 0$, *then* $S_\alpha^{CD}(\kappa) = (2\mathrm{P} - 1)\left(\begin{smallmatrix} i & 0 \\ 0 & -i \end{smallmatrix}\right)$, *where* P *is the orthogonal projection on* $\ker(D)^\perp \equiv \ker(C)$, *see* (4.24).

4.7 Final remarks

As mentioned before, the parametrization of the self-adjoint extensions of H_α with the pair (C, D) satisfying (4.7) is highly none unique. For the sake of convenience, we recall here a one-to-one parametrization of all self-adjoint extensions and reinterpret a part of the results obtained before in this framework.

So, let $U \in U(2)$ and set

$$C = C(U) := \frac{1}{2}(1 - U) \quad \text{and} \quad D = D(U) = \frac{i}{2}(1 + U). \tag{4.26}$$

It is easy to check that C and D satisfy both conditions (4.7). In addition, two different elements U, U' of $U(2)$ lead to two different self-adjoint operators H_α^{CD} and $H_\alpha^{C'D'}$ with $C = C(U), D = D(U), C' = C(U')$ and $D' = D(U')$, *cf.* [52]. Thus, without ambiguity we can write H_α^U for the operator H_α^{CD} with C, D given by (4.26). Moreover, the set $\{H_\alpha^U \mid U \in U(2)\}$ describes all self-adjoint extensions of H_α, and, by (4.10), the map $U \to H_\alpha^U$ is continuous in the norm resolvent topology. Let us finally mention that the normalization of the above map has been chosen such that $H_\alpha^{-1} \equiv H_\alpha^{10} = H_\alpha^{AB}$.

Obviously, we could use various parametrizations for the set $U(2)$. For example, one could set

$$U = U(\eta, a, b) = e^{i\eta}\begin{pmatrix} a & -\bar{b} \\ b & \bar{a} \end{pmatrix}$$

with $\eta \in [0, 2\pi)$ and $a, b \in \mathbb{C}$ satisfying $|a|^2 + |b|^2 = 1$, which is the parametrization used in [2] (note nevertheless that the role of the unitary parameter was quite different). We could also use the parametrization inspired by [32]:

$$U = U(\omega, a, b, q) = e^{i\omega}\begin{pmatrix} q\,e^{ia} & -(1-q^2)^{1/2}\,e^{-ib} \\ (1-q^2)^{1/2}\,e^{ib} & q\,e^{-ia} \end{pmatrix}$$

with $\omega, a, b \in [0, 2\pi)$ and $q \in [0, 1]$. However, the following formulae look much simpler without such an arbitrary choice, and such a particularization can always be performed later on.

We can now rewrite part of the previous results in terms of U :

Lemma 4.7.1. *Let* $U \in U(2)$. *Then,*

i) For $z \in \rho(H_\alpha^{AB}) \cap \rho(H_\alpha^U)$ *the resolvent equation holds:*

$$(H_\alpha^U - z)^{-1} - (H_\alpha^{AB} - z)^{-1} = -\gamma(z)\big[(1 + U)M(z) + i(1 - U)\big]^{-1}(1 + U)\gamma(\bar{z})^*\ ,$$

ii) The number of negative eigenvalues of H_α^U *coincides with the number of negative eigenvalues of the matrix* $i(U - U^*)$, *iii) The value* $z \in \mathbb{R}_-$ *is an eigenvalue of* H_α^U *if and only if* $\det\big((1+U)M(z)+i(1-U)\big) = 0$, *and in that case one has*

$$\ker(H_\alpha^U - z) = \gamma(z)\ker\big((1+U)M(z)+i(1-U)\big)\ .$$

The wave operators can also be rewritten in terms of the single parameter U. We shall not do it here but simply express the asymptotic values of the scattering operator $S_\alpha^U := S(H_\alpha^U, H_0)$ in terms of U. If $\lambda \in \mathbb{C}$ is an eigenvalue of U, we denote by $\mathcal{V}_\lambda$ the corresponding eigenspace.

Proposition 4.7.2. *One has:*

i) If $U = -1$, *then* $S_\alpha^U(\kappa) \equiv S_\alpha^{AB} = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$,

ii) If $-1 \notin \sigma(U)$, *then* $S_\alpha^U(+\infty) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

iii) If $-1 \in \sigma(U)$ *with multiplicity one and* $\alpha = 1/2$, *then* $S_\alpha^U(+\infty) = (2\mathrm{P}-1)\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$, *where* P *is the orthogonal projection onto* $\mathcal{V}_{-1}^\perp$,

iv) If $\mathcal{V}_{-1} = \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$ *or if* $-1 \in \sigma(U)$ *with multiplicity one,* $\alpha < 1/2$ *and* $\mathcal{V}_{-1} \neq \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$, *then* $S_\alpha^U(+\infty) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

v) If $\mathcal{V}_{-1} = \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$ *or if* $-1 \in \sigma(U)$ *with multiplicity one,* $\alpha > 1/2$ *and* $\mathcal{V}_{-1} \neq \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$, *then* $S_\alpha^U(+\infty) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$.

Furthermore,

a) If $U = 1$, *then* $S_\alpha^U(0) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

b) If $1 \notin \sigma(U)$, *then* $S_\alpha^U(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$,

c) If $1 \in \sigma(U)$ *with multiplicity one and* $\alpha = 1/2$, *then* $S_\alpha^U(0) = (1-2\Pi)\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$, *where* Π *is the orthogonal projection on* $\mathcal{V}_1^\perp$.

d) If $\mathcal{V}_1 = \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$ *or if* $1 \in \sigma(U)$ *with multiplicity one,* $\alpha > 1/2$ *and* $\mathcal{V}_1 \neq \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$, *then* $S_\alpha^U(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

e) If $\mathcal{V}_1 = \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$ *or if* $1 \in \sigma(U)$ *with multiplicity one,* $\alpha < 1/2$ *and* $\mathcal{V}_1 \neq \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$, *then* $S_\alpha^U(0) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$.

Remark 4.7.3. *The scattering matrix is independent of the energy in the following cases only:*

- $U = -1$, *then* $S_\alpha^U(\kappa) \equiv S_\alpha^{AB} = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$,
- $U = 1$, *then* $S_\alpha^U(\kappa) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$, *see* (4.21),

- $U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, *then* $S_\alpha^U(\kappa) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$, *see* (4.25),
- $U = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$, *then* $S_\alpha^U(\kappa) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$, *see* (4.25),
- $\alpha = 1/2$ *and* $\sigma(U) = \{-1, 1\}$, *then* $S_\alpha^U = (2\mathrm{P} - 1) \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$, *where* P *is the orthogonal projection on* $\mathcal{V}_1$, *see* (4.24).

Chapter 5

Levinson's theorem and higher degree traces for Aharonov-Bohm operators

5.1 Introduction

In recent work [60, 61, 62, 64, 90] it was advocated that Levinson's theorem is of topological nature, namely that it should be viewed as an index theorem. The relevant index theorem occurs naturally in the framework of non-commutative topology, that is, C^*-algebras, their K-theory and higher traces (unbounded cyclic cocycles). The analytical hypothesis which has to be fulfilled for the index theoretic formulation to hold is that the wave operators of the scattering system lie in a certain C^*-algebra. In the examples considered until now, the index theorem substantially extends the usual Levinson's theorem which relates the number of bound states of a physical system to an expression depending on the scattering part of the system. In particular it sheds new light on the corrections due to resonances and on the regularization which are often involved in the proof of this relation. It also emphasizes the influence of the restriction of the waves operators at thresholds energies.

In the present paper we extend these investigations in two directions. On the one hand, we apply the general idea for the first time to a magnetic system. Indeed, the Aharonov-Bohm operators describe a two-dimensional physical system involving a singular magnetic field located at the origin and perpendicular to the plane of motion. On the other hand, due to the large number of parameters present in this model, we can develop a new topological equality involving higher degree traces. Such an equality, which we call a *higher degree Levinson's theorem*, extends naturally the usual Levinson's theorem (which corresponds to a relation between an 0-trace and a 1-trace) and it is apparently the first time that a relation between a 2-trace and a 3-trace is put into evidence in a physical context. While the precise physical meaning of this equality deserves more investigations, we have no doubt that it can play a role in the theory of topological transport and/or of adiabatic pumping [24].

Let us describe more precisely the content of this paper. In Section 5.2 we recall the contruction of the Aharonov-Bohm operators and present part of the results obtained in the previous chapter. Earlier references for the basic properties of these operators are [2, 3, 32, 89, 100]. In particular, we recall the explicit expressions for the wave operators in terms of functions of the free Laplacian and of the generator of the dilation group in $\mathbb{R}^2$. Let us mention that the theory of boundary triples, as presented in [27] was extensively used in the previous chapter for the computation of these explicit expressions.

In Section 5.3 we state and prove a version of Levinson's theorem adapted to our model, see Theorem 5.3.1. It will become clear at that moment that a naive approach of this theorem involving only the scattering operator would lead to a completely wrong result. Indeed, the corrections due to the restriction of the wave operators at 0-energy and at energy equal to $+\infty$ will be explicitly computed. Adding these different contributions leads to a first proof of Levinson's theorem. All the various situations, which depend on the parameters related to the flux of the magnetic field and to the description of the self-adjoint extensions, are summarized in Section 5.3.3. Let us stress that this proof is rather lengthy but that it leads to a very precise result. Note that up to this point, no C^*-algebraic knowledge is required, all proofs are purely analytical.

The last two sections of the paper contain the necessary algebraic framework, the two topological statements and their proofs. So Section 5.4 contains a very short introduction to K-theory, cyclic cohomology, n-traces, Connes' pairing and the dual boundary maps. Obviously, only the very few necessary information on these subjects is presented, and part of the constructions are over-simplified. However, the authors tried to give a flavor of this necessary background for non-experts, but any reader familiar with these constructions can skip Section 5.4 without any loss of understanding in the last part of the paper.

In the first part of Section 5.5, we construct a suitable C^*-algebra $\mathcal{E}$ which contains the wave operators. For computational reasons, this algebra should neither be too small nor too large. In the former case, the computation of its quotient by the ideal of compact operators would be too difficult and possibly not understandable, in the latter case the deducible information would become too vague. In fact, the algebra we propose is very natural once the explicit form of the wave operators is known. Once the quotient of the algebra $\mathcal{E}$ by the compact operators is computed, the new topological version of Levinson's theorem can be stated. This is done in Theorem 5.5.3 and in that case its proof is contained in a few lines. Note furthermore that there is a big difference between Theorem 5.3.1 and the topological statement (and its corollary). In the former case, the proof consisted in checking that the sum of various explicit contributions is equal to the number of bound states of the corresponding system. In the latter case, the proof involves a topological argument and it clearly shows the topological nature of Levinson's theorem. However, the statement is global, and the contributions due to the scattering operator and to the restrictions at 0-energy and at energy $+\infty$ can not be distinguished. For that reason, both approaches are complementary. Note that the topological approach opens the way towards generalisations which could hardly be guessed from the purely analytical approach.

Up to this point, the flux of the magnetic field as well as the parameters involved in the description of the self-adjoint extension were fixed. In the second topological statement, we shall consider a smooth boundaryless submanifold of the parameter space and perform some computations as these parameters vary on the manifold. More precisely, we first state an equality between a continuous family of projections on the bound states and the image through the index map of a continuous family of unitary operators deduced from the wave operators, see Theorem 5.5.5. These unitary operators contain a continuous family of scattering operators, but also the corresponding continuous family of restrictions at energies 0 and $+\infty$. Note that this result is still abstract, in the sense that it gives an equality between an equivalent class in the K_0-theory related to the bounded part of the system with an equivalent class in the K_1-theory related to the scattering part of the system, but nothing prevents this equality from being trivial in the sense that it yields $0 = 0$.

In the final part of the paper, we choose a 2-dimensional submanifold and show that the second topological result is not trivial. More precisely, we explicitly compute the pairings of the K-equivalent classes with their respective higher degree traces. On the one hand this leads to the computation of the Chern number of a bundle defined by the family of projections. For the chosen manifold this number is equal to 1, and thus is not trivial. By duality of the boundary maps, it follows that the natural 3-trace applied on the family of unitary operators is also not trivial. The resulting statement is provided in Proposition 5.5.7. Note that this statement is again global. A distinction of each contribution could certainly be interesting for certain applications, but its computation could be rather tedious and therefore no further investigations have been performed in that direction.

5.2 The Aharonov-Bohm model

In this section, we briefly recall the construction of the Aharonov-Bohm operators and present a part of the results obtained in the previous chapter to which we refer for details. We also mention [2, 32, 100] for earlier works on these operators.

5.2.1 The self-adjoint extensions

Let $\mathcal{H}$ denote the Hilbert space $\mathsf{L}^2(\mathbb{R}^2)$ with its scalar product $\langle\cdot,\cdot\rangle$ and its norm $\|\cdot\|$. For any $\alpha \in (0,1)$, we set $A_\alpha : \mathbb{R}^2 \setminus \{0\} \to \mathbb{R}^2$ by

$$A_\alpha(x,y) = -\alpha\Big(\frac{-y}{x^2+y^2}, \frac{x}{x^2+y^2}\Big),$$

corresponding formally to the magnetic field $B = \alpha\delta$ (δ is the Dirac delta function), and consider the operator

$$H_\alpha := (-i\nabla - A_\alpha)^2, \qquad \mathcal{D}(H_\alpha) = C_c^\infty\big(\mathbb{R}^2 \setminus \{0\}\big) .$$

Here $C_c^\infty(\Xi)$ denotes the set of smooth functions on Ξ with compact support. The closure of this operator in $\mathcal{H}$, which is denoted by the same symbol, is symmetric and has deficiency indices $(2,2)$.

We briefly recall the parametrization of the self-adjoint extensions of H_α from the previous chapter. Some elements of the domain of the adjoint operator H_α^* admit singularities at the origin. For dealing with them, one defines linear functionals Φ_0, Φ_{-1}, Ψ_0, Ψ_{-1} on $\mathcal{D}(H_\alpha^*)$ such that for $\mathfrak{f} \in \mathcal{D}(H_\alpha^*)$ one has, with $\theta \in [0,2\pi)$ and $r \searrow 0$,

$$2\pi\mathfrak{f}(r\cos\theta, r\sin\theta) = \Phi_0(\mathfrak{f})r^{-\alpha} + \Psi_0(\mathfrak{f})r^{\alpha} + e^{-i\theta}\Big(\Phi_{-1}(\mathfrak{f})r^{\alpha-1} + \Psi_{-1}(\mathfrak{f})r^{1-\alpha}\Big) + O(r).$$

The family of all self-adjoint extensions of the operator H_α is then indexed by two matrices $C, D \in M_2(\mathbb{C})$ which satisfy the following conditions:

$$\text{(i) } CD^* \text{ is self-adjoint,} \qquad \text{(ii) } \det(CC^* + DD^*) \neq 0, \tag{5.1}$$

and the corresponding extensions H_α^{CD} are the restrictions of H_α^* onto the functions $\mathfrak{f}$ satisfying the boundary conditions

$$C \begin{pmatrix} \Phi_0(\mathfrak{f}) \\ \Phi_{-1}(\mathfrak{f}) \end{pmatrix} = 2D \begin{pmatrix} \alpha\Psi_0(\mathfrak{f}) \\ (1-\alpha)\Psi_{-1}(\mathfrak{f}) \end{pmatrix}.$$

For simplicity, we call *admissible* a pair of matrices (C, D) satisfying the above conditions.

Remark 5.2.1. *The parametrization of the self-adjoint extensions of H_α with all admissible pairs (C, D) is very convenient but non-unique. At a certain point, it will be useful to have a one-to-one parametrization of all self-adjoint extensions. So, let us consider $U \in U(2)$ and set*

$$C(U) := \tfrac{1}{2}(1-U) \quad \text{and} \quad D(U) = \tfrac{i}{2}(1+U).$$

It is easy to check that $C(U)$ and $D(U)$ satisfy both conditions (5.1)*. In addition, two different elements U, U' of $U(2)$ lead to two different self-adjoint operators $H_\alpha^{C(U)\,D(U)}$ and $H_\alpha^{C(U')\,D(U')}$, cf. [52]. Thus, without ambiguity we can write H_α^U for the operator $H_\alpha^{C(U)\,D(U)}$. Moreover, the set $\{H_\alpha^U \mid U \in U(2)\}$ describes all self-adjoint extensions of H_α. Let us also mention that the normalization of the above maps has been chosen such that $H_\alpha^{-1} \equiv H_\alpha^{10} = H_\alpha^{AB}$ which corresponds to the standard Aharonov-Bohm operator studied in [3, 100].*

The essential spectrum of H_α^{CD} is absolutely continuous and covers the positive half line $[0, +\infty)$. The discrete spectrum consists of at most two negative eigenvalues. More precisely, the number of negative eigenvalues of H_α^{CD} coincides with the number of negative eigenvalues of the matrix CD^*.

The negative eigenvalues are the real negative solutions of the equation

$$\det\bigl(DM(z) - C\bigr) = 0$$

where $M(z)$ is, for $z < 0$,

$$M(z) = -\frac{2}{\pi}\sin(\pi\alpha) \begin{pmatrix} \Gamma(1-\alpha)^2\Bigl(-\frac{z}{4}\Bigr)^{\alpha} & 0 \\ 0 & \Gamma(\alpha)^2\Bigl(-\frac{z}{4}\Bigr)^{1-\alpha} \end{pmatrix},$$

and there exists an injective map $\gamma(z) : \mathbb{C}^2 \to \mathcal{H}$ depending continuously on $z \in \mathbb{C} \setminus [0, +\infty)$ and calculated explicitly in the previous chapter such that for each $z < 0$ one has $\ker(H_\alpha^{CD} - z) = \gamma(z) \ker\bigl(DM(z) - C\bigr)$.

5.2.2 Wave and scattering operators

One of the main result of the previous chapter is an explicit description of the wave operators. We shall recall this result below, but we first need to introduce the decomposition of the Hilbert space $\mathcal{H}$ with respect to a special basis. For any $m \in \mathbb{Z}$, let ϕ_m be the complex function defined by $[0, 2\pi) \ni \theta \mapsto \phi_m(\theta) := \frac{e^{im\theta}}{\sqrt{2\pi}}$. One has then the canonical isomorphism

$$\mathcal{H} \cong \bigoplus_{m\in\mathbb{Z}} \mathcal{H}_r \otimes [\phi_m] \, , \tag{5.2}$$

where $\mathcal{H}_r := \mathsf{L}^2(\mathbb{R}_+, r\,\mathrm{d}r)$ and $[\phi_m]$ denotes the one dimensional space spanned by ϕ_m. For shortness, we write $\mathcal{H}_m$ for $\mathcal{H}_r \otimes [\phi_m]$, and often consider it as a subspace of $\mathcal{H}$. Let us still set $\mathcal{H}_{\text{int}} := \mathcal{H}_0 \oplus \mathcal{H}_{-1}$ which is clearly isomorphic to $\mathcal{H}_r \otimes \mathbb{C}^2$.

Let us also recall that the unitary dilation group $\{U_\tau\}_{\tau\in\mathbb{R}}$ is defined on any $\mathfrak{f} \in \mathcal{H}$ and $x \in \mathbb{R}^2$ by

$$[U_\tau \mathfrak{f}](x) = e^\tau \mathfrak{f}(e^\tau x) \, .$$

Its self-adjoint generator A is formally given by $\frac{1}{2}(X \cdot (-i\nabla) + (-i\nabla) \cdot X)$, where X is the position operator and $-i\nabla$ is its conjugate operator. All these operators are essentially self-adjoint on the Schwartz space on $\mathbb{R}^2$. Clearly, the group of dilations as well as its generator leave each subspace $\mathcal{H}_m$ invariant.

Let us now consider the wave operators

$$W_-^{CD} := W_-(H_\alpha^{CD}, H_0) = s - \lim_{t\to-\infty} e^{itH_\alpha^{CD}} e^{-itH_0} \, .$$

where $H_0 := -\Delta$. It is well known that for any admissible pair (C, D) the operator $W_\pm^{CD}$ is reduced by the decomposition $\mathcal{H} = \mathcal{H}_{\text{int}} \oplus \mathcal{H}_{\text{int}}^\perp$ and that $W_-^{CD}|_{\mathcal{H}_{\text{int}}^\perp} = W_-^{AB}|_{\mathcal{H}_{\text{int}}^\perp}$. The restriction to $\mathcal{H}_{\text{int}}^\perp$ is further reduced by the decomposition (5.2) and it is proved in Proposition 4.5.4 that the channel wave operators satisfy for each $m \in \mathbb{Z}$,

$$W_{-,m}^{AB} = \varphi_m^-(A) \, ,$$

with φ_m^- explicitly given for $x \in \mathbb{R}$ by

$$\varphi_m^-(x) := e^{i\delta_m^\alpha} \frac{\Gamma\big(\frac{1}{2}(|m| + 1 + ix)\big)}{\Gamma\big(\frac{1}{2}(|m| + 1 - ix)\big)} \frac{\Gamma\big(\frac{1}{2}(|m + \alpha| + 1 - ix)\big)}{\Gamma\big(\frac{1}{2}(|m + \alpha| + 1 + ix)\big)}$$

and

$$\delta_m^\alpha = \tfrac{1}{2}\pi\big(|m| - |m + \alpha|\big) = \begin{cases} -\frac{1}{2}\pi\alpha & \text{if } m \geq 0 \\ \frac{1}{2}\pi\alpha & \text{if } m < 0 \end{cases} .$$

It is also proved in Theorem 4.5.5 that

$$W_-^{CD}|_{\mathcal{H}_{\text{int}}} = \begin{pmatrix} \varphi_0^-(A) & 0 \\ 0 & \varphi_{-1}^-(A) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(A) & 0 \\ 0 & \tilde{\varphi}_{-1}(A) \end{pmatrix} \widetilde{S}_\alpha^{CD}\big(\sqrt{H_0}\big) \tag{5.3}$$

with $\tilde{\varphi}_m(x)$ given for $m \in \{0, -1\}$ by

$$\frac{1}{2\pi} e^{-i\pi|m|/2} e^{\pi x/2} \frac{\Gamma\big(\frac{1}{2}(|m| + 1 + ix)\big)}{\Gamma\big(\frac{1}{2}(|m| + 1 - ix)\big)} \Gamma\big(\tfrac{1}{2}(1 + |m + \alpha| - ix)\big) \Gamma\big(\tfrac{1}{2}(1 - |m + \alpha| - ix)\big) \, .$$

Clearly, the functions φ_m^- and $\tilde\varphi_m$ are continuous on $\mathbb{R}$. Furthermore, these functions admit limits at $\pm\infty$: $\varphi_m^-(-\infty)=1$, $\varphi_m^-(+\infty)=e^{2i\delta_m^\alpha}$, $\tilde\varphi_m(-\infty)=0$ and $\tilde\varphi_m(+\infty)=1$. Note also that the expression for the function $\widetilde{S}_\alpha^{CD}(\cdot)$ is given for $\kappa\in\mathbb{R}_+$ by

$$\begin{aligned}\widetilde{S}_\alpha^{CD}(\kappa) := 2i\sin(\pi\alpha)&\begin{pmatrix}\frac{\Gamma(1-\alpha)e^{-i\pi\alpha/2}}{2^\alpha}\kappa^\alpha & 0\\ 0 & \frac{\Gamma(\alpha)e^{-i\pi(1-\alpha)/2}}{2^{1-\alpha}}\kappa^{(1-\alpha)}\end{pmatrix}\\
&\cdot\left(D\begin{pmatrix}\frac{\Gamma(1-\alpha)^2e^{-i\pi\alpha}}{4^\alpha}\kappa^{2\alpha} & 0\\ 0 & \frac{\Gamma(\alpha)^2e^{-i\pi(1-\alpha)}}{4^{1-\alpha}}\kappa^{2(1-\alpha)}\end{pmatrix}+\frac{\pi}{2\sin(\pi\alpha)}C\right)^{-1}D\\
&\cdot\begin{pmatrix}\frac{\Gamma(1-\alpha)e^{-i\pi\alpha/2}}{2^\alpha}\kappa^\alpha & 0\\ 0 & -\frac{\Gamma(\alpha)e^{-i\pi(1-\alpha)/2}}{2^{1-\alpha}}\kappa^{(1-\alpha)}\end{pmatrix}.\end{aligned}$$

As usual, the scattering operator is defined by the formula

$$S_\alpha^{CD} := \left[W_+^{CD}\right]^* W_-^{CD}.$$

Then, the relation between this operator and $\widetilde{S}_\alpha^{CD}$ is of the form

$$S_\alpha^{CD}|_{\mathcal{H}_{\text{int}}} = S_\alpha^{CD}(\sqrt{H_0}) \quad\text{with}\quad S_\alpha^{CD}(\kappa) := \begin{pmatrix}e^{-i\pi\alpha} & 0\\ 0 & e^{i\pi\alpha}\end{pmatrix} + \widetilde{S}_\alpha^{CD}(\kappa)\,. \tag{5.4}$$

The following result has been obtained in Proposition 4.6.2 and will be necessary further on:

Proposition 5.2.2. *The map*

$$\mathbb{R}_+ \ni \kappa \mapsto S_\alpha^{CD}(\kappa) \in U(2)$$

is continuous and has explicit asymptotic values for $\kappa=0$ and $\kappa=+\infty$. More explicitly, depending on C, D and α one has:

i) If $D=0$, then $S_\alpha^{CD}(\kappa)=\begin{pmatrix}e^{-i\pi\alpha} & 0\\ 0 & e^{i\pi\alpha}\end{pmatrix}$,

ii) If $\det(D)\neq 0$, then $S_\alpha^{CD}(+\infty)=\begin{pmatrix}e^{i\pi\alpha} & 0\\ 0 & e^{-i\pi\alpha}\end{pmatrix}$,

iii) If $\dim[\ker(D)]=1$ and $\alpha=1/2$, then $S_\alpha^{CD}(+\infty)=(2\mathrm{P}-1)\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}$, where P is the orthogonal projection onto $\ker(D)^\perp$,

iv) If $\ker(D)=\begin{pmatrix}\mathbb{C}\\ 0\end{pmatrix}$ or if $\dim[\ker(D)]=1$, $\alpha<1/2$ and $\ker(D)\neq\begin{pmatrix}0\\ \mathbb{C}\end{pmatrix}$, then $S_\alpha^{CD}(+\infty)=\begin{pmatrix}e^{-i\pi\alpha} & 0\\ 0 & e^{-i\pi\alpha}\end{pmatrix}$,

v) If $\ker(D)=\begin{pmatrix}0\\ \mathbb{C}\end{pmatrix}$ or if $\dim[\ker(D)]=1$, $\alpha>1/2$ and $\ker(D)\neq\begin{pmatrix}\mathbb{C}\\ 0\end{pmatrix}$, then $S_\alpha^{CD}(+\infty)=\begin{pmatrix}e^{i\pi\alpha} & 0\\ 0 & e^{i\pi\alpha}\end{pmatrix}$.

Furthermore,

a) If $C=0$, then $S_\alpha^{CD}(0)=\begin{pmatrix}e^{i\pi\alpha} & 0\\ 0 & e^{-i\pi\alpha}\end{pmatrix}$, *b) If* $\det(C) \neq 0$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$,

c) If $\dim[\ker(C)] = 1$ *and* $\alpha = 1/2$*, then* $S_\alpha^{CD}(0) = (1 - 2\Pi)\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$*, where* Π *is the orthogonal projection on* $\ker(C)^\perp$.

d) If $\ker(C) = \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$ *or if* $\dim[\ker(C)] = 1$*,* $\alpha > 1/2$ *and* $\ker(C) \neq \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{-i\pi\alpha} & 0 \\ 0 & e^{-i\pi\alpha} \end{pmatrix}$,

e) If $\ker(C) = \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$ *or if* $\dim[\ker(C)] = 1$*,* $\alpha < 1/2$ *and* $\ker(C) \neq \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$*, then* $S_\alpha^{CD}(0) = \begin{pmatrix} e^{i\pi\alpha} & 0 \\ 0 & e^{i\pi\alpha} \end{pmatrix}$.

5.3 The 0-degree Levinson's theorem, a pedestrian approach

In this section, we state a Levinson's type theorem adapted to our model. The proof is quite ad-hoc and will look like a recipe, but a much more conceptual one will be given subsequently. The main interest in this pedestrian approach is that it shows the importance of the restriction of the wave operators at 0-energy and at energy equal to $+\infty$. Let us remind the reader interested in the algebraic approach that the present proof can be skipped without any loss of understanding in the following sections.

Let us start by considering again the expression (5.3) for the operator $W_-^{CD}|_{\mathcal{H}_{\rm int}}$. It follows from the explicit expressions for the functions φ_m^-, $\tilde{\varphi}_m$ and $\widetilde{S}_\alpha^{CD}$ that $W_-^{CD}|_{\mathcal{H}_{\rm int}}$ is a linear combination of product of functions of two non-commuting operators with functions that are respectively continuous on $[-\infty, \infty]$ and on $[0, \infty]$ and which take values in $M_2(\mathbb{C})$. For a reason that will become limpid in the algebraic framework, we shall consider the restrictions of these products of functions on the endpoints of the closed intervals. Namely, let us first set for $x \in \mathbb{R}$ and $\kappa \in \mathbb{R}_+$

$$\Gamma_1(C,D,\alpha,x) := \begin{pmatrix} \varphi_0^-(x) & 0 \\ 0 & \varphi_{-1}^-(x) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(x) & 0 \\ 0 & \tilde{\varphi}_{-1}(x) \end{pmatrix} \widetilde{S}_\alpha^{CD}(0)\ , \tag{5.5}$$

$$\Gamma_2(C,D,\alpha,\kappa) := S_\alpha^{CD}(\kappa)\ , \tag{5.6}$$

$$\Gamma_3(C,D,\alpha,x) := \begin{pmatrix} \varphi_0^-(x) & 0 \\ 0 & \varphi_{-1}^-(x) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(x) & 0 \\ 0 & \tilde{\varphi}_{-1}(x) \end{pmatrix} \widetilde{S}_\alpha^{CD}(+\infty)\ , \tag{5.7}$$

$$\Gamma_4(C,D,\alpha,\kappa) := 1. \tag{5.8}$$

Clearly, $\Gamma_1(C,D,\alpha,\cdot)$ and $\Gamma_3(C,D,\alpha,\cdot)$ are continuous functions on $[-\infty,\infty]$ with values in $M_2(\mathbb{C})$, and $\Gamma_2(C,D,\alpha,\cdot)$ and $\Gamma_4(C,D,\alpha,\cdot)$ are continuous functions on $[0,\infty]$ with values in $M_2(\mathbb{C})$. Now, we set $\square \subset [0,\infty] \times [-\infty,\infty]$ for the union of the four parts: $\square = B_1 \cup B_2 \cup B_3 \cup B_4$, with $B_1 = \{0\} \times [-\infty,\infty]$, $B_2 = [0,\infty] \times \{+\infty\}$, $B_3 = \{+\infty\} \times [-\infty,\infty]$ and $B_4 = [0,\infty] \times \{-\infty\}$. Then, we naturally define the function $\Gamma(C,D,\alpha,\cdot) : \square \to M_2(\mathbb{C})$ by the relations $\Gamma\big(C,D,\alpha,(0,x)\big) = \Gamma_1(C,D,\alpha,x)$, $\Gamma\big(C,D,\alpha,(\kappa,\infty)\big) = \Gamma_2(C,D,\alpha,\kappa)$, $\Gamma\big(C,D,\alpha,(\infty,x)\big) = \Gamma_3(C,D,\alpha,x)$ and finally $\Gamma\big(C,D,\alpha,(\kappa,-\infty)\big) = \Gamma_4(C,D,\alpha,\kappa)$. In fact, since the following relations hold: $\Gamma_1(C,D,\alpha,\infty) = \Gamma_2(C,D,\alpha,0)$, $\Gamma_2(C,D,\alpha,\infty) = \Gamma_3(C,D,\alpha,\infty)$, $\Gamma_3(C,D,\alpha,-\infty) = \Gamma_4(C,D,\alpha,\infty)$, $\Gamma_4(C,D,\alpha,0) = \Gamma_1(C,D,\alpha,-\infty)$, one easily observes that $\Gamma(C,D,\alpha,\cdot)$ is a continuous function on $\square$ with values in $U(2)$. Thus, since $\Gamma(C,D,\alpha,\cdot)\in C\big(\square,U(2)\big)$, we can define the winding number $\mathrm{wind}\big[\Gamma(C,D,\alpha,\cdot)\big]$ of the map

$$\square\ni\zeta\mapsto\det[\Gamma(C,D,\alpha,\zeta)]\in\mathbb{T}$$

with orientation of $\square$ chosen clockwise. Here $\mathbb{T}$ denotes the set of complex numbers of modulus 1. The following statement is our Levinson's type theorem.

Theorem 5.3.1. *For any $\alpha\in(0,1)$ and any admissible pair (C,D) one has*

$$\mathrm{wind}\big[\Gamma(C,D,\alpha,\cdot)\big]=-\#\sigma_p(H_\alpha^{CD})=-\#\{\textit{negative eigenvalues of } CD^*\}\ .$$

Proof. The first equality is proved below by a case-by-case study. The equality between the cardinality of $\sigma_p(H_\alpha^{CD})$ and the number of negative eigenvalues of the matrix CD^* has been shown in Lemma 4.3.2. ☐

We shall now calculate separately the contribution to the winding number from the functions $\Gamma_1(C,D,\alpha,\cdot)$, $\Gamma_2(C,D,\alpha,\cdot)$ and $\Gamma_3(C,D,\alpha,\cdot)$. The contribution due to the scattering operator is the one given by $\Gamma_2(C,D,\alpha,\cdot)$. It will be rather clear that a naive approach of Levinson's theorem involving only the contribution of the scattering operator would lead to a completely wrong result. The final results are presented in Section 5.3.3.

5.3.1 Contributions of $\Gamma_1(C,D,\alpha,\cdot)$ and $\Gamma_3(C,D,\alpha,\cdot)$

In this section we calculate the contributions due to $\Gamma_1(C,D,\alpha,\cdot)$ and $\Gamma_3(C,D,\alpha,\cdot)$ which were introduced in (5.5) and (5.7). For that purpose, recall first the relation

$$S_\alpha^{CD}(\kappa):=\begin{pmatrix}e^{-i\pi\alpha}&0\\0&e^{i\pi\alpha}\end{pmatrix}+\widetilde{S}_\alpha^{CD}(\kappa)\ .$$

Since $S_\alpha^{CD}(0)$ and $S_\alpha^{CD}(+\infty)$ are diagonal in most of the situations, as easily observed in Proposition 5.2.2, let us define for $a\in\mathbb{C}$ and $m\in\{0,-1\}$ the following functions:

$$\varphi_m(\cdot,a):=\varphi_m^-(\cdot)+a\,\tilde{\varphi}_m(\cdot)\ .$$

Then, by a simple computation one obtains

$$\begin{aligned}\varphi_m(x,a)\ =\ &\frac{\Gamma\big(\frac12(|m|+1+ix)\big)}{\Gamma\big(\frac12(|m|+1-ix)\big)}\,\frac{\Gamma\big(\frac12(|m+\alpha|+1-ix)\big)}{\Gamma\big(\frac12(|m+\alpha|+1+ix)\big)}\ \cdot\\ &\cdot\Big[e^{i\delta_m^\alpha}+a\,e^{-i\pi|m|/2}\,\frac{e^{\pi x/2}}{2\sin\big(\frac{\pi}{2}(1+|m+\alpha|+ix)\big)}\Big].\end{aligned}$$

Let us mention that the equality

$$\Gamma(z)\Gamma\big(1-z\big)=\frac{\pi}{\sin(\pi z)}\tag{5.9}$$

for $z=\frac12(1+|m+\alpha|+ix)$ has been used for this calculation. In the case $a=0$, the function $\varphi_m(\cdot,0)$ clearly takes its values in $\mathbb{T}$. We shall now consider the other two special cases $\varphi_0(\cdot, e^{i\pi\alpha} - e^{-i\pi\alpha})$ and $\varphi_{-1}(\cdot, e^{-i\pi\alpha} - e^{i\pi\alpha})$ which will appear naturally subsequently. Few more calculations involving some trigonometric relations and the same relation (5.9) lead to

$$\begin{aligned}\varphi_0(x, e^{i\pi\alpha} - e^{-i\pi\alpha}) &= e^{i\pi\alpha/2} \frac{\Gamma\big(\frac{1}{2}(1+ix)\big)}{\Gamma\big(\frac{1}{2}(1-ix)\big)} \frac{\Gamma\big(\frac{1}{2}(1+\alpha-ix)\big)}{\Gamma\big(\frac{1}{2}(1+\alpha+ix)\big)} \frac{\sin\big(\frac{\pi}{2}(1+\alpha-ix)\big)}{\sin\big(\frac{\pi}{2}(1+\alpha+ix)\big)} \\ &= e^{i\pi\alpha/2} \frac{\Gamma\big(\frac{1}{2}(1+ix)\big)}{\Gamma\big(\frac{1}{2}(1-ix)\big)} \frac{\Gamma\big(\frac{1}{2}(1-\alpha-ix)\big)}{\Gamma\big(\frac{1}{2}(1-\alpha+ix)\big)}\end{aligned}$$

and to

$$\begin{aligned}\varphi_{-1}(x, e^{-i\pi\alpha} - e^{i\pi\alpha}) &= -e^{-i\pi\alpha/2} \frac{\Gamma\big(1+\frac{1}{2}ix\big)}{\Gamma\big(1-\frac{1}{2}ix\big)} \frac{\Gamma\big(1-\frac{1}{2}(\alpha+ix)\big)}{\Gamma\big(1-\frac{1}{2}(\alpha-ix)\big)} \frac{\sin\big(\frac{\pi}{2}(\alpha+ix)\big)}{\sin\big(\frac{\pi}{2}(\alpha-ix)\big)} \\ &= -e^{-i\pi\alpha/2} \frac{\Gamma\big(1+\frac{1}{2}ix\big)}{\Gamma\big(1-\frac{1}{2}ix\big)} \frac{\Gamma\big(\frac{1}{2}(\alpha-ix)\big)}{\Gamma\big(\frac{1}{2}(\alpha+ix)\big)}\ .\end{aligned}$$

Clearly, both functions are continuous and take values in $\mathbb{T}$. Furthermore, since φ_m^- and $\tilde{\varphi}_m$ have limits at $\pm\infty$, so does the functions $\varphi_m(\cdot, a)$. It follows that the variation of the arguments of the previous functions can be defined. More generally, for any continuously differentiable function $\varphi : [-\infty, \infty] \to \mathbb{T}$ we set

$$\mathrm{Var}[\varphi] := \frac{1}{i} \int_{-\infty}^{\infty} \varphi(x)^{-1} \varphi'(x)\, \mathrm{d}x\ .$$

Let us first state a convenient formula. Its proof is given in the Appendix 5.6.1.

Lemma 5.3.2. *Let* $a, b > 0$. *For* $\varphi_{a,b}(x) := \frac{\Gamma(a+ix)}{\Gamma(a-ix)} \frac{\Gamma(b-ix)}{\Gamma(b+ix)}$ *one has* $\mathrm{Var}[\varphi_{a,b}] = 2\pi(a-b)$.

As an easy corollary one obtains

Corollary 5.3.3. *The following equalities hold:*

i) $\mathrm{Var}[\varphi_m(\cdot, 0)] = 2\delta_m^\alpha$ *for* $m \in \{0, -1\}$,

ii) $\mathrm{Var}[\varphi_0(\cdot, e^{i\pi\alpha} - e^{-i\pi\alpha})] = \pi\alpha$,

iii) $\mathrm{Var}[\varphi_{-1}(\cdot, e^{-i\pi\alpha} - e^{i\pi\alpha})] = \pi(2-\alpha)$.

Let us now set

$$\phi_1(C, D, \alpha) := \mathrm{Var}\big[\det\big(\Gamma_1(C, D, \alpha, \cdot)\big)\big]$$

and

$$\phi_3(C, D, \alpha) := -\mathrm{Var}\big[\det\big(\Gamma_3(C, D, \alpha, \cdot)\big)\big].$$

The sign " $-$ " in the second definition comes from the sense of the computation of the winding number: from $+\infty$ to $-\infty$. By taking into account the above information and the expression $S_\alpha^{CD}(0)$ and $S_\alpha^{CD}(+\infty)$ recalled in Proposition 5.2.2 one can prove:

Proposition 5.3.4. *One has*

i) If $D = 0$*, then* $\phi_3(C, D, \alpha) = 0$*,*

ii) If $\det(D) \neq 0$*, then* $\phi_3(C, D, \alpha) = -2\pi$*,*

iii) If $\ker(D) = \binom{\mathbb{C}}{0}$ *or if* $\dim[\ker(D)] = 1$*,* $\alpha < 1/2$ *and* $\ker(D) \neq \binom{0}{\mathbb{C}}$*, then* $\phi_3(C, D, \alpha) = -2\pi(1 - \alpha)$*,*

iv) If $\ker(D) = \binom{0}{\mathbb{C}}$ *or if* $\dim[\ker(D)] = 1$*,* $\alpha > 1/2$ *and* $\ker(D) \neq \binom{\mathbb{C}}{0}$*, then* $\phi_3(C, D, \alpha) = -2\pi\alpha$*,*

v) If $\dim[\ker(D)] = 1$ *and* $\alpha = 1/2$*, then* $\phi_3(C, D, \alpha) = -\pi$*.*

Furthermore,

a) If $C = 0$*, then* $\phi_1(C, D, \alpha) = 2\pi$*,*

b) If $\det(C) \neq 0$*, then* $\phi_1(C, D, \alpha) = 0$*,*

c) If $\ker(C) = \binom{0}{\mathbb{C}}$ *or if* $\dim[\ker(C)] = 1$*,* $\alpha > 1/2$ *and* $\ker(C) \neq \binom{\mathbb{C}}{0}$*, then* $\phi_1(C, D, \alpha) = 2\pi(1 - \alpha)$*,*

d) If $\ker(C) = \binom{\mathbb{C}}{0}$ *or if* $\dim[\ker(C)] = 1$*,* $\alpha < 1/2$ *and* $\ker(C) \neq \binom{0}{\mathbb{C}}$*, then* $\phi_1(C, D, \alpha) = 2\pi\alpha$*,*

e) If $\dim[\ker(C)] = 1$ *and* $\alpha = 1/2$*, then* $\phi_1(C, D, \alpha) = \pi$*.*

Proof. Statements i) to iv) as well as statements a) to d) are easily obtained simply by taking the asymptotic values of $S^{CD}_\alpha(\cdot)$ into account. So let us concentrate on the remaining statements.

Let $p = (p_1, p_2) \in \mathbb{C}^2$ with $\|p\| = 1$, and let

$$\mathrm{P} = \begin{pmatrix} |p_2|^2 & -p_1\bar{p}_2 \\ -\bar{p}_1 p_2 & |p_1|^2 \end{pmatrix}$$

be the orthogonal projection onto $p^\perp$. For $x \in \mathbb{R}$, let us also set

$$\varphi(\mathrm{P}, x) := \begin{pmatrix} \varphi_0^-(x) & 0 \\ 0 & \varphi_{-1}^-(x) \end{pmatrix} + \begin{pmatrix} \tilde{\varphi}_0(x) & 0 \\ 0 & \tilde{\varphi}_{-1}(x) \end{pmatrix} 2\mathrm{P} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

whose determinant is equal to

$$g(x) := \varphi_0^-(x)\,\varphi_{-1}^-(x) + 2i\tilde{\varphi}_0(x)\,\varphi_{-1}^-(x)\,|p_2|^2 - 2i\varphi_0^-(x)\,\tilde{\varphi}_{-1}(x)|p_1|^2\,.$$

By taking the explicit expressions for these functions one obtains

$$\begin{aligned} g(x) \;=\; & \frac{\Gamma\big(\frac{1}{2}(1+ix)\big)}{\Gamma\big(\frac{1}{2}(1-ix)\big)} \frac{\Gamma\big(\frac{1}{2}(\frac{3}{2}-ix)\big)}{\Gamma\big(\frac{1}{2}(\frac{3}{2}+ix)\big)} \frac{\Gamma\big(\frac{1}{2}(2+ix)\big)}{\Gamma\big(\frac{1}{2}(2-ix)\big)} \frac{\Gamma\big(\frac{1}{2}(\frac{3}{2}-ix)\big)}{\Gamma\big(\frac{1}{2}(\frac{3}{2}+ix)\big)} \\ & \cdot \Big(1 + i\,e^{i\pi/4}\,\frac{e^{\pi x/2}}{\pi}\,\Gamma\big(\tfrac{1}{2}(\tfrac{1}{2}-ix)\big)\Gamma\big(\tfrac{1}{2}(\tfrac{3}{2}+ix)\big)\Big). \end{aligned}$$

Now, by setting $z = \frac{3}{4} + i\frac{x}{2}$ and by some algebraic computations one obtains

$$\begin{aligned}
&1 + ie^{i\pi/4}\frac{e^{\pi x/2}}{\pi}\Gamma\big(\tfrac{1}{2}(\tfrac{1}{2}-ix)\big)\Gamma\big(\tfrac{1}{2}(\tfrac{3}{2}+ix)\big)\\
&= 1 + \frac{i}{\pi}e^{-i\pi(z-1)}\Gamma(1-z)\Gamma(z) = 1 - i\frac{e^{-i\pi z}}{\sin(\pi z)}\\
&= -i\frac{\cos(\pi z)}{\sin(\pi z)} = -i\frac{1}{\tan\big(\frac{3\pi}{4} + i\frac{\pi x}{2}\big)}\\
&= -i\frac{\tanh(\frac{\pi x}{2}) - i}{\tanh(\frac{\pi x)}{2}) + i}\ .
\end{aligned}$$

Thus, one finally obtains that

$$g(x) = -i\frac{\Gamma\big(\frac{1}{2}(1+ix)\big)}{\Gamma\big(\frac{1}{2}(1-ix)\big)}\frac{\Gamma\big(\frac{1}{2}(\frac{3}{2}-ix)\big)}{\Gamma\big(\frac{1}{2}(\frac{3}{2}+ix)\big)}\frac{\Gamma\big(\frac{1}{2}(2+ix)\big)}{\Gamma\big(\frac{1}{2}(2-ix)\big)}\frac{\Gamma\big(\frac{1}{2}(\frac{3}{2}-ix)\big)}{\Gamma\big(\frac{1}{2}(\frac{3}{2}+ix)\big)}\frac{\tanh(\frac{\pi x}{2}) - i}{\tanh(\frac{\pi x}{2}) + i}\ .$$

Note that this function does not depend on the projection P at all.

Clearly one has

$$\mathrm{Var}[g] = \mathrm{Var}[\varphi_{\frac{1}{2},\frac{3}{4}}] + \mathrm{Var}[\varphi_{1,\frac{3}{4}}] + \mathrm{Var}\Big[\frac{\tanh(\frac{\pi\cdot}{2}) - i}{\tanh(\frac{\pi\cdot}{2}) + i}\Big] = -\frac{\pi}{2} + \frac{\pi}{2} + \pi = \pi.$$

Now, by observing that $\phi_3(C,D,\alpha) = -\mathrm{Var}[g]$ in the case v), one concludes that in this special case $\phi_3(C,D,\alpha) = -\pi$.

For the case e), observe that by setting $\mathrm{P} := 1 - \Pi$, one easily obtains that in this special case $\Gamma_1(C,D,\alpha,\cdot) = \varphi(\mathrm{P},\cdot)$. It follows that $\phi_1(C,D,\alpha) = \mathrm{Var}[g]$ and then $\phi_1(C,D,\alpha) = \pi$. □

5.3.2 Contribution of $\Gamma_2(C,D,\alpha,\cdot)$

Recall first that $\Gamma_2(C,D,\alpha,\cdot)$ defined in (5.6) is equal to $S^{CD}_\alpha(\cdot)$. We are interested here in the phase of $\det\big(S^{CD}_\alpha(\kappa)\big)$ acquired as κ runs from 0 to $+\infty$; we denote this phase by $\phi_2(C,D,\alpha)$. Note that if $\det\big(S^{CD}_\alpha(\kappa)\big) = \frac{\bar{f}(\kappa)}{f(\kappa)}$ for a non-vanishing continuous function $f : \mathbb{R}_+ \to \mathbb{C}^*$, then

$$\phi_2(C,D,\alpha) = -2\big(\arg f(+\infty) - \arg f(0)\big)\ ,$$

where $\arg : \mathbb{R}_+ \to \mathbb{R}$ is a continuous function defined by the argument of f. In the sequel, we shall also use the notation $\theta : \mathbb{C}^* \to (-\pi,\pi]$ for the principal argument of a complex number different from 0.

Now, let us consider $\kappa > 0$ and set $S(\kappa) := S^{CD}_\alpha(\kappa)$. For shortness, we also set $L := \frac{\pi}{2\sin(\pi\alpha)}C$ and

$$B := \begin{pmatrix} b_1(\kappa) & 0 \\ 0 & b_2(\kappa)\end{pmatrix} = \begin{pmatrix} \frac{\Gamma(1-\alpha)}{2^\alpha}\kappa^\alpha & 0 \\ 0 & \frac{\Gamma(\alpha)}{2^{1-\alpha}}\kappa^{(1-\alpha)}\end{pmatrix}, \quad \Phi := \begin{pmatrix} e^{-i\pi\alpha/2} & 0 \\ 0 & e^{-i\pi(1-\alpha)/2}\end{pmatrix},$$

and $J := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Note that the matrices B, Φ and J commute with each other, that the matrix B is self-adjoint and invertible, and that J and Φ are unitary.

I) If $D = 0$, then S_α^{CD} is constant and $\phi_2(C, D, \alpha) = 0$.

II) Let us assume $\det(D) \neq 0$, *i.e.* D is invertible. Without loss of generality, we may assume that $D = 1$, as explained in Section 4.3, and that C and hence L are self-adjoint. We write $C = (c_{jk})$, $L = (l_{jk})$ and we then use the expression

$$S(\kappa) = \Phi \, \frac{B^{-1} L B^{-1} + \cos(\pi\alpha) J + i \sin(\pi\alpha)}{B^{-1} L B^{-1} + \cos(\pi\alpha) J - i \sin(\pi\alpha)} \, \Phi \, J \,, \tag{5.10}$$

derived in the previous chapter. By direct calculation one obtains $\det\big(S(\kappa)\big) = \frac{\bar{f}(\kappa)}{f(\kappa)}$ with

$$\begin{aligned} f(\kappa) &= \det\big(B^{-1} L B^{-1} + \cos(\pi\alpha) J - i \sin(\pi\alpha)\big) \\ &= \det(L)\, b_1^{-2}(\kappa)\, b_2^{-2}(\kappa) - 1 + \cos(\pi\alpha)\big(l_{22}\, b_2^{-2}(\kappa) - l_{11}\, b_1^{-2}(\kappa)\big) \\ &\quad - i \sin(\pi\alpha)\big(l_{11}\, b_1^{-2}(\kappa) + l_{22}\, b_2^{-2}(\kappa)\big) \end{aligned} \tag{5.11}$$

and f is non-vanishing as the determinant of an invertible matrix.

For the computation of $\phi_2(C, D, \alpha)$ we shall have to consider several cases. We first assume that $\det(C) \neq 0$, which is equivalent to $\det(L) \neq 0$. In that case one clearly has $\det\big(S_\alpha^{CD}(0)\big) = \det\big(S_\alpha^{CD}(+\infty)\big)$, and then $\phi_2(C, D, \alpha)$ will be a multiple of 2π. Furthermore, note that $\theta\big(f(+\infty)\big) = \pi$ and that $\theta\big(f(0)\big) = 0$ if $\det(L) > 0$ and $\theta\big(f(0)\big) = \pi$ if $\det(L) < 0$.

Assuming that $l_{11}\, l_{22} \geq 0$ (which means that $\Im f$ is either non-negative or non-positive, and its sign is opposite to that of $\mathrm{tr}(L)$), one has the following cases:

II.1) If $\mathrm{tr}(C) > 0$ and $\det(C) > 0$, then $\Im f < 0$ and $\phi_2(C, D, \alpha) = 2\pi$,

II.2) If $\mathrm{tr}(C) > 0$ and $\det(C) < 0$, then $\Im f < 0$ and $\phi_2(C, D, \alpha) = 0$,

II.3) If $\mathrm{tr}(C) < 0$ and $\det(C) > 0$, then $\Im f > 0$ and $\phi_2(C, D, \alpha) = -2\pi$,

II.4) If $\mathrm{tr}(C) < 0$ and $\det(C) < 0$, then $\Im f > 0$ and $\phi_2(C, D, \alpha) = 0$,

II.5) If $c_{11} = c_{22} = 0$ (automatically $\det(C) < 0$), then f is real and non-vanishing, hence $\phi_2(C, D, \alpha) = 0$.

Now, if $l_{11} l_{22} < 0$ the main difference is that the parameter α has to be taken into account. On the other hand, one has $\det(L) < 0$ which implies that $\arg f(+\infty) - \arg f(0)$ has to be a multiple of 2π. For the computation of this difference, observe that the equation $\Im f(\kappa) = 0$ (for $\kappa \geq 0$) is equivalent to

$$\frac{b_1^{-2}(\kappa)}{b_2^{-2}(\kappa)} = -\frac{l_{22}}{l_{11}} \iff \kappa^{2\alpha-1} = 2^{2\alpha-1} \frac{\Gamma(\alpha)}{\Gamma(1-\alpha)} \sqrt{-\frac{l_{11}}{l_{22}}}. \tag{5.12}$$

For $\alpha \neq 1/2$ this equation has a unique solution κ_0, and it follows that the sign of $\Im f(\kappa)$ will be different for $\kappa < \kappa_0$ and for $\kappa > \kappa_0$ (and will depend on α and on the relative sign of l_{11} and l_{22}).

Let us now estimate $\Re f(\kappa_0)$. We have

$$\begin{aligned}
\Re f(\kappa) &= \det(L)\, b_1^{-2}(\kappa)\, b_2^{-2}(\kappa) - 1 + \cos(\pi\alpha)\big(l_{22}\, b_2^{-2}(\kappa) - l_{11}\, b_1^{-2}(\kappa)\big) \\
&\leq -|l_{11}\, l_{22}|\, b_1^{-2}(\kappa)\, b_2^{-2}(\kappa) - 1 + |\cos(\pi\alpha)|\big(|l_{22}|\, b_2^{-2}(\kappa) + |l_{11}|\, b_1^{-2}(\kappa)\big) \\
&= -\Big(|l_{11}\, l_{22}|\, b_1^{-2}(\kappa)\, b_2^{-2}(\kappa) + 1 - |\cos(\pi\alpha)|\big(|l_{22}|\, b_2^{-2}(\kappa) + |l_{11}|\, b_1^{-2}(\kappa)\big)\Big) \\
&= -\big(1 - |\cos(\pi\alpha)|\big)\big(|l_{11}\, l_{22}|\, b_1^{-2}(\kappa)\, b_2^{-2}(\kappa) + 1\big) \\
&\quad - |\cos(\pi\alpha)|\big(|l_{11}|\, b_1^{-2}(\kappa) - 1\big)\big(|l_{22}\,| b_2^{-2}(\kappa) - 1\big).
\end{aligned}$$

Hence using (5.12) and the equality $-\frac{l_{22}}{l_{11}} = \frac{|l_{22}|}{|l_{11}|}$ one obtains

$$\begin{aligned}
\Re f(\kappa_0) &\leq -\big(1 - |\cos(\pi\alpha)|\big)\big(|l_{11}l_{22}|\, b_1^{-2}(\kappa_0) b_2^{-2}(\kappa_0) + 1\big) - |\cos(\pi\alpha)|\big(|l_{22}| b_2^{-2}(\kappa_0) - 1\big)^2 \\
&< 0.
\end{aligned}$$

This estimate implies that 0 is not contained in the interior of the curve $f(\mathbb{R}_+)$, which means that $\arg f(+\infty) - \arg f(0) = 0$ for all $\alpha \neq 1/2$.

For the special case $\alpha = 1/2$, the equation (5.12) has either no solution or holds for all $\kappa \in \mathbb{R}_+$. In the former situation, $\Im f$ has always the same sign, which means that the $\arg f(+\infty) - \arg f(0) = 0$. In the latter situation, f is real, and obviously $\arg f(+\infty) - \arg f(0) = 0$. In summary, one has obtained:

II.6) If $c_{11}\, c_{22} < 0$, then $\phi_2(C, D, \alpha) = 0$.

Let us now assume that $\det(C) = 0$ but $C \neq 0$, *i.e.* $\det(L) = 0$ but $L \neq 0$. In that case one simply has

$$f(\kappa) = -1 + \cos(\pi\alpha)\big(l_{22}\, b_2^{-2}(\kappa) - l_{11}\, b_1^{-2}(\kappa)\big) - i\sin(\pi\alpha)\big(l_{11}\, b_1^{-2}(\kappa) + l_{22}\, b_2^{-2}(\kappa)\big).$$

Furthermore, one always has $l_{11}l_{22} \geq 0$, which means that $\Im f$ is either non-negative or non-positive. Then, since $\theta\big(f(+\infty)\big) = \pi$, it will be sufficient to calculate the value $\theta\big(f(0)\big)$.

i) Assume first that $l_{11} = 0$, which automatically implies that $l_{22} \neq 0$ and $l_{12} = l_{21} = 0$. Then one has

$$f(\kappa) = -1 + \cos(\pi\alpha)\, l_{22}\, b_2^{-2}(\kappa) - i\sin(\pi\alpha)\, l_{22}\, b_2^{-2}(\kappa)$$

and

$$\theta\big(f(0)\big) = \begin{cases} -\pi\alpha & \text{if } l_{22} > 0 \\ \pi(1-\alpha) & \text{if } l_{22} < 0 \end{cases}.$$

By taking into account the sign of $\Im f$, one then obtains

$$\arg f(+\infty) - \arg f(0) = \begin{cases} -\pi(1-\alpha) & \text{if } l_{22} > 0 \\ \pi\alpha & \text{if } l_{22} < 0 \end{cases}.$$

ii) Similarly, if we assume now that $l_{22} = 0$, we then have $l_{11} \neq 0$, $l_{12} = l_{21} = 0$ and

$$f(\kappa) = -1 - \cos(\pi\alpha)\, l_{11}\, b_1^{-2}(\kappa) - i\sin(\pi\alpha)\, l_{11}\, b_1^{-2}(\kappa).$$

It then follows that

$$\theta\big(f(0)\big) = \begin{cases} \pi\alpha & \text{if } l_{11} < 0 \\ -\pi(1-\alpha) & \text{if } l_{11} > 0 \end{cases}$$

and

$$\arg f(+\infty) - \arg f(0) = \begin{cases} \pi(1-\alpha) & \text{if } l_{11} < 0 \\ -\pi\alpha & \text{if } l_{11} > 0 \end{cases}.$$

iii) Assume now that $l_{11}\, l_{22} \neq 0$ (which means automatically $l_{11}l_{22} > 0$) and that $\alpha = 1/2$. Since $b_1(\kappa) = b_2(\kappa) =: b(\kappa)$ one then easily observes that $f(\kappa) = -1 - i\,\mathrm{tr}(L)\, b^{-2}(\kappa)$, $\theta\big(f(0)\big) = -\frac{\pi}{2}\,\mathrm{sign}\big(\mathrm{tr}(L)\big)$ and $\arg f(+\infty) - \arg f(0) = -\frac{\pi}{2}\,\mathrm{sign}\big(\mathrm{tr}(L)\big)$.

iv) Assume that $l_{11}\, l_{22} \neq 0$ and that $\alpha < 1/2$. In this case one can rewrite

$$f(\kappa) = -1 + \cos(\pi\alpha)\, b_2^{-2}(\kappa)\Big(l_{22} - l_{11}\frac{b_2^2(\kappa)}{b_1^2(\kappa)}\Big) - i\sin(\pi\alpha)\, b_2^{-2}(\kappa)\Big(l_{22} + l_{11}\frac{b_2^2(\kappa)}{b_1^2(\kappa)}\Big).$$

Since $b_2(\kappa)/b_1(\kappa) \to 0$ as $\kappa \searrow 0$, one has the same limit values and phases as in i).

v) Similarly, if $l_{11}\, l_{22} \neq 0$ and $\alpha > 1/2$, we have the same limit and phases as in ii).

In summary, if $\det(C) = 0$ and $C \neq 0$ one has obtained:

II.7) If $c_{11} = 0$ and $\mathrm{tr}(C) > 0$, or if $c_{11}\, c_{22} \neq 0$, $\mathrm{tr}(C) > 0$ and $\alpha < 1/2$, then $\phi_2(C, D, \alpha) = 2\pi(1-\alpha)$,

II.8) If $c_{11} = 0$ and $\mathrm{tr}(C) < 0$, or if $c_{11}\, c_{22} \neq 0$, $\mathrm{tr}(C) < 0$ and $\alpha < 1/2$, then $\phi_2(C, D, \alpha) = -2\pi\alpha$,

II.9) If $c_{22} = 0$ and $\mathrm{tr}(C) > 0$, or if $c_{11}\, c_{22} \neq 0$, $\mathrm{tr}(C) > 0$ and $\alpha > 1/2$, then $\phi_2(C, D, \alpha) = 2\pi\alpha$,

II.10) If $c_{22} = 0$ and $\mathrm{tr}(C) < 0$, or if $c_{11}\, c_{22} \neq 0$, $\mathrm{tr}(C) < 0$ and $\alpha > 1/2$, then $\phi_2(C, D, \alpha) = -2\pi(1-\alpha)$,

II.11) If $c_{11}\, c_{22} \neq 0$, $\mathrm{tr}(C) > 0$ and $\alpha = 1/2$, then $\phi_2(C, D, \alpha) = \pi$,

II.12) If $c_{11}\, c_{22} \neq 0$, $\mathrm{tr}(C) < 0$ and $\alpha = 1/2$, then $\phi_2(C, D, \alpha) = -\pi$.

III) If $C = 0$, then S_α^{CD} is constant and $\phi_2(C, D, \alpha) = 0$.

IV) We shall now consider the situation $\det(D) = 0$ but $D \neq 0$. Obviously, $\ker(D)$ is of dimension 1. So let $p = (p_1, p_2)$ be a vector in $\ker(D)$ with $\|p\| = 1$. Let us also introduce

$$c(\kappa) = b_1^2(\kappa)\, |p_2|^2\, e^{-i\pi\alpha} - b_2^2(\kappa)\, |p_1|^2\, e^{i\pi\alpha}$$

and

$$X_- := \big(b_1^2(\kappa)\, |p_2|^2 - b_2^2(\kappa)\, |p_1|^2\big), \qquad X_+ := \big(b_1^2(\kappa)\, |p_2|^2 + b_2^2(\kappa)\, |p_1|^2\big)\ .$$

In that case it has been shown in the previous chapter that

$$S = \Phi\,\big(c(\kappa) + \ell\big)^{-1} M(\kappa)\,\Phi\, J\ ,$$

where

$$M(\kappa) := \begin{pmatrix} e^{i\pi\alpha} X_- + \ell & -2i\sin(\pi\alpha)\, b_1(\kappa)\, b_2(\kappa)\, p_1\, \bar{p}_2 \\ -2i\sin(\pi\alpha)\, b_1(\kappa)\, b_2(\kappa)\, \bar{p}_1\, p_2 & e^{-i\pi\alpha} X_- + \ell \end{pmatrix}$$

and ℓ is a real number which will be specified below. Note that $\det\big(M(\kappa)\big) = |c(\kappa) + \ell|^2$ which ensures that S is a unitary operator. Therefore, by setting

$$\begin{aligned} g(\kappa) &:= c(\kappa) + \ell \\ &= \cos(\pi\alpha)\Big(b_1^2(\kappa)\,|p_2|^2 - b_2^2(\kappa)\,|p_1|^2\Big) + \ell - i\sin(\pi\alpha)\Big(b_1^2(\kappa)\,|p_2|^2 + b_2^2(\kappa)\,|p_1|^2\Big), \end{aligned}$$

one has

$$\phi_2(C, D, \alpha) = -2\big(\arg g(+\infty) - \arg g(0)\big),$$

where $\arg : \mathbb{R}_+ \to \mathbb{R}$ is a continuous function defined by the argument of g. Note already that we always have $\Im g < 0$.

We first consider the special case $\alpha = 1/2$. In that case we have $b_1(\kappa) = b_2(\kappa) =: b(\kappa)$, and then

$$g(\kappa) = \ell - ib^2(\kappa).$$

If $\ell \neq 0$, we have $\theta\big(g(0)\big) = \theta(\ell)$ and $\theta\big(g(+\infty)\big) = -\pi/2$. Therefore

$$\arg g(+\infty) - \arg g(0) = \begin{cases} -\pi/2 & \text{if } \ell > 0 \\ \pi/2 & \text{if } \ell < 0 \end{cases}.$$

If $\ell = 0$, then g is pure imaginary, hence $\arg g(+\infty) - \arg g(0) = 0$. In summary, for $\det(D) = 0$ but $D \neq 0$, one has already obtained:

IV.1) If $\ell > 0$ and $\alpha = 1/2$, then $\phi_2(C, D, \alpha) = \pi$,

IV.2) If $\ell = 0$ and $\alpha = 1/2$, then $\phi_2(C, D, \alpha) = 0$,

IV.3) If $\ell < 0$ and $\alpha = 1/2$, then $\phi_2(C, D, \alpha) = -\pi$.

Let us now consider the case $\alpha < 1/2$, and assume first that $\ell \neq 0$. It follows that $\theta\big(g(0)\big) = \theta(\ell)$. To calculate $\theta\big(g(+\infty)\big)$ one has to consider two subcases. So, on the one hand let us assume in addition that $p_1 \neq 0$. Then one has

$$g(\kappa) = \ell - \cos(\pi\alpha)\, b_2^2(\kappa)\Big(|p_1|^2 - \frac{b_1^2(\kappa)}{b_2^2(\kappa)}\,|p_2|^2\Big) - i\sin(\pi\alpha)\, b_2^2(\kappa)\Big(|p_1|^2 + \frac{b_1^2(\kappa)}{b_2^2(\kappa)}\,|p_2|^2\Big).$$

Since $b_1(\kappa)/b_2(\kappa) \to 0$ as $\kappa \to +\infty$, one obtains $\theta\big(g(+\infty)\big) = -\pi(1-\alpha)$ and

$$\arg g(+\infty) - \arg g(0) = \begin{cases} -\pi(1-\alpha), & \text{if } \ell > 0 \\ \pi\alpha, & \text{if } \ell < 0 \end{cases}.$$

On the other hand, if $p_1 = 0$, then one has

$$g(\kappa) = \ell + b_1^2(\kappa)\big(\cos(\pi\alpha) - i\sin(\pi\alpha)\big),$$

which implies that $\theta\big(g(+\infty)\big) = -\pi\alpha$ and that

$$\arg g(+\infty) - \arg g(0) = \begin{cases} -\pi\alpha, & \text{if } \ell > 0 \\ \pi(1-\alpha), & \text{if } \ell < 0 \end{cases}.$$

Now, let us assume that $\ell = 0$. In this case the above limits for $\kappa \to +\infty$ still hold, so we only need to calculate $\theta\big(g(0)\big)$. Firstly, if $p_2 \neq 0$, we have

$$g(\kappa) = \cos(\pi\alpha)\, b_1^2(\kappa)\Big(|p_2|^2 - \frac{b_2^2(\kappa)}{b_1^2(\kappa)}\,|p_1|^2\Big) - i\sin(\pi\alpha)\, b_1^2(\kappa)\Big(|p_2|^2 + \frac{b_2^2(\kappa)}{b_1^2(\kappa)}\,|p_1|^2\Big),$$

and since $b_2(\kappa)/b_1(\kappa) \to 0$ as $\kappa \searrow 0$ it follows that $\theta\big(g(0)\big) = -\pi\alpha$. Secondly, if $p_2 = 0$, then

$$g(\kappa) = -b_2^2(\kappa)\Big(\cos(\pi\alpha) + i\sin(\pi\alpha)\Big)\Big),$$

and we get $\theta\big(g(0)\big) = -\pi(1-\alpha)$.

In summary, for $\det(D) = 0$, $D \neq 0$ and $\alpha < 1/2$, we have obtained

IV.4) if $\ell < 0$ and $p_1 \neq 0$, then $\phi_2(C, D, \alpha) = -2\pi\alpha$,

IV.5) if $\ell < 0$ and $p_1 = 0$, then $\phi_2(C, D, \alpha) = -2\pi(1-\alpha)$,

IV.6) if $\ell > 0$ and $p_1 \neq 0$, then $\phi_2(C, D, \alpha) = 2\pi(1-\alpha)$,

IV.7) if $\ell > 0$ and $p_1 = 0$, then $\phi_2(C, D, \alpha) = 2\pi\alpha$,

IV.8) if $\ell = 0$, $p_1 \neq 0$ and $p_2 \neq 0$ then $\phi_2(C, D, \alpha) = 2\pi(1-2\alpha)$,

IV.9) if $\ell = 0$ and $p_1 = 0$ or if $\ell = 0$ and $p_2 = 0$, then $\phi_2(C, D, \alpha) = 0$.

The case $\det(D) = 0$, $D \neq 0$ and $\alpha > 1/2$ can be treated analogously. We simply state the results:

IV.10) if $\ell < 0$ and $p_2 \neq 0$, then $\phi_2(C, D, \alpha) = -2\pi(1-\alpha)$,

IV.11) if $\ell < 0$ and $p_2 = 0$, then $\phi_2(C, D, \alpha) = -2\pi\alpha$,

IV.12) if $\ell > 0$ and $p_2 \neq 0$, then $\phi_2(C, D, \alpha) = 2\pi\alpha$,

IV.13) if $\ell > 0$ and $p_2 = 0$, then $\phi_2(C, D, \alpha) = 2\pi(1-\alpha)$,

IV.14) if $\ell = 0$, $p_1 \neq 0$ and $p_2 \neq 0$ then $\phi_2(C, D, \alpha) = -2\pi(1-2\alpha)$,

IV.15) if $\ell = 0$ and $p_1 = 0$ or if $\ell = 0$ and $p_2 = 0$, then $\phi_2(C, D, \alpha) = 0$.

Let us finally recall some relationship between the constant ℓ and the matrices C and D in the case IV). As explained before, we can always assume that $C = (1-U)/2$ and $D = i(1+U)/2$ for some $U \in U(2)$. Recall that in deriving the equalities (IV.1)–(IV.15) we assumed $\dim[\ker(D)] = 1$, *i.e.* -1 is an eigenvalue of U of multiplicity 1. Let $e^{i\theta}$,

$\theta \in (-\pi, \pi)$ be the other eigenvalue of U. Then by the construction explained in the previous chapter, one has

$$\ell = \frac{\pi}{2\sin(\pi\alpha)}\,\frac{1-e^{i\theta}}{i(1+e^{i\theta})} = -\frac{\pi}{2\sin(\pi\alpha)}\frac{\sin\left(\frac{\theta}{2}\right)}{\cos\left(\frac{\theta}{2}\right)}.$$

On the other hand, the eigenvalues of the matrix $CD^* = i(U-U^*)/4$ are $\lambda_1 = 0$ and

$$\lambda_2 = i(e^{i\theta} - e^{-i\theta})/4 = -\tfrac{1}{2}\sin(\theta) = -\sin\left(\tfrac{\theta}{2}\right)\cos\left(\tfrac{\theta}{2}\right).$$

It follows that λ_2 and ℓ have the same sign. Therefore, in (IV.1)–(IV.15) one has: $\ell < 0$ if CD^* has one zero eigenvalue and one negative eigenvalue, $\ell = 0$ if $CD^* = 0$ and $\ell > 0$ if CD^* has one zero eigenvalue and one positive eigenvalue.

5.3.3 Case-by-case results

In this section we finally collect all previous results and prove the case-by-case version of Levinson's theorem. The interest of this analysis is that the contribution of the 0-energy operator $\Gamma_1(C, D, \alpha, \cdot)$ and the contribution of the operator $\Gamma_3(C, D, \alpha, \cdot)$ at $+\infty$-energy are explicit. Here, Levinson's theorem corresponds to the equality between the number of bound states of H_α^{CD} and $-\frac{1}{2\pi}\sum_{j=1}^4 \phi_j(C, D, \alpha)$. This is proved again by comparing the column 3 with the column 7 (the contribution of $\Gamma_4(C, D, \alpha, \cdot)$ defined in (5.8) is always trivial).

For simplicity, we shall write H for H_α^{CD} and ϕ_j for $\phi_j(C, D, \alpha)$. We also recall that the number $\#\sigma_p(H)$ of eigenvalues of H is equal to the number of negative eigenvalues of the matrix CD^*, as shown in Lemma 4.3.2.

We consider first the very special situations:

No	Conditions	$\#\sigma_p(H)$	ϕ_1	ϕ_2	ϕ_3	$\sum_j \phi_j$
I	$D = 0$	0	0	0	0	0
III	$C = 0$	0	2π	0	-2π	0

Now, if $\det(D) \neq 0$ and $\det(C) \neq 0$, we set $E := D^{-1}C =: (e_{jk})$ and obtains:

No	Conditions	$\#\sigma_p(H)$	ϕ_1	ϕ_2	ϕ_3	$\sum_j \phi_j$
II.1	$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) > 0$, $\det(E) > 0$	0	0	2π	-2π	0
II.2	$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) > 0$, $\det(E) < 0$	1	0	0	-2π	-2π
II.3	$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) < 0$, $\det(E) > 0$	2	0	-2π	-2π	-4π
II.4	$e_{11}e_{22} \geq 0$, $\mathrm{tr}(E) < 0$, $\det(E) < 0$	1	0	0	-2π	-2π
II.5	$e_{11} = e_{22} = 0, \det(E) < 0$	1	0	0	-2π	-2π
II.6	$e_{11}\,e_{22} < 0$	1	0	0	-2π	-2π

If $\det(D) \neq 0$, $\det(C) = 0$ and if we still set $E := D^{-1}C$ one has:

No	Conditions	$\#\sigma_p(H)$	ϕ_1	ϕ_2	ϕ_3	$\sum_j \phi_j$
II.7.a	$e_{11} = 0, \mathrm{tr}(E) > 0$	0	$2\pi\alpha$	$2\pi(1-\alpha)$	-2π	0
II.7.b	$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) > 0, \alpha < 1/2$	0	$2\pi\alpha$	$2\pi(1-\alpha)$	-2π	0
II.8.a	$e_{11} > 0, \mathrm{tr}(E) < 0$	1	$2\pi\alpha$	$-2\pi\alpha$	-2π	-2π
II.8.b	$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) < 0, \alpha < 1/2$	1	$2\pi\alpha$	$-2\pi\alpha$	-2π	-2π
II.9.a	$e_{22} = 0, \mathrm{tr}(E) > 0$	0	$2\pi(1-\alpha)$	$2\pi\alpha$	-2π	0
II.9.b	$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) > 0, \alpha > 1/2$	0	$2\pi(1-\alpha)$	$2\pi\alpha$	-2π	0
II.10.a	$e_{22} = 0, \mathrm{tr}(E) < 0$	1	$2\pi(1-\alpha)$	$-2\pi(1-\alpha)$	-2π	-2π
II.10.b	$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) < 0, \alpha > 1/2$	1	$2\pi(1-\alpha)$	$-2\pi(1-\alpha)$	-2π	-2π
II.11	$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) > 0, \alpha = 1/2$	0	π	π	-2π	0
II.12	$e_{11}\, e_{22} \neq 0, \mathrm{tr}(E) < 0, \alpha = 1/2$	1	π	$-\pi$	-2π	-2π

On the other hand, if $\dim[\ker(D)] = 1$ and $\alpha = 1/2$ one has:

No	Conditions	$\#\sigma_p(H)$	ϕ_1	ϕ_2	ϕ_3	$\sum_j \phi_j$
IV.1	$\ell > 0$	0	0	π	$-\pi$	0
IV.2	$\ell = 0$	0	π	0	$-\pi$	0
IV.3	$\ell < 0$	1	0	$-\pi$	$-\pi$	-2π

If $\dim[\ker(D)] = 1$, $\alpha < 1/2$ and if $(p_1, p_2) \in \ker(D)$ one obtains:

No	Conditions	$\#\sigma_p(H)$	ϕ_1	ϕ_2	ϕ_3	$\sum_j \phi_j$
IV.4	$\ell < 0, p_1 \neq 0$	1	0	$-2\pi\alpha$	$-2\pi(1-\alpha)$	-2π
IV.5	$\ell < 0, p_1 = 0$	1	0	$-2\pi(1-\alpha)$	$-2\pi\alpha$	-2π
IV.6	$\ell > 0, p_1 \neq 0$	0	0	$2\pi(1-\alpha)$	$-2\pi(1-\alpha)$	0
IV.7	$\ell > 0, p_1 = 0$	0	0	$2\pi\alpha$	$-2\pi\alpha$	0
IV.8	$\ell = 0, p_1 p_2 \neq 0$	0	$2\pi\alpha$	$2\pi(1-2\alpha)$	$-2\pi(1-\alpha)$	0
IV.9.a	$\ell = 0, p_1 = 0$	0	$2\pi\alpha$	0	$-2\pi\alpha$	0
IV.9.b	$\ell = 0, p_2 = 0$	0	$2\pi(1-\alpha)$	0	$-2\pi(1-\alpha)$	0

Finally, if $\dim[\ker(D)] = 1$, $\alpha > 1/2$ and $(p_1, p_2) \in \ker(D)$ one has:

No	Conditions	$\#\sigma_p(H)$	ϕ_1	ϕ_2	ϕ_3	$\sum_j \phi_j$
IV.10	$\ell < 0, p_2 \neq 0$	1	0	$-2\pi(1-\alpha)$	$-2\pi\alpha$	-2π
IV.11	$\ell < 0, p_2 = 0$	1	0	$-2\pi\alpha$	$-2\pi(1-\alpha)$	-2π
IV.12	$\ell > 0, p_2 \neq 0$	0	0	$2\pi\alpha$	$-2\pi\alpha$	0
IV.13	$\ell > 0, p_2 = 0$	0	0	$2\pi(1-\alpha)$	$-2\pi(1-\alpha)$	0
IV.14	$\ell = 0, p_1 p_2 \neq 0$	0	$2\pi(1-\alpha)$	$-2\pi(1-2\alpha)$	$-2\pi\alpha$	0
IV.15.a	$\ell = 0, p_1 = 0$	0	$2\pi\alpha$	0	$-2\pi\alpha$	0
IV.15.b	$\ell = 0, p_2 = 0$	0	$2\pi(1-\alpha)$	0	$-2\pi(1-\alpha)$	0

5.4 K-groups, n-traces and their pairings

In this section, we give a very short account on the K-theory for C^*-algebras and on various constructions related to it. Our aim is not to present a thorough introduction to these subjects but to recast the result obtained in the previous section in the most suitable framework. For the first part, we refer to [99] for an enjoyable introduction to the subject.

5.4.1 K-groups and boundary maps

The K_0-group of a unital C^*-algebra $\mathcal{E}$ is constructed from the homotopy classes of projections in the set of square matrices with entries in $\mathcal{E}$. Its addition is induced from the addition of two orthogonal projections: if p and q are orthogonal projections, *i.e.* $pq = 0$, then also $p+q$ is a projection. Thus, the sum of two homotopy classes $[p]_0 + [q]_0$ is defined as the class of the sum of the block matrices $[p \oplus q]_0$ on the diagonal. This new class does not depend on the choice of the representatives p and q. $K_0(\mathcal{E})$ is defined as the Grothendieck group of this set of homotopy classes of projections endowed with the mentioned addition. In other words, the elements of the K_0-group are given by formal differences: $[p]_0 - [q]_0$ is identified with $[p']_0 - [q']_0$ if there exists a projection r such that $[p]_0 + [q']_0 + [r]_0 = [p']_0 + [q]_0 + [r]_0$. In the general non-unital case the construction is a little bit more subtle.

The K_1-group of a C^*-algebra $\mathcal{E}$ is constructed from the homotopy classes of unitaries in the set of square matrices with entries in the unitisation of $\mathcal{E}$. Its addition is again defined by: $[u]_1 + [v]_1 = [u \oplus v]_1$ as a block matrix on the diagonal. The homotopy class of the added identity is the neutral element.

Now, let us consider three C^*-algebras $\mathcal{J}, \mathcal{E}$ and $\mathcal{Q}$ such that $\mathcal{J}$ is an ideal of $\mathcal{E}$ and $\mathcal{Q}$ is isomorphic to the quotient $\mathcal{E}/\mathcal{J}$. Another way of saying this is that $\mathcal{J}$ and $\mathcal{Q}$ are the left and right part of an exact sequence of C^*-algebras

$$0 \to \mathcal{J} \xrightarrow{\mathtt{i}} \mathcal{E} \xrightarrow{\mathtt{q}} \mathcal{Q} \to 0, \tag{5.13}$$

$\mathtt{i}$ being an injective morphism and $\mathtt{q}$ a surjective morphism satisfying $\ker \mathtt{q} = \mathrm{im}\, \mathtt{i}$. There might not be any reasonable algebra morphism between $\mathcal{J}$ and $\mathcal{Q}$ but algebraic topology provides us with homomorphisms between their K-groups: $\mathrm{ind} : K_1(\mathcal{Q}) \to K_0(\mathcal{J})$ and $\exp : K_0(\mathcal{Q}) \to K_1(\mathcal{J})$, the index map and the exponential map. These maps are also referred to as boundary maps. For the sequel we shall be concerned only with the index map. It can be computed as follows: If u is a unitary in $\mathcal{Q}$ then there exists a unitary $w \in M_2(\mathcal{E})$ such that $\mathtt{q}(w) = \left(\begin{smallmatrix} u & 0 \\ 0 & u^* \end{smallmatrix}\right)$. It turns out that $w \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right) w^*$ lies in the unitisation of $\mathtt{i}\big(M_2(\mathcal{J})\big)$ so that $\big([w \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right) w^*]_0 - [\left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)]_0\big)$ defines an element of $K_0(\mathcal{J})$. $\mathrm{ind}([u]_1)$ is that element. With a little luck there exists even a partial isometry $w \in \mathcal{E}$ such that $\mathtt{q}(w) = u$. Then $(1 - w^*w)$ and $(1 - ww^*)$ are projections in $\mathcal{J}$ and we have the simpler formula

$$\mathrm{ind}[u]_1 = \big[1 - w^*w\big]_0 - \big[1 - ww^*\big]_0 \,. \tag{5.14}$$

5.4.2 Cyclic cohomology, n-traces and Connes' pairing

For this part, we refer to [31, Sec. III] or to the short surveys presented in [65, Sec. 5] or in [66, Sec. 4 & 5]. For simplicity, we denote by $\mathbb{N}$ the set of natural number including 0.

Given a complex algebra $\mathcal{B}$ and any $n \in \mathbb{N}$, let $C^n_\lambda(\mathcal{B})$ be the set of $(n+1)$-linear functional on $\mathcal{B}$ which are cyclic in the sense that any $\eta \in C^n_\lambda(\mathcal{B})$ satisfies for each $w_0, \dots, w_n \in \mathcal{B}$:

$$\eta(w_1, \dots, w_n, w_0) = (-1)^n \eta(w_0, \dots, w_n)\ .$$

Let $\mathtt{b} : C^n_\lambda(\mathcal{B}) \to C^{n+1}_\lambda(\mathcal{B})$ be the Hochschild coboundary map defined for $w_0, \dots, w_{n+1} \in \mathcal{B}$ by

$$\begin{aligned}&[\mathtt{b}\eta](w_0, \dots, w_{n+1})\\ &:= \sum_{j=0}^{n} (-1)^j \eta(w_0, \dots, w_j w_{j+1}, \dots, w_{n+1}) + (-1)^{n+1} \eta(w_{n+1} w_0, \dots, w_n)\ .\end{aligned}$$

An element $\eta \in C^n_\lambda(\mathcal{B})$ satisfying $\mathtt{b}\eta = 0$ is called a cyclic n-cocyle, and the cyclic cohomology $HC(\mathcal{B})$ of $\mathcal{B}$ is the cohomology of the complex

$$0 \to C^0_\lambda(\mathcal{B}) \to \dots \to C^n_\lambda(\mathcal{B}) \xrightarrow{\mathtt{b}} C^{n+1}_\lambda(\mathcal{B}) \to \dots\ .$$

A convenient way of looking at cyclic n-cocycles is in terms of characters of a graded differential algebra over $\mathcal{B}$. So, let us first recall that a graded differential algebra $(\mathcal{A}, \mathtt{d})$ is a graded algebra $\mathcal{A}$ together with a map $\mathtt{d} : \mathcal{A} \to \mathcal{A}$ of degree $+1$. More precisely, $\mathcal{A} := \oplus_{j=0}^\infty \mathcal{A}_j$ with each $\mathcal{A}_j$ an algebra over $\mathbb{C}$ satisfying the property $\mathcal{A}_j\, \mathcal{A}_k \subset \mathcal{A}_{j+k}$, and $\mathtt{d}$ is a graded derivation satisfying $\mathtt{d}^2 = 0$. In particular, the derivation satisfies $\mathtt{d}(w_1 w_2) = (\mathtt{d}w_1)w_2 + (-1)^{\deg(w_1)} w_1 (\mathtt{d}w_2)$, where $\deg(w_1)$ denotes the degree of the homogeneous element w_1.

A cycle $(\mathcal{A}, \mathtt{d}, \int)$ of dimension n is a graded differential algebra $(\mathcal{A}, \mathtt{d})$, with $\mathcal{A}_j = 0$ for $j > n$, endowed with a linear functional $\int : \mathcal{A} \to \mathbb{C}$ satisfying $\int \mathtt{d}w = 0$ if $w \in \mathcal{A}_{n-1}$ and for $w_j \in \mathcal{A}_j$, $w_k \in \mathcal{A}_k$:

$$\int w_j w_k = (-1)^{jk} \int w_k w_j\ .$$

Given an algebra $\mathcal{B}$, a cycle of dimension n over $\mathcal{B}$ is a cycle $(\mathcal{A}, \mathtt{d}, \int)$ of dimension n together with a homomorphism $\rho : \mathcal{B} \to \mathcal{A}_0$. In the sequel, we will assume that this map is injective and hence identify $\mathcal{B}$ with a subalgebra of $\mathcal{A}_0$ (and do not write ρ anymore). Now, if $w_0, \dots, w_n$ are $n+1$ elements of $\mathcal{B}$, one can define the character $\eta(w_0, \dots, w_n) \in \mathbb{C}$ by the formula:

$$\eta(w_0, \dots, w_n) := \int w_0\, (\mathtt{d}w_1) \dots (\mathtt{d}w_n)\ . \tag{5.15}$$

As shown in [31, Prop.III.1.4], the map $\eta : \mathcal{B}^{n+1} \to \mathbb{C}$ is a cyclic $(n+1)$-linear functional on $\mathcal{B}$ satisfying $\mathtt{b}\eta = 0$, *i.e.* η is a cyclic n-cocycle. Conversely, any cyclic n-cocycle arises as the character of a cycle of dimension n over $\mathcal{B}$. Let us also mention that a third description of any cyclic n-cocycle is presented in [31, Sec. III.1.α] in terms of the universal differential algebra associated with $\mathcal{B}$.

We can now introduce the precise definition of a n-trace over a Banach algebra. For an algebra $\mathcal{B}$ that is not necessarily unital, we denote by $\widetilde{\mathcal{B}} := \mathcal{B} \oplus \mathbb{C}$ the algebra obtained by adding a unit to $\mathcal{B}$.

Definition 5.4.1. *A n-trace on a Banach algebra $\mathcal{B}$ is the character of a cycle $(\mathcal{A}, \mathtt{d}, \int)$ of dimension n over a dense subalgebra $\mathcal{B}'$ of $\mathcal{B}$ such that for all $w_1, \dots, w_n \in \mathcal{B}'$ and any $x_1, \dots, x_n \in \widetilde{\mathcal{B}'}$ there exists a constant $c = c(w_1, \dots, w_n)$ such that*

$$\left| \int (x_1 \mathtt{d} w_1) \dots (x_n \mathtt{d} w_n) \right| \leq c \|x_1\| \dots \|x_n\| \, .$$

Remark 5.4.2. *Typically, the elements of $\mathcal{B}'$ are suitably smooth elements of $\mathcal{B}$ on which the derivation $\mathtt{d}$ is well defined and for which the r.h.s. of* (5.15) *is also well defined. However, the n-trace η can sometimes be extended to more general elements $(w_0, \dots, w_n) \in \mathcal{B}^{n+1}$ by a suitable reinterpretation of the l.h.s. of* (5.15).

The importance of n-traces relies on their duality relation with K-groups. Recall first that $M_q(\mathcal{B}) \cong M_q(\mathbb{C}) \otimes \mathcal{B}$ and that tr denotes the standard trace on matrices. Now, let $\mathcal{B}$ be a C^*-algebra and let η_n be a n-trace on $\mathcal{B}$ with $n \in \mathbb{N}$ even. If $\mathcal{B}'$ is the dense subalgebra of $\mathcal{B}$ mentioned in Definition 5.4.1 and if p is a projection in $M_q(\mathcal{B}')$, then one sets

$$\langle \eta_n, p \rangle := c_n \, [\mathrm{tr} \otimes \eta_n](p, \dots, p).$$

Similarly, if $\mathcal{B}$ is a unital C^*-algebra and if η_n is a n-trace with $n \in \mathbb{N}$ odd, then for any unitary u in $M_q(\mathcal{B}')$ one sets

$$\langle \eta_n, u \rangle := c_n \, [\mathrm{tr} \otimes \eta_n](u^*, u, u^*, \dots, u)$$

the entries on the r.h.s. alternating between u and u^*. The constants c_n are given by

$$c_{2k} = \frac{1}{(2\pi i)^k} \frac{1}{k!}, \qquad c_{2k+1} = \frac{1}{(2\pi i)^{k+1}} \frac{1}{2^{2k+1}} \frac{1}{(k + \frac{1}{2})(k - \frac{1}{2}) \cdots \frac{1}{2}} \, .$$

There relations are referred to as Connes' pairing between K-theory and cyclic cohomology of $\mathcal{B}$ because of the following property, see [30, Thm. 2.7] for a precise statement and for its proof: In the above framework, the values $\langle \eta_n, p \rangle$ and $\langle \eta_n, u \rangle$ depend only of the K_0-class $[p]_0$ of p and of the K_1-class $[u]_1$ of u, respectively.

We now illustrate these notions with two basic examples which will be of importance in the sequel.

Example 5.4.3. *If $\mathcal{B} = \mathcal{K}(\mathcal{H})$, the algebra of compact operators on a Hilbert space $\mathcal{H}$, then the linear functional $\int$ on $\mathcal{B}$ is given by the usual trace Tr on the set $\mathcal{K}_1$ of trace class elements of $\mathcal{K}(\mathcal{H})$. Furthermore, since any projection $p \in \mathcal{K}(\mathcal{H})$ is trace class, it follows that $\langle \eta_0, p \rangle \equiv \langle \mathrm{Tr}, p \rangle$ is well defined for any such p and that this expression gives the dimension of the projection p.*

For the next example, let us recall that $\det$ denotes the usual determinant of elements of $M_q(\mathbb{C})$.

Example 5.4.4. *If $\mathcal{B} = C\big(\mathbb{S}^1, M_q(\mathbb{C})\big)$ for some $q \geq 1$, let us fix $\mathcal{B}' := C^1\big(\mathbb{S}^1, M_q(\mathbb{C})\big)$. We parameterize $\mathbb{S}^1$ by the real numbers modulo 2π using θ as local coordinate. As usual, for any $w \in \mathcal{B}'$ (which corresponds to an homogeneous element of degree 0), one sets $[\mathtt{d}w](\theta) :=$*

$w'(\theta)\,\mathrm{d}\theta$ (which is now an homogeneous element of degree 1). Furthermore, we define the graded trace $\int v\,\mathrm{d}\theta := \int_{-\pi}^{\pi}\mathrm{tr}[v(\theta)]\,\mathrm{d}\theta$ for an arbitrary element $v\,\mathrm{d}\theta$ of degree 1. This defines the 1-trace η_1. A unitary element in $u \in C^1\big(\mathbb{S}^1, M_q(\mathbb{C})\big)$ (or rather its class) pairs as follows:

$$\langle \eta_1, u\rangle = c_1[\mathrm{tr}\otimes\eta_1](u^*, u) := \frac{1}{2\pi i}\int_{-\pi}^{\pi}\mathrm{tr}[u(\theta)^*\,u'(\theta)]\,\mathrm{d}\theta\,. \tag{5.16}$$

For this example, the extension of this expression for any unitary $u \in C\big(\mathbb{S}^1, M_q(\mathbb{C})\big)$ is quite straightforward. Indeed, let us first rewrite $u =: e^{i\varphi}$ for some $\varphi \in C^1\big(\mathbb{S}^1, M_q(\mathbb{R})\big)$ and set $\beta(\theta) := \det[u(\theta)]$. By using the equality $\det[e^{i\varphi}] = e^{i\,\mathrm{tr}[\varphi]}$, one then easily observed that the quantity (5.16) is equal to

$$\frac{1}{2\pi i}\int_{-\pi}^{\pi}\beta(\theta)^*\,\beta'(\theta)\,\mathrm{d}\theta\,.$$

But this quantity is known to be equal to the winding number of the map $\beta : \mathbb{S}^1 \to \mathbb{T}$, a quantity which is of topological nature and which only requires that the map β is continuous. Altogether, one has thus obtained that the l.h.s. of (5.16) is nothing but the winding number of the map $\det[u] : \mathbb{S}^1 \to \mathbb{T}$, valid for any unitary $u \in C\big(\mathbb{S}^1, M_q(\mathbb{C})\big)$.

5.4.3 Dual boundary maps

We have seen that an n-trace η over $\mathcal{B}$ gives rise to a functional on $K_i(\mathcal{B})$ for $i = 1$ or $i = 2$, *i.e.* the map $\langle \eta, \cdot\rangle$ is an element of $Hom(K_i(\mathcal{B}), \mathbb{C})$. In that sense n-traces are dual to the elements of the (complexified) K-groups. An important question is whether this dual relation is functorial in the sense that morphisms between the K-groups of different algebras yield dual morphisms on higher traces. Here we are in particular interested in a map on higher traces which is dual to the index map, *i.e.* a map $\#$ which assigns to an even trace η an odd trace $\#\eta$ such that

$$\langle \eta, \mathrm{ind}(\cdot)\rangle = \langle \#\eta, \cdot\rangle. \tag{5.17}$$

This situation gives rise to equalities between two numerical topological invariants.

Such an approach for relating two topological invariants has already been used at few occasions. For example, it has been recently shown that Levinson's theorem corresponds to a equality of the form (5.17) for a 0-trace and a 1-trace [62]. In Section 5.5.3 we shall develop such an equality for a 2-trace and a 3-trace. On the other hand, let us mention that similar equalities have also been developed for the exponential map in (5.17) instead of the index map. In this framework, an equality involving a 0-trace and a 1-trace has been put into evidence in [58]. It gives rise to a relation between the pressure on the boundary of a quantum system and the integrated density of states. Similarly, a relation involving 2-trace and a 1-trace was involved in the proof of the equality between the bulk-Hall conductivity and the conductivity of the current along the edge of the sample, see [65, 66].

5.5 Topological Levinson's theorems

In this section we introduce the algebraic framework suitable for the Aharonov-Bohm model. In fact, the following algebras were already introduced in [61] for the study of the wave operators in potential scattering on $\mathbb{R}$. The similar form of the wave operators in the Aharonov-Bohm model and in the model studied in that reference allows us to reuse part of the construction and the abstract results. Let us stress that the following construction holds for fixed α and (C, D). These parameters will vary only at the end of the section.

5.5.1 The algebraic framework

For the construction of the C^*-algebras, let us introduce the operator $B := \frac{1}{2}\ln(H_0)$, where $H_0 = -\Delta$ is the usual Laplace operator on $\mathbb{R}^2$. The crucial property of the operators A and B is that they satisfy the canonical commutation relation $[A, B] = i$ so that A generates translations in B and vice versa,

$$e^{iBt}Ae^{-iBt} = A + t, \quad e^{iAs}Be^{-iAs} = B - s.$$

Furthermore, both operators leave the subspaces $\mathcal{H}_m$ invariant. More precisely, for any essentially bounded functions φ and η on $\mathbb{R}$, the operator $\varphi(A)\eta(B)$ leaves each of these subspaces invariant. Since all the interesting features of the Aharonov-Bohm model take place in the subspace $\mathcal{H}_{\text{int}} \cong \mathsf{L}^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes \mathbb{C}^2$, we shall subsequently restrict our attention to this subspace and consider functions φ, η defined on $\mathbb{R}$ and taking values in $M_2(\mathbb{C})$.

Now, let $\mathcal{E}$ be the closure in $\mathcal{B}(\mathcal{H}_{\text{int}})$ of the algebra generated by elements of the form $\varphi(A)\psi(H_0)$, where φ is a continuous function on $\mathbb{R}$ with values in $M_2(\mathbb{C})$ which converges at $\pm\infty$, and ψ is a continuous function $\mathbb{R}_+$ with values in $M_2(\mathbb{C})$ which converges at 0 and at $+\infty$. Stated differently, $\varphi \in C\big(\overline{\mathbb{R}}, M_2(\mathbb{C})\big)$ with $\overline{\mathbb{R}} = [-\infty, +\infty]$, and $\psi \in C\big(\overline{\mathbb{R}_+}, M_2(\mathbb{C})\big)$ with $\overline{\mathbb{R}_+} = [0, +\infty]$. Let $\mathcal{J}$ be the norm closed algebra generated by $\varphi(A)\psi(H_0)$ with functions φ and ψ for which the above limits vanish. Obviously, $\mathcal{J}$ is an ideal in $\mathcal{E}$, and the same algebras are obtained if $\psi(H_0)$ is replaced by $\eta(B)$ with $\eta \in C\big(\overline{\mathbb{R}}, M_2(\mathbb{C})\big)$ or $\eta \in C_0\big(\mathbb{R}, M_2(\mathbb{C})\big)$, respectively. Furthermore, the ideal $\mathcal{J}$ is equal to the algebra of compact operators $\mathcal{K}(\mathcal{H}_{\text{int}})$, as shown in [61, Sec. 4].

Let us already mention the reason of our interest in defining the above algebra $\mathcal{E}$. Since for $m \in \{0, -1\}$ the functions φ_m^- and $\tilde{\varphi}_m$ have limits at $\pm\infty$, and since $\widetilde{S}_\alpha^{CD}$ also has limits at 0 and $+\infty$, it follows from (5.3) that the operator $W_-^{CD}|_{\mathcal{H}_{\text{int}}}$ belongs to $\mathcal{E}$. Since $\mathcal{J} = \mathcal{K}(\mathcal{H}_{\text{int}})$, the image of $W_-^{CD}|_{\mathcal{H}_{\text{int}}}$ by the quotient map $\mathsf{q} : \mathcal{E} \to \mathcal{E}/\mathcal{J}$ corresponds to the image of $W_-^{CD}|_{\mathcal{H}_{\text{int}}}$ in the Calkin algebra. This motivates the following computation of the quotient $\mathcal{E}/\mathcal{J}$.

To describe the quotient $\mathcal{E}/\mathcal{J}$ we consider the square $\blacksquare := \overline{\mathbb{R}_+} \times \overline{\mathbb{R}}$ whose boundary $\square$ is the union of four parts: $\square = B_1 \cup B_2 \cup B_3 \cup B_4$, with $B_1 = \{0\} \times \overline{\mathbb{R}}$, $B_2 = \overline{\mathbb{R}_+} \times \{+\infty\}$, $B_3 = \{+\infty\} \times \overline{\mathbb{R}}$ and $B_4 = \overline{\mathbb{R}_+} \times \{-\infty\}$. We can then view $\mathcal{Q} := C\big(\square, M_2(\mathbb{C})\big)$ as the subalgebra of

$$C\big(\overline{\mathbb{R}}, M_2(\mathbb{C})\big) \oplus C\big(\overline{\mathbb{R}_+}, M_2(\mathbb{C})\big) \oplus C\big(\overline{\mathbb{R}}, M_2(\mathbb{C})\big) \oplus C\big(\overline{\mathbb{R}_+}, M_2(\mathbb{C})\big)$$

given by elements $(\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ which coincide at the corresponding end points, that is, $\Gamma_1(+\infty) = \Gamma_2(0)$, $\Gamma_2(+\infty) = \Gamma_3(+\infty)$, $\Gamma_3(-\infty) = \Gamma_4(+\infty)$, $\Gamma_4(0) = \Gamma_1(-\infty)$. The following lemma corresponds to results obtained in [43, Sec. 3.5] rewritten in our framework.

Lemma 5.5.1. *$\mathcal{E}/\mathcal{J}$ is isomorphic to $\mathcal{Q}$. Furthermore, for any $\varphi \in C\big(\overline{\mathbb{R}}, M_2(\mathbb{C})\big)$ and for any $\psi \in C\big(\overline{\mathbb{R}_+}, M_2(\mathbb{C})\big)$, the image of $\varphi(A)\psi(H_0)$ through the quotient map $\mathsf{q} : \mathcal{E} \to \mathcal{Q}$*

is given by $\Gamma_1(\cdot) = \varphi(\cdot)\psi(0)$*,* $\Gamma_2(\cdot) = \varphi(+\infty)\psi(\cdot)$*,* $\Gamma_3(\cdot) = \varphi(\cdot)\psi(+\infty)$ *and* $\Gamma_4(\cdot) = \varphi(-\infty)\psi(\cdot)$*.*

Stated differently, the algebras $\mathcal{J}, \mathcal{E}$ and $\mathcal{Q}$ are part of the short exact sequence of C^*-algebras (5.13). And as already mentioned, the operator $W_-^{CD}|_{\mathcal{H}_{\rm int}}$ clearly belongs to $\mathcal{E}$. Furthermore, its image through the quotient map $\mathtt{q}$ can be easily computed, and in fact has already been computed. Indeed, the function $\Gamma(C, D, \alpha, \cdot)$ introduced in Section 5.3 is precisely $\mathtt{q}\big(W_-^{CD}|_{\mathcal{H}_{\rm int}}\big)$, as we shall see it in the following section.

Remark 5.5.2. *We still would like to provide an alternative description of the above algebras and of the corresponding short exact sequence. Since* $\square$ *is isomorphic to* $\mathbb{T}$*, one first observes that* $\mathcal{Q} \equiv C\big(\square, M_2(\mathbb{C})\big)$ *is isomorphic to* $C\big(\mathbb{T}, M_2(\mathbb{C})\big)$*. Furthermore, by Stone-Weierstrass Theorem one clearly has that* $C(\mathbb{T})$ *is the* C^**-algebra generated by the continuous bijective function* $u : \mathbb{T} \ni \lambda \mapsto u(\lambda) := \lambda \in \mathbb{T} \subset \mathbb{C}$ *with winding number* 1*. Then, up to a natural equivalence there are not so many* C^**-algebras* $\mathcal{B}$ *which fit into an exact sequence of the form* $0 \to \mathcal{K} \to \mathcal{B} \to C(\mathbb{T}) \to 0$*, with* $\mathcal{K}$ *the algebra of compact operators. In fact, it turns out that they are classified by the Fredholm-index of a lift* $\hat{u}$ *of* u *[33, Thm. IX.3.3]. In the present case we can use an exactly solvable model to find out that* $\hat{u}$ *can be taken to be an isometry of co-rank* 1 *and hence this index is* -1 *[61]. Our extension is thus what one refers to as the Toeplitz extension. This means that* $\mathcal{E}$ *is the tensor product of* $M_2(\mathbb{C})$ *with the* C^**-algebra generated by an element* $\hat{u}$ *satisfying* $\hat{u}^*\hat{u} = 1$ *and* $\hat{u}\hat{u}^* = 1 - e_{00}$ *where* e_{00} *is a rank* 1 *projection. The surjection* $\mathtt{q}$ *is uniquely defined by* $\mathtt{q}(\hat{u}) = u$*. Our exact sequence is thus the tensor product with* $M_2(\mathbb{C})$ *of the exact sequence*

$$0 \to \mathcal{K} \xrightarrow{\mathtt{i}} C^*(\hat{u}) \xrightarrow{\mathtt{q}} C^*(u) \to 0. \tag{5.18}$$

5.5.2 The 0-degree Levinson's theorem, the topological approach

We can now state the topological version of Levinson's theorem.

Theorem 5.5.3. *For each* $\alpha \in (0, 1)$ *and each admissible pair* (C, D)*, one has* $W_-^{CD}|_{\mathcal{H}_{\rm int}} \in \mathcal{E}$*. Furthermore,* $\mathtt{q}\big(W_-^{CD}|_{\mathcal{H}_{\rm int}}\big) = \Gamma(C, D, \alpha, \cdot) \in \mathcal{Q}$ *and the following equality holds*

$$\mathrm{ind}[\Gamma(C, D, \alpha, \cdot)]_1 = -[P_\alpha^{CD}]_0 ,$$

where P_α^{CD} *is the orthogonal projection on the space spanned by the bound states of* H_α^{CD}*.*

Remark 5.5.4. *Recall that by Atkinson's theorem the image of any Fredholm operator* $F \in \mathcal{B}(\mathcal{H}_{\rm int})$ *in the Calkin algebra* $\mathcal{B}(\mathcal{H}_{\rm int})/\mathcal{K}(\mathcal{H}_{\rm int})$ *is invertible. Then, since the wave operators* $W_-^{CD}|_{\mathcal{H}_{\rm int}}$ *is an isometry and a Fredholm operator, it follows that each function* $\Gamma_j(C, D, \alpha, \cdot)$ *takes values in* $U(2)$*. In fact, this was already mentioned when the functions* $\Gamma_j(C, D, \alpha, \cdot)$ *were introduced.*

Proof of Theorem 5.5.3. The image of $W_-^{CD}|_{\mathcal{H}_{\rm int}}$ through the quotient map $\mathtt{q}$ is easily obtained by taking the formulae recalled in Lemma 5.5.1 into account. Then, since $W_-^{CD}|_{\mathcal{H}_{\rm int}}$ is a lift for $\Gamma(C, D, \alpha, \cdot)$, the image of $[\Gamma(C, D, \alpha, \cdot)]_1$ though the index map is obtained by the formula (5.14):

$$\begin{aligned}\mathrm{ind}[\Gamma(C,D,\alpha,\cdot)]_1 &= \big[1-\big(W_-^{CD}|_{\mathcal{H}_{\rm int}}\big)^* W_-^{CD}|_{\mathcal{H}_{\rm int}}\big]_0 - \big[1-W_-^{CD}|_{\mathcal{H}_{\rm int}}\big(W_-^{CD}|_{\mathcal{H}_{\rm int}}\big)^*\big]_0 \\ &= [0]_0 - \big[P_\alpha^{CD}\big]_0 \,.\end{aligned}$$

□

Theorem 5.5.3 covers the K-theoretic part of Levinson's theorem. In order to get a genuine Levinson's theorem, by which we mean an equality between topological numbers, we need to add the dual description, *i.e.* identify higher traces on $\mathcal{J}$ and $\mathcal{Q}$ and a dual boundary map. As a matter of fact, the algebras considered so far are too simple to allow for non-trivial results in higher degree and so we must content ourselves here to identify a suitable 0-trace and 1-trace which can be applied to P_α^{CD} and $\Gamma(C,D,\alpha,\cdot)$, respectively. Clearly, only the usual trace Tr can be applied on the former term, *cf.* Example 5.4.3 of Section 5.4. On the other hand, since $\Gamma(C,D,\alpha,\cdot)\in C\big(\square,U(2)\big)$, we can define the winding number $\mathrm{wind}\big[\Gamma(C,D,\alpha,\cdot)\big]$ of the map

$$\square \ni \zeta \mapsto \det[\Gamma(C,D,\alpha,\zeta)] \in \mathbb{T}$$

with orientation of □ chosen clockwise, *cf.* Example 5.4.4 of Section 5.4. Then, the already stated Theorem 5.3.1 essentially reformulates the fact that the 0-trace is mapped to the 1-trace by the dual of the index map. The first equality of Theorem 5.3.1 can then be found in Proposition 7 of [61] and the equality between the cardinality of $\sigma_p(H_\alpha^{CD})$ and the number of negative eigenvalues of the matrix CD^* has been shown in Lemma 4.3.2.

5.5.3 Higher degree Levinson's theorem

The previous theorem is a pointwise 0-degree Levinson's theorem. More precisely, it was obtained for fixed C,D and α. However, it clearly calls for making these parameters degrees of freedom and thus to include them into the description of the algebras. In the context of our physical model this amounts to considering families of self-adjoint extensions of H_α. For that purpose we use the one-to-one parametrization of these extensions with elements $U\in U(2)$ introduced in Remark 5.2.1. We denote the self-adjoint extension corresponding to $U\in U(2)$ by H_α^U.

So, let us consider a smooth and compact orientable n-dimensional manifold X without boundary. Subsequently, we will choose for X a two-dimensional submanifold of $U(2)\times(0,1)$. Taking continuous functions over X we get a new short exact sequence

$$0\to C(X,\mathcal{J})\to C(X,\mathcal{E})\to C(X,\mathcal{Q})\to 0\,. \tag{5.19}$$

Furthermore, recall that $\mathcal{J}$ is endowed with a 0-trace and the algebra $\mathcal{Q}$ with a 1-trace. There is a standard construction in cyclic cohomology, the cup product, which provides us with a suitable n-trace on the algebra $C(X,\mathcal{J})$ and a corresponding $n+1$-trace on the algebra $C(X,\mathcal{Q})$, see [31, Sec. III.1.α]. We describe it here in terms of cycles.

Recall that any smooth and compact manifold Y of dimension d naturally defines a structure of a graded differential algebra $(\mathcal{A}_Y,\mathrm{d}_Y)$, the algebra of its smooth differential k-forms. If we assume in addition that Y is orientable so that we can choose a global volume form, then the linear form $\int_Y$ can be defined by integrating the d-forms over Y. In that case, the algebra $C(Y)$ is naturally endowed with the d-trace defined by the character of the cycle $(\mathcal{A}_Y, \mathtt{d}_Y, \int_Y)$ of dimension d over the dense subalgebra $C^\infty(Y)$.

For the algebra $C(X, \mathcal{J})$, let us recall that $\mathcal{J}$ is equal to the algebra $\mathcal{K}(\mathcal{H}_{\mathsf{int}})$ and that the 0-trace on $\mathcal{J}$ was simply the usual trace Tr. So, let $\mathcal{K}_1$ denote the trace class elements of $\mathcal{K}(\mathcal{H}_{\mathsf{int}})$. Then, the natural graded differential algebra associated with $C^\infty(X, \mathcal{K}_1)$ is given by $(\mathcal{A}_X \otimes \mathcal{K}_1, \mathtt{d}_X)$. The resulting n-trace on $C(X, \mathcal{J})$ is then defined by the character of the cycle $(\mathcal{A}_X \otimes \mathcal{K}_1, \mathtt{d}_X, \int_X \otimes \mathrm{Tr})$ over the dense subalgebra $C^\infty(X, \mathcal{K}_1)$ of $C(X, \mathcal{J})$. We denote it by η_X.

For the algebra $C(X, \mathcal{Q})$, let us recall that $\mathcal{Q} = C\big(\square, M_2(\mathbb{C})\big)$ with $\square \cong \mathbb{S}^1$, and thus $C(X, \mathcal{Q}) \cong C\big(X \times \mathbb{S}^1, M_2(\mathbb{C})\big) \cong C(X \times \mathbb{S}^1) \otimes M_2(\mathbb{C})$. Since $X \times \mathbb{S}^1$ is a compact orientable manifold without boundary, the above construction applies also to $C\big(X \times \mathbb{S}^1, M_2(\mathbb{C})\big)$. More precisely, the exterior derivation on $X \times \mathbb{S}^1$ is the sum of $\mathtt{d}_X$ and $\mathtt{d}_{\mathbb{S}^1}$ (the latter was denoted simply by $\mathtt{d}$ in Example 5.4.4). Furthermore, we consider the natural volume form on $X \times \mathbb{S}^1$. Note because of the factor $M_2(\mathbb{C})$ the graded trace of the cycle involves the usual matrix trace tr. Thus the resulting $n+1$-trace is the character of the cycle $(\mathcal{A}_{X \times \mathbb{S}^1} \otimes M_2(\mathbb{C}), \mathtt{d}_X + \mathtt{d}_{\mathbb{S}^1}, \int_{X \times \mathbb{S}^1} \otimes \mathrm{tr})$. We denote it by $\#\eta_X$.

Having these constructions at our disposal we can now state the main result of this section. For the statement, we use the one-to-one parametrization of the extensions of H_α introduced in Remark 5.2.1 and let $\alpha \in (0,1)$. We consider a family $\{W_-(H_\alpha^U, H_0)\}_{(U,\alpha) \in X} \in \mathcal{B}(\mathcal{H}_{\mathsf{int}})$, parameterized by some compact orientable and boundaryless submanifold X of $U(2) \times (0,1)$. This family defines a map $\mathbf{W} : X \to \mathcal{E}$, $\mathbf{W}(U,\alpha) = W_-(H_\alpha^U, H_0)$, a map $\mathbf{\Gamma} : X \to \mathcal{Q}$, $\mathbf{\Gamma}(U, \alpha, \cdot) = \Gamma\big(C(U), D(U), \alpha, \cdot\big) = \mathtt{q}(W_-(H_\alpha^U, H_0))$, and a map $\mathbf{P} : X \to \mathcal{J}$, $\mathbf{P}(U, \alpha) = P_\alpha^U$ the orthogonal projection of the subspace of $\mathcal{H}_{\mathsf{int}}$ spanned by the bound states of H_α^U.

Theorem 5.5.5. *Let X be a smooth, compact and orientable n-dimensional submanifold of $U(2) \times (0,1)$ without boundary. Let us assume that the map $\mathbf{W} : X \to \mathcal{E}$ is continuous. Then the following equality holds:*

$$\mathrm{ind}[\mathbf{\Gamma}]_1 = -[\mathbf{P}]_0$$

where ind *is the index map from $K_1\big(C(X, \mathcal{Q})\big)$ to $K_0\big(C(X, \mathcal{J})\big)$. Furthermore, the numerical equality*

$$\big\langle \#\eta_X, [\mathbf{\Gamma}]_1 \big\rangle = -\big\langle \eta_X, [\mathbf{P}]_0 \big\rangle \tag{5.20}$$

also holds.

Proof. For the first equality we can simply repeat pointwise the proof of Theorem 5.5.3. Since we required $\mathbf{W}$ to be continuous, its kernel projection $\mathbf{P}$ is continuous as well. The second equality follows from of a more general formula stating that the map $\eta_X \mapsto \#\eta_X$ is dual to the boundary maps [39]. We also mention that another proof can be obtained by mimicking the calculation given in the Appendix of [65]. For the convenience of the reader, we sketch it in the Appendix 5.6.2 and refer to [65] for details. ☐

Let us point out that r.h.s. of (5.20) is the Chern number of the vector bundle given by the eigenstates of H_α^U. The next section is devoted to a computation of this number for a special choice of manifold X.

5.5.4 An example of a non trivial Chern number

We shall now choose a 2-dimensional manifold X and show that the above relation between the corresponding 2-trace and 3-trace is not trivial. More precisely, we shall choose a manifold X such that the r.h.s. of (5.20) is not equal to 0.

For that purpose, let us fix two complex numbers λ_1, λ_2 of modulus 1 with $\Im\lambda_1 < 0 < \Im\lambda_2$ and consider the set $X \subset U(2)$ defined by :

$$X = \left\{ V \left(\begin{smallmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{smallmatrix}\right) V^* \mid V \in U(2) \right\}.$$

Clearly, X is a two-dimensional smooth and compact manifold without boundary, which can be parameterized by

$$X = \left\{ \begin{pmatrix} \rho^2\lambda_1 + (1-\rho^2)\lambda_2 & \rho(1-\rho^2)^{1/2}\, e^{i\phi}(\lambda_1 - \lambda_2) \\ \rho(1-\rho^2)^{1/2}\, e^{-i\phi}(\lambda_1-\lambda_2) & (1-\rho^2)\lambda_1 + \rho^2\lambda_2 \end{pmatrix} \mid \rho \in [0,1] \text{ and } \phi \in [0,2\pi) \right\}. \tag{5.21}$$

Note that the (θ, ϕ)-parametrization of X is complete in the sense that it covers all the manifold injectively away from a subset of codimension 1, but it has coordinate singularities at $\rho \in \{0, 1\}$.

By Lemma 4.7.1, for each $U \equiv U(\rho, \phi) \in X$ the operator H^U_α has a single negative eigenvalue $z \equiv z(U)$ defined by the equality $\det\big((1+U)M(z) + i(1-U)\big) = 0$, and one has

$$\ker(H^U_\alpha - z) = \gamma(z) \ker\big((1+U)M(z) + i(1-U)\big). \tag{5.22}$$

Here, $M(z)$ is the Weyl function which is a 2×2 diagonal matrix and $\gamma(z) : \mathbb{C}^2 \to \mathcal{H}$ an injective linear map (see subsection 5.2.1). The orthogonal projection onto $\ker(H^U_\alpha - z)$ is denoted by P^U_α and we shall consider $E = \{\mathsf{Im}\, P^U_\alpha \mid U \in X\}$ which is a subbundle of the trivial bundle $X \times \mathcal{H}$. Our next aim is to calculate its Chern number $\mathrm{ch}(E)$, first in terms of the Chern number of a simpler bundle. In view of (5.22) $X \times \mathbb{C}^2 \ni (U, \xi) \mapsto (U, \gamma(z(U))\xi) \in X \times \mathcal{H}$ defines a continuous isomorphism between the subbundle F of the trivial bundle $X \times \mathbb{C}^2$ defined by

$$F = \big\{ \ker\big((1+U)M(z) + i(1-U)\big) \mid U \in X \big\}.$$

and E, and hence $\mathrm{ch}(E) = \mathrm{ch}(F)$. Now, the assumptions on λ_1 and λ_2 imply that for any $U \in X$ the matrix $(1+U)$ is invertible and one can then consider the self-adjoint operator

$$T(U) = i\,\frac{1-U}{1+U}\,.$$

By setting $\lambda_j =: e^{i\varphi_j}$ with $\varphi_1 \in (-\pi, 0)$ and $\varphi_2 \in (0, \pi)$, and then $r_i = \tan\frac{\varphi_i}{2}$ we get

$$T(U) = \begin{pmatrix} \rho^2 r_1 + (1-\rho^2) r_2 & \rho(1-\rho^2)^{1/2} e^{i\phi}(r_1 - r_2) \\ \rho(1-\rho^2)^{1/2} e^{-i\phi}(r_1 - r_2) & (1-\rho^2) r_1 + \rho^2 r_2 \end{pmatrix}$$

for some $\rho \in [0,1]$ and $\phi \in [0,2\pi)$ given by (5.21). Thus, by using the parametrization of U and z in terms of (ρ,ϕ) one obtains that the bundle E is isomorphic to the bundle G defined by

$$G = \big\{ \ker\big(G(\rho,\phi)\big) \mid \rho \in [0,1] \text{ and } \phi \in [0,2\pi)\big\}.$$

with

$$G(\rho,\phi) := \begin{pmatrix} M_{11}\big(z(\rho,\phi)\big) + \rho^2 r_1 + (1-\rho^2) r_2 & \rho(1-\rho^2)^{1/2} e^{i\phi}(r_1 - r_2) \\ \rho(1-\rho^2)^{1/2} e^{-i\phi}(r_1-r_2) & M_{22}\left(z(\rho,\phi)\right) + (1-\rho^2) r_1 + \rho^2 r_2 \end{pmatrix}.$$

Recall that $z(\rho,\phi)$ is defined by the condition $\det\big(G(\rho,\phi)\big) = 0$, *i.e.*

$$\big(M_{11}\big(z(\rho,\phi)\big)+\rho^2 r_1+(1-\rho^2)r_2\big)\cdot\big(M_{22}\left(z(\rho,\phi)\right)+(1-\rho^2)r_1+\rho^2 r_2\big) = (r_1-r_2)^2(1-\rho^2)\rho^2. \tag{5.23}$$

Finally, since $M(z)$ is self-adjoint for $z \in \mathbb{R}_-$, the matrix $G(\rho,\phi)$ is self-adjoint, and hence $\ker G(\rho,\phi) = \big(\operatorname{Im} G(\rho,\phi)\big)^{\perp}$. In particular, if one defines the bundle

$$H = \big\{ \operatorname{Im} G(\rho,\phi) \mid \rho \in [0,1] \text{ and } \phi \in [0,2\pi)\big\} \tag{5.24}$$

one obviously has $G + H = X \times \mathbb{C}^2$, and then $\operatorname{ch}(G) = -\operatorname{ch}(H)$ as the Chern number of the trivial bundle $X \times \mathbb{C}^2$ is zero. In summary, $\operatorname{ch}(E) = -\operatorname{ch}(H)$, which we are going to calculate after the following remark.

Remark 5.5.6. *Let $A : X \to M_2(\mathbb{C})$ be a continuously differentiable map with $A(x)$ of rank 1 for all $x \in X$. Let us recall how to calculate the Chern number of the bundle $B = \{\operatorname{Im} A(x) \mid x \in X\}$. Assume that the first column A_1 of A vanishes only on a finite set Y. If Y is empty, the bundle is trivial and $\operatorname{ch}(B) = 0$. So let us assume that Y is non-empty. Let $P(x)$ be the matrix of the orthogonal projection onto $\operatorname{Im} A(x)$ in $\mathbb{C}^2$. By definition, one has*

$$\operatorname{ch}(B) = \frac{1}{2\pi i}\int_X \operatorname{tr}\big(P \,\mathtt{d}_X P \wedge \mathtt{d}_X P\big).$$

Now, for $\epsilon > 0$ consider an open set $V_\epsilon \subset X$ with $Y \subset V_\epsilon$, having a C^1 boundary and such that $\operatorname{vol}_X V_\epsilon \to 0$ as $\epsilon \to 0$. By continuity and compactness, the differential form $\operatorname{tr}\big(P \,\mathtt{d}_X P \wedge \mathtt{d}_X P\big)$ is bounded, and then

$$\operatorname{ch}(B) = \frac{1}{2\pi i}\lim_{\epsilon\to 0}\int_{X\setminus V_\epsilon} \operatorname{tr}\big(P \,\mathtt{d}_X P \wedge \mathtt{d}_X P\big).$$

For $x \in X \setminus V_\epsilon$ one can consider the vector

$$\psi(x) = \frac{A_1(x)}{\|A_1(x)\|}$$

and by a direct calculation, one obtains $\operatorname{tr}\big(P \,\mathtt{d}_X P \wedge \mathtt{d}_X P\big) = \mathtt{d}_X\bar{\psi} \wedge \mathtt{d}_X\psi$. Since the differential form $\mathtt{d}_X\bar{\psi} \wedge \mathtt{d}_X\psi$ is exact, then $\mathtt{d}_X\bar{\psi} \wedge \mathtt{d}_X\psi = \mathtt{d}_X(\bar{\psi}\,\mathtt{d}_X\psi)$ and by Stokes' theorem, one obtains

$$\operatorname{ch}(B) = \frac{1}{2\pi i}\lim_{\epsilon\to 0}\int_{\partial V_\epsilon} \bar{\psi}\,\mathtt{d}_X\psi.$$

Let us apply the above constructions to the bundle (5.24). Since $(r_1 - r_2) \neq 0$ the first column $G_1(\rho,\phi)$ of the matrix $G(\rho,\phi)$ can potentially vanish only for $\rho = 0$ or for $\rho = 1$. As already mentioned, these two points are the coordinate singularities of the parametrization. But by a local change of parametrization, one easily get rid of this pathology. Thus, we first consider $\rho = 1$ and let $(\theta_1,\theta_2) \in (-1,1)^2$ be a local parametrization of a neighbourhood of the point $\rho = 1$ which coincides with $(\theta_1,\theta_2) = (0,0)$. Let $\widetilde{G}$ be the expression of the function G in the coordinates (θ_1,θ_2) and in a neighbourhood of the point $\rho = 1$. For this function one has

$$\widetilde{G}_1(0,0) = \begin{pmatrix} M_{11}\big(z(0,0)\big) + r_1 \\ 0 \end{pmatrix}$$

Now, note that under our assumptions one has $r_1 < 0$ and $r_2 > 0$. As seen from the explicit expressions for M, the entries of $M(z)$ are negative for $z < 0$. Then the term $M_{11}\big(z(0,0)\big)+r_1$ can not be equal to 0 and this also holds for the first coefficient of $\widetilde{G}_1(0,0)$.

For $\rho = 0$ let $(\vartheta_1,\vartheta_2) \in (-1,1)^2$ be a local parametrization of a neighbourhood of the point $\rho = 0$ which coincides with $(\vartheta_1,\vartheta_2) = (0,0)$. Let again $\widehat{G}$ be the expression of the function G in the coordinates $(\vartheta_1,\vartheta_2)$ and in a neighbourhood of the point $\rho = 0$. Then one has

$$\widehat{G}_1(0,0) = \begin{pmatrix} M_{11}\big(z(0,0)\big) + r_2 \\ 0 \end{pmatrix} .$$

In that case, since $M_{22}(z) + r_1$ is strictly negative for any $z \in \mathbb{R}_-$ one has $M_{11}\big(z(0,0)\big) + r_2 = 0$ in order to satisfy Equation (5.23). Therefore, the corresponding point $\rho = 0$ belongs to Y, as introduced in Remark 5.5.6. Therefore, in our case Y consists in a single point y corresponding to $\rho = 0$.

Now, for $\epsilon > 0$ consider the set

$$V_\epsilon = \Big\{ \begin{pmatrix} \rho^2\lambda_1 + (1-\rho^2)\lambda_2 & \rho(1-\rho^2)^{1/2}\, e^{i\phi}(\lambda_1-\lambda_2) \\ \rho(1-\rho^2)^{1/2}\, e^{-i\phi}(\lambda_1-\lambda_2) & (1-\rho^2)\lambda_1 + \rho^2\lambda_2 \end{pmatrix} \\ \mid \rho \in [0,\epsilon) \text{ and } \phi \in [0,2\pi) \Big\}.$$

Obviously, this set satisfies the conditions of Remark 5.5.6. We can then represent

$$G_1(\rho,\phi) = \begin{pmatrix} M_{11}\big(z(\rho,\phi)\big) + \rho^2 r_1 + (1-\rho^2) r_2 \\ \rho(1-\rho^2)^{1/2} e^{-i\phi}(r_1 - r_2) \end{pmatrix} =: \begin{pmatrix} g(\rho,\phi) \\ f(\rho)e^{-i\phi} \end{pmatrix}$$

with f, g real, and set

$$\psi(\rho,\phi) := \frac{G_1(\rho,\phi)}{\|G_1(\rho,\phi)\|} = \begin{pmatrix} \dfrac{g(\rho,\phi)}{\sqrt{f^2(\rho)+g^2(\rho,\phi)}} \\ \dfrac{f(\rho)e^{-i\phi}}{\sqrt{f^2(\rho)+g^2(\rho,\phi)}} \end{pmatrix} .$$

Then one has

$$\begin{aligned}&\int_{\partial V_\epsilon(y)} \bar{\psi}\, \mathtt{d}_X \psi \\ &= \int_0^{2\pi} \Big[\frac{g}{\sqrt{f^2+g^2}}\,\partial_\phi\Big(\frac{g}{\sqrt{f^2+g^2}}\Big) + \frac{f e^{i\cdot}}{\sqrt{f^2+g^2}}\,\partial_\phi\Big(\frac{f e^{-i\cdot}}{\sqrt{f^2+g^2}}\Big)\Big](\epsilon,\phi)\,\mathrm{d}\phi \\ &= -i\int_0^{2\pi} \Big[\frac{f^2}{f^2+g^2}\Big](\epsilon,\phi)\mathrm{d}\phi\end{aligned}$$

Thus, one has obtained that

$$\mathrm{ch}(H) = -\frac{1}{2\pi}\lim_{\epsilon\to 0}\int_0^{2\pi} \frac{f^2(\epsilon)}{f^2(\epsilon)+g^2(\epsilon,\phi)}\,\mathrm{d}\phi. \tag{5.25}$$

Furthermore, note that Equation (5.23) can be rewritten as $g(\rho,\phi)h(\rho,\phi) = f^2(\rho)$, where $h(\rho,\phi) = \big(M_{22}\,(z(\rho,\phi)) + (1-\rho^2)r_1 + \rho^2 r_2\big)$ does not vanish in a sufficiently small neighbourhood of the point $\rho = 0$. Then one has $g(\rho,\phi) = o\big(f(\rho)\big)$ uniformly in ϕ as r tends to 0. By substituting this observation into (5.25) one obtains

$$\mathrm{ch}(H) = -\frac{1}{2\pi}\int_0^{2\pi}\lim_{\epsilon\to 0}\frac{f^2(\epsilon)}{f^2(\epsilon)+g^2(\epsilon,\phi)}\,\mathrm{d}\phi = -\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi = -1.$$

As a consequence, by returning to the original bundle E, one has obtained $\mathrm{ch}(E) = -\mathrm{ch}(H) = 1$.

As a corollary, one easily prove:

Proposition 5.5.7. *Let λ_1, λ_2 be two complex numbers of modulus 1 with $\Im\lambda_1 < 0 < \Im\lambda_2$ and consider the set $X \subset U(2)$ defined by* (5.21)*. Then the map $\mathbf{W} : X \to \mathcal{E}$ is continuous and the following equality holds:*

$$\frac{1}{24\pi^2}\int_{X\times\square} \mathrm{tr}\left[\mathbf{\Gamma}^*\, \mathtt{d}_{X\times\square}\mathbf{\Gamma} \wedge \mathtt{d}_{X\times\square}\mathbf{\Gamma}^* \wedge \mathtt{d}_{X\times\square}\mathbf{\Gamma}\right] = 1$$

Proof. Continuity of $X \ni U \mapsto W_-(H^U_\alpha, H_0) \in \mathcal{E}$ is proved in Appendix 5.6.3. The equation is an application of Theorem 5.5.5 with $n = 2$ with η_X defined by the first Chern character over X: $\langle \eta_X, [\mathbf{P}]_0\rangle = \frac{1}{2\pi i}\int_X \mathrm{Tr}\big[\mathbf{P}\,\mathtt{d}_X\mathbf{P}\wedge \mathtt{d}_X\mathbf{P}\big] = \mathrm{ch}(E)$. □

5.6 Appendix

5.6.1 Proof of Lemma 5.3.2

Denote for brevity $\varphi = \varphi_{a,b}$. We first observe that

$$\varphi(x)^{-1}\varphi'(x) = i\Big(\frac{\Gamma'(a+ix)}{\Gamma(a+ix)} + \frac{\Gamma'(a-ix)}{\Gamma(a-ix)} - \frac{\Gamma'(b-ix)}{\Gamma(b-ix)} - \frac{\Gamma'(b+ix)}{\Gamma(b+ix)}\Big).$$

Since the function Γ is real on the real positive axis, let us choose a continuous determination of the logarithm, denoted by $\log$, such that $\log\big(\Gamma(y+ix)\big)|_{x=0}\in\mathbb{R}$ for any $y\in\mathbb{R}_+^*$. Then, one observes that

$$\varphi(x)^{-1}\varphi'(x)=\frac{\mathrm{d}}{\mathrm{d}x}I(x,a,b)$$

with

$$I(x,a,b):=\log\big(\Gamma(a+ix)\big)-\log\big(\Gamma(a-ix)\big)+\log\big(\Gamma(b-ix)\big)-\log\big(\Gamma(b+ix)\big)\ .$$

It follows that

$$\mathrm{Var}[\varphi]=\frac{1}{i}\big[\lim_{x\to\infty}I(x,a,b)-\lim_{x\to-\infty}I(x,a,b)\big]=\frac{2}{i}\lim_{x\to\infty}I(x,a,b)\ .$$

Now, let us denote by $\ln$ the principal determination of the logarithm, *i.e.* $\ln(z)=\ln(|z|)+i\theta(z)$, where $\theta:\mathbb{C}^*\to(-\pi,\pi]$ is the principal argument of z. We recall from [1, Eq. 6.1.37] that for $z\to\infty$ with $|\theta(z)|<\pi$:

$$\Gamma(z)\cong e^{-z}\,e^{(z-1/2)\ln(z)}\,(2\pi)^{1/2}\big(1+O(z^{-1})\big)\ .$$

For $z=y+ix$, the term $e^{-z}\,e^{(z-1/2)\ln(z)}$ can be rewritten as

$$e^{-y}\,e^{(y-1/2)\ln(\sqrt{x^2+y^2})}\,e^{-x\theta(y+ix)}\exp\big\{-i\big(x-x\ln\big(\sqrt{x^2+y^2}\big)-(y-1/2)\theta(y+ix)\big)\big\}\ .$$

It follows that for $|x|$ large enough, one has

$$\begin{aligned}\log\big(\Gamma(y+ix)\big)\;\cong\;&-y+(y-1/2)\ln\big(\sqrt{x^2+y^2}\big)-x\theta(y+ix)+\tfrac{1}{2}\ln(2\pi)\\&-i\big(x-x\ln\big(\sqrt{x^2+y^2}\big)-(y-1/2)\theta(y+ix)\big)\ .\end{aligned}$$

By taking this asymptotic development into account, one obtains:

$$\begin{aligned}I(x,a,b)\;\cong\;&-x\big[\theta(a+ix)+\theta(a-ix)-\theta(b-ix)-\theta(b+ix)\big]\\&+ix\big[2\ln\big(\sqrt{a^2+x^2}\big)-2\ln\big(\sqrt{b^2+x^2}\big)\big]\\&+i(a-\tfrac{1}{2})\big[\theta(a+ix)-\theta(a-ix)\big]+i(b-\tfrac{1}{2})\big[\theta(b-ix)-\theta(b+ix)\big]\ .\end{aligned}$$

Clearly, for any x one has

$$\theta(a+ix)+\theta(a-ix)-\theta(b-ix)-\theta(b+ix)=0\ .$$

Furthermore, some calculations of asymptotic developments show that

$$\lim_{|x|\to\infty}x\big[2\ln\big(\sqrt{a^2+x^2}\big)-2\ln\big(\sqrt{b^2+x^2}\big)\big]=0\ .$$

It thus follows that

$$\begin{aligned}&\lim_{x\to\infty}I(x,a,b)\\&=i\lim_{x\to\infty}\Big\{(a-\tfrac{1}{2})\big[\theta(a+ix)-\theta(a-ix)\big]+(b-\tfrac{1}{2})\big[\theta(b-ix)-\theta(b+ix)\big]\Big\}\\&=i(a-\tfrac{1}{2})\big[\tfrac{\pi}{2}-\big(-\tfrac{\pi}{2}\big)\big]+i(b-\tfrac{1}{2})\big[\big(-\tfrac{\pi}{2}\big)-\tfrac{\pi}{2}\big]\\&=i\pi(a-b)\ .\end{aligned}$$

5.6.2 Proof of Theorem 5.5.5

As already mentioned, we simply sketch the proof of the second equality of Theorem 5.5.5 mimicking the approach of the Appendix of [65]. Note that this proof is based on the alternative description of the C^*-algebras provided in Remark 5.5.2.

Proof of the second statement of Theorem 5.5.5. 1) Let us first observe that the short exact sequence (5.18) illuminates better the K-theory associated with the relevant algebras. Indeed, the relations for $\hat{u}$ tell us immediately that $1 - e_{00}$ and 1 are Murray-von Neumann equivalent and hence define the same K_0-element in $\mathcal{E}$. It follows that the two maps $K_0(\mathtt{i}) : K_0(\mathcal{K}) \to K_0\big(C^*(\hat{u})\big)$ and $K_1(\mathtt{i}) : K_1(\mathcal{K}) \to K_1\big(C^*(\hat{u})\big)$ are the zero maps, so that the six-term exact sequence splits into two short exact sequences, see [99, Chap. 12] for more information on the six-term exact sequence. From this one may conclude that the inclusion $\mathtt{j} : \mathbb{C} \ni 1 \mapsto 1 \in C^*(\hat{u})$ induces an isomorphism in K-theory. The two exact sequences in K-theory therefore become for $i = 0, 1 \bmod 2$:

$$0 \to K_i(\mathbb{C}) \xrightarrow{K_i(\mathtt{j})} K_i(C^*(u)) \xrightarrow{\delta_i} K_{i-1}(\mathcal{K}) \to 0,$$

where δ_i are the boundary maps, and in particular $\delta_1 = \mathrm{ind}$.

Let us now consider a smooth and compact orientable n-dimensional manifold X without boundary and the associated short exact sequence introduced in Section 5.5.3. The above description has the following generalisation: $C(X, \mathcal{E}) \cong C\big(X, M_2(\mathbb{C})\big) \otimes C^*(\hat{u})$ and the map $\mathtt{j}' : C\big(X, M_2(\mathbb{C})\big) \to C\big(X, M_2(\mathbb{C})\big) \otimes C^*(\hat{u})$, $f \mapsto \mathtt{j}'(f) \equiv f \otimes 1$, induces an isomorphism in K-theory. Furthermore, the short exact sequence (5.19) is isomorphic to the following one:

$$0 \to C\big(X, M_2(\mathbb{C})\big) \otimes \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big) \to C\big(X, M_2(\mathbb{C})\big) \otimes C^*(\hat{u}) \to C\big(X, M_2(\mathbb{C})\big) \otimes C^*(u) \to 0\,. \tag{5.26}$$

This short exact sequence is the Toeplitz extension of the crossed product of the algebra $C\big(X, M_2(\mathbb{C})\big)$ by the trivial action of $\mathbb{Z}$. Note that Pimsner and Voiculescu have considered the general case of an action of $\mathbb{Z}$ on a C^*-algebra [83]. Our interest in (5.26) relies on the study of a more general short exact sequence performed in the Appendix of [65] (in that reference, the action of $\mathbb{Z}$ is general) and on the corresponding dual boundary maps.

2) Once this framework is settled, the next part of the proof consists in constructing a right inverse for ind. The map $\mathfrak{j} : C\big(X, M_2(\mathbb{C})\big) \to C\big(X, M_2(\mathbb{C})\big) \otimes \mathcal{K}\big(\mathsf{L}^2(\mathbb{R}_+)\big)$, $\mathfrak{j}(f) = f \otimes e_{00}$ induces an isomorphism in K-theory [99]. It is hence sufficient to construct a preimage under ind of an element of the form $[\mathfrak{j}(P)]_0$ where P is a projection in $C\big(X, M_2(\mathbb{C})\big) \otimes M_k(\mathbb{C})$. Here k is arbitrary and in principle higher k are needed, but for simplicity of the notation we shall set $k = 1$, the more general case being a simple adaptation. Let $U \in C\big(X, M_2(\mathbb{C})\big) \otimes C^*(u)$ be given by $U = 1 \otimes u$, and set $U_P := U\mathfrak{j}(P) + \big(1 - \mathfrak{j}(P)\big)$. Then one has to show that U_P is a unitary in $C\big(X, M_2(\mathbb{C})\big) \otimes C^*(u)$ and that $\mathrm{ind}[U_P]_1 = [\mathfrak{j}(P)]_0$. However, this calculation is well-known and in particular is performed in [65, Prop. A.1]) to which we refer. Note that since the action of $\mathbb{Z}$ is trivial, the expression of U_P introduced here is even simpler than the formula presented in that reference.

3) The last step consists in checking that the numerical equality

$$\big\langle \#\eta_X, [U_P]_1 \big\rangle = \big\langle \eta_X, [P]_0 \big\rangle$$

holds. Again this direct computation has already been performed in [65, Thm. A.10] to which we refer for details. Note that the constants c_{2k} and c_{2k+1} introduced in Section 5.4.2 follow from this computation. Since the above equality has been proved for arbitrary elements of the corresponding algebras, we can then apply the result to $\mathbf{P} \in C(X, \mathcal{J})$ and recall that $\mathbf{\Gamma} \in C(X, \mathcal{Q})$ is a right inverse to $-\mathbf{P}$ for the map ind, *i.e.* $\mathrm{ind}[\mathbf{\Gamma}]_1 = -[\mathbf{P}]_0$. $\square$

5.6.3 Continuity of the wave operator

In this section we show that the map $X \ni U \mapsto W_-(H^U_\alpha, H_0) \in \mathcal{E}$ is continuous under the assumptions of Proposition 5.5.7. In view of the representations (5.3) and (5.4) for the wave operators it is sufficient to show the continuity of the map $X \ni U \mapsto S^U \in \mathcal{B}$, where $\mathcal{B}$ is the space of bounded continuous matrix-valued functions $S : [0, +\infty] \to M_2(\mathbb{C})$ endowed with the norm

$$\left\| \begin{pmatrix} s_{11}(\cdot) & s_{12}(\cdot) \\ s_{21}(\cdot) & s_{22}(\cdot) \end{pmatrix} \right\| = \max_{1\leq j,k\leq 2} \sup_{\kappa\geq 0} \left| s_{jk}(\kappa) \right|.$$

Note that we use the notation S^U for S^{CD}_α with $C = C(U)$ and $D = D(U)$ defined in Remark 5.2.1. Let us set

$$L = L(U) = \frac{\pi}{2\sin(\pi\alpha)} \frac{1-U}{i(1+U)} =: (l_{jk})$$

and use again the representation (5.10):

$$S^U(\kappa) = \Phi \frac{B^{-1} L B^{-1} + \cos(\pi\alpha) J + i\sin(\pi\alpha)}{B^{-1} L B^{-1} + \cos(\pi\alpha) J - i\sin(\pi\alpha)} \Phi J\,,$$

with

$$B \equiv B(\kappa) := \begin{pmatrix} \frac{\Gamma(1-\alpha)}{2^\alpha}\kappa^\alpha & 0 \\ 0 & \frac{\Gamma(\alpha)}{2^{1-\alpha}}\kappa^{(1-\alpha)} \end{pmatrix}, \quad \Phi := \begin{pmatrix} e^{-i\pi\alpha/2} & 0 \\ 0 & e^{-i\pi(1-\alpha)/2} \end{pmatrix}, \quad J := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Then by observing that the map $X \ni U \mapsto L(U) \in M_2(\mathbb{C})$ is continuous in the usual matrix norm, it follows that the map

$$L(X) \times [0,\infty] \ni (L,\kappa) \mapsto \frac{B(\kappa)^{-1} L B(\kappa)^{-1} + \cos(\pi\alpha) J + i\sin(\pi\alpha)}{B(\kappa)^{-1} L B(\kappa)^{-1} + \cos(\pi\alpha) J - i\sin(\pi\alpha)} \in M_2(\mathbb{C}).$$

is also continuous. This implies the required continuity of the map $X \ni U \mapsto S^U \in \mathcal{B}$.

Bibliography

[1] M. Abramowitz and I. Stegun. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, National Bureau of Standards Applied Mathematics Series 55, U.S. Government Printing Office, Washington D.C., 1964.

[2] R. Adami and A. Teta. On the Aharonov-Bohm Hamiltonian. *Lett. Math. Phys.* 43: 43–54, 1998.

[3] Y. Aharonov and D. Bohm. Significance of electromagnetic potentials in the quantum theory. *Phys. Rev.* 115: 485–491, 1959.

[4] T. Aktosun. On the Schrödinger equation with steplike potentials. *J. Math. Phys.* 40(11): 5289–5305, 1999.

[5] S. Albeverio, F. Gesztesy, R. Høegh-Krohn and H. Holden. *Solvable models in quantum mechanics*, 2nd ed. with an Appendix by P. Exner, AMS, Providence, Rhode Island, 2005.

[6] S. Albeverio and K. Pankrashkin. A remark on Krein's resolvent formula and boundary conditions. *J. Phys. A* 38: 4859–4864, 2005.

[7] W. O. Amrein, A. Boutet de Monvel and V. Georgescu. *C_0-groups, commutator methods and spectral theory of N-body Hamiltonians*, volume 135 of *Progress in Math.* Birkhäuser, Basel, 1996.

[8] W. O. Amrein and M. B. Cibils. Global and Eisenbud-Wigner time delay in scattering theory. *Helv. Phys. Acta* 60: 481–500, 1987.

[9] W. O. Amrein, M. B. Cibils and K. B. Sinha. Configuration space properties of the S-matrix and time delay in potential scattering. *Ann. Inst. Henri Poincaré* 47: 367–382, 1987.

[10] W. O. Amrein and Ph. Jacquet. Time delay for one-dimensional quantum systems with steplike potentials. *Phys. Rev. A* 75(2): 022106, 2007.

[11] W.O. Amrein, J.M. Jauch and K.B. Sinha. *Scattering theory in quantum mechanics*. Lecture Notes and Supplements in Physics 16, W. A. Benjamin, Inc., Reading, Mass.-London-Amsterdam, 1977.

[12] W. O. Amrein and K. B. Sinha. Time delay and resonances in potential scattering. *J. Phys. A* 39(29): 9231–9254, 2006.

[13] I. Antoniou, I. Prigogine, V. Sadovnichii and S. A. Shkarin. Time operator for diffusion. *Chaos Solitons Fractals* 11(4): 465–477, 2000.

[14] A. Arai. Generalized Weyl relation and decay of quantum dynamics. *Rev. Math. Phys.* 17(9): 1071–1109, 2005.

[15] M. Ballesteros and R. Weder. High-velocity estimates for the scattering operator and Aharonov-Bohm effect in three dimensions. *Commun. Math. Phys.* 285: 345–398, 2009.

[16] M. Ballesteros and R. Weder. Aharonov-Bohm effect and Tonomura et al. experiments, rigorous results. *Journal of Math. Phys.* 50: 122108, 2009.

[17] H. Baumgärtel and M. Wollenberg. *Mathematical scattering theory*, volume 9 of *Operator Theory: Advances and Applications*. Birkhäuser Verlag, Basel, 1983.

[18] M.V. Berry. Aptly named Aharonov-Bohm effect has classical analogue, long history. *Letter in Physics Today* August 2010.

[19] M. Sh. Birman and M. Z. Solomjak. *Spectral theory of selfadjoint operators in Hilbert space*. Mathematics and its Applications (Soviet Series). D. Reidel Publishing Co., Dordrecht, 1987. Translated from the 1980 Russian original by S. Khrushchëv and V. Peller.

[20] D. Bollé, F. Gesztesy and H. Grosse. Time delay for long-range interactions. *J. Math. Phys.* 24(6): 1529–1541, 1983.

[21] D. Bollé and T. A. Osborn. Time delay in N-body scattering. *J. Math. Phys.* 20: 1121–1134, 1979.

[22] A. Boutet de Monvel and V. Georgescu. The method of differential inequalities. In *Recent developments in quantum mechanics* pp. 279–298. Math. Phys. Stud. 12, Kluwer Acad. Publ., Dordrecht, 1991.

[23] A. Boutet de Monvel, G. Kazantseva and M. Măntoiu. Some anisotropic Schrödinger operators without singular spectrum. *Helv. Phys. Acta* 69(1): 13–25, 1996.

[24] G. Bräunlich, G.M. Graf and G. Ortelli. Equivalence of topological and scattering approaches to quantum pumping. *Comm. Math. Phys.* 295: 243–259, 2010.

[25] L. Bruneau, J. Dereziński and V. Georgescu. Homogeneous Schrödinger operators on half-line. *Annales Henri Poincaré* 12(3): 547-590, 2011.

[26] J. Brüning and V. Geyler. Scattering on compact manifolds with infinitely thin horns. *J. Math. Phys.* 44: 371–405, 2003.

[27] J. Brüning, V. Geyler and K. Pankrashkin. Spectra of self-adjoint extensions and applications to solvable Schrödinger operators. *Rev. Math. Phys.* 20: 1–70, 2008.

[28] T. Christiansen. Resonances for steplike potentials: forward and inverse results. *Trans. Amer. Math. Soc.* 358(5): 2071–2089 (electronic), 2006.

[29] A. Cohen and T. Kappeler. Scattering and inverse scattering for steplike potentials in the Schrödinger equation. *Indiana Univ. Math. J.* 34(1): 127–180, 1985.

[30] A. Connes. Cyclic cohomology and the transverse fundamental class of a foliation. In *Geometric methods in operator algebras (Kyoto, 1983)*, 52–144, Pitman Res. Notes Math. Ser. 123, Longman Sci. Tech., Harlow, 1986.

[31] A. Connes. *Noncommutative geometry*, Academic Press, Inc., San Diego, CA, 1994.

[32] L. Dąbrowski and P. Stovícek. Aharonov-Bohm effect with δ-type interaction. *J. Math. Phys.* 39: 47–62, 1998.

[33] K. Davidson. *C^*-algebras by example*. American Mathematical Society, 1996.

[34] E. B. Davies. *Spectral theory and differential operators*, volume 42 of *Cambridge Studies in Advanced Mathematics* Cambridge University Press, Cambridge, 1995.

[35] C. A. A. de Carvalho and H. M. Nussenzveig. Time delay. *Phys. Rep.* 364(2): 83–174, 2002.

[36] J. Dereziński and C. Gérard. *Scattering theory of classical and quantum N-particle systems*. Texts and Monographs in Physics. Springer-Verlag, Berlin, 1997.

[37] V.A. Derkach and M.M. Malamud. Generalized resolvents and the boundary value problems for Hermitian operators with gaps. *J. Funct. Anal.* 95: 1–95, 1991.

[38] L. Eisenbud. *Dissertation*. Princeton University, 1948.

[39] G. Elliott, T. Natsume and R. Nest. Cyclic cohomology for one-parameter smooth crossed products. *Acta Math.* 160: 285–305, 1988.

[40] P. Exner, P. Stovícek and P. Vytras. Generalised boundary conditions for the Aharonov-Bohm effect combined with a homogeneous magnetic field. *J. Math. Phys.* 43: 2151–2168, 2002.

[41] G. B. Folland. *A course in abstract harmonic analysis*. Studies in Advanced Mathematics. CRC Press, Boca Raton, 1995.

[42] E. A. Galapon. Pauli's theorem and quantum canonical pairs: the consistency of a bounded, self-adjoint time operator canonically conjugate to a Hamiltonian with non-empty point spectrum. *R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci.* 458: 451–472, 2002.

[43] V. Georgescu and A. Iftimovici. C^*-algebras of quantum Hamiltonians. In *Operator Algebras and Mathematical Physics*. Conference Proceedings: Constanţa (Romania) July 2001, 123–167, Theta Foundation, Bucharest, 2003.

[44] V. Georgescu and C. Gérard. On the virial theorem in quantum mechanics. *Commun. Math. Phys.* 208: 275–281, 1999.

[45] C. Gérard and R. Tiedra de Aldecoa. Generalized definition of time delay in scattering theory. *J. Math. Phys.* page 122101, 2007.

[46] F. Gesztesy. Scattering theory for one-dimensional systems with nontrivial spatial asymptotics. In *Schrödinger operators, Aarhus 1985*, volume 1218 of *Lecture Notes in Math.* pages 93–122. Springer, Berlin, 1986.

[47] S. Golénia and S. Moroianu. Spectral analysis of magnetic Laplacians on conformally cusp manifolds. *Ann. Henri Poincaré* 9(1): 131–179, 2008.

[48] N. Goloshchapova and L. Oridoroga. The one-dimensional Schrödinger operator with point δ- and δ'-interactions. *Math. Notes* 84: 125–129, 2008.

[49] F. Gómez. Self-adjoint time operators and invariant subspaces. *Rep. Math. Phys.* 61(1): 123–148, 2008.

[50] T. Gotō, K. Yamaguchi and N. Sudō. On the time operator in quantum mechanics. Three typical examples. *Progr. Theoret. Phys.* 66(5): 1525–1538, 1981.

[51] K. Gustafson and K. Sinha. On the Eisenbud-Wigner formula for time-delay. *Lett. Math. Phys.* 4(5): 381–385, 1980.

[52] M. Harmer. Hermitian symplectic geometry and extension theory. *J. Phys. A* 33: 9193–9203, 2000.

[53] F. Hiroshima, S. Kuribayashi and Y. Matsuzawa. Strong time operators associated with generalized Hamiltonians. *Lett. Math. Phys.* 87(1-2): 115–123, 2009.

[54] J. M. Jauch, K. B. Sinha and B. N. Misra. Time-delay in scattering processes. *Helv. Phys. Acta* 45: 398–426, 1972.

[55] A. Jensen. Time-delay in potential scattering theory. Some "geometric" results. *Comm. Math. Phys.* 82(3): 435–456, 1981/82.

[56] P. T. Jørgensen and P. S. Muhly. Selfadjoint extensions satisfying the Weyl operator commutation relations. *J. Analyse Math.* 37: 46–99, 1980.

[57] T. Kato. *Perturbation theory for linear operators*, Reprint of the 1980 edition, Classics in Mathematics, Springer-Verlag, Berlin, 1995.

[58] J. Kellendonk. Gap labelling and the pressure on the boundary. *Commun. Math. Phys.* 258(3): 751–768, 2005.

[59] J. Kellendonk, K. Pankrashkin and S. Richard. Levinson's theorem and higher degree traces for Aharonov-Bohm operators. *J. Math. Phys.* 52: 052102, 2011.

[60] J. Kellendonk and S. Richard. Levinson's theorem for Schrödinger operators with point interaction: a topological approach. *J. Phys. A* 39(46)L 14397–14403, 2006.

[61] J. Kellendonk and S. Richard. On the structure of the wave operators in one dimensional potential scattering. *Mathematical Physics Electronic Journal* 14: 1–21, 2008.

[62] J. Kellendonk and S. Richard. The topological meaning of Levinson's theorem, half-bound states included. *J. Phys. A: Math. Theor.* 41: 295207, 2008.

[63] J. Kellendonk and S. Richard. Weber-Schafheitlin type integrals with exponent 1. *Int. Transf. Spec. Funct.* 20: 147–153, 2009.

[64] J. Kellendonk and S. Richard. On the wave operators and Levinson's theorem for potential scattering in $\mathbb{R}^3$. To appear in Asian-European Journal of Mathematics. .

[65] J. Kellendonk, T. Richter and H. Schulz-Baldes. Edge current channels and Chern numbers in the integer quantum Hall effect. *Rev. Math. Phys.* 14(1): 87–119, 2002.

[66] J. Kellendonk and H. Schulz-Baldes. Boundary maps for C^*-crossed products with $\mathbb{R}$ with an application to the quantum Hall effect. *Comm. Math. Phys.* 249(3): 611–637, 2004.

[67] O. Lisovyy. Aharonov-Bohm effect on the Poincaré disk. *J. Math. Phys.* 48: 052112, 2007.

[68] M. Măntoiu, S. Richard and R. Tiedra de Aldecoa. Spectral analysis for adjacency operators on graphs. *Ann. Henri Poincaré* 8(7): 1401–1423, 2007.

[69] M. Măntoiu and R. Tiedra de Aldecoa. Spectral analysis for convolution operators on locally compact groups. *J. Funct. Anal.* 253(2): 675–691, 2007.

[70] P. A. Martin. Scattering theory with dissipative interactions and time delay. *Nuovo Cimento B* 30: 217–238, 1975.

[71] P. A. Martin. On the time-delay of simple scattering systems. *Comm. Math. Phys.* 47(3): 221–227, 1976.

[72] P. A. Martin. Time delay in quantum scattering processes. *Acta Phys. Austriaca Suppl., XXIII*, pages 157–208, 1981.

[73] M. Miyamoto. A generalized Weyl relation approach to the time operator and its connection to the survival probability. *J. Math. Phys.* 42(3): 1038–1052, 2001.

[74] A. Mohapatra, K. B. Sinha and W. O. Amrein. Configuration space properties of the scattering operator and time delay for potentials decaying like $|x|^{-\alpha}$, $\alpha > 1$. *Ann. Inst. H. Poincaré Phys. Théor.* 57(1): 89–113, 1992.

[75] J. S. Møller and M. Westrich. Regularity of eigenstates in regular Mourre theory. *J. Funct. Anal.* 260(3): 852–878, 2011.

[76] E. Mourre. Absence of singular continuous spectrum for certain selfadjoint operators. *Comm. Math. Phys.* 78(3): 391–408, 1980/81.

[77] J. G. Muga and C. R. Leavens. Arrival time in quantum mechanics. *Phys. Rep.* 338(4): 353–438, 2000.

[78] J. G. Muga, R. Sala Mayato and Í. L. Egusquiza, editors. *Time in quantum mechanics. Vol. 1*, volume 734 of *Lecture Notes in Physics*. Springer, Berlin, second edition, 2008.

[79] F. Oberhettinger. *Tables of Mellin transforms*, Springer-Verlag, New York–Heidelberg, 1974.

[80] T. A. Osborn and D. Bollé. The three-body time-delay operator. *J. Math. Phys.* 16: 1533–1549, 1975.

[81] K. Pankrashkin. Resolvents of self-adjoint extensions with mixed boundary conditions. *Rep. Math. Phys.* 58: 207–221, 2006.

[82] K. Pankrashkin and S. Richard. Spectral and scattering theory for the Aharonov-Bohm operators. *Rev. Math. Phys.* 23: 53–81, 2011.

[83] M. Pimsner and D. Voiculescu. Exact sequences for K-groups and Ext-groups of certain cross-products of C^*-algebras. *J. Op. Theory* 4: 93–118, 1980.

[84] A. Posilicano. Self-adjoint extensions of restrictions. *Oper. Matrices* 2: 483–506, 2008.

[85] M. Razavy. Time of arrival operator. *Canad. J. Phys.* 49: 3075–3081, 1971.

[86] M. Reed and B. Simon. *Methods of modern mathematical physics I, Functional analysis*. Academic Press Inc. [Harcourt Brace Jovanovich Publishers], New York, second edition, 1980.

[87] M. Reed and B. Simon. *Methods of modern mathematical physics II, Fourier analysis, Self-adjointness*. Academic Press Inc. [Harcourt Brace Jovanovich Publishers], New York, 1975.

[88] S. Richard. Spectral and scattering theory for Schrödinger operators with Cartesian anisotropy. *Publ. Res. Inst. Math. Sci.* 41(1): 73–111, 2005.

[89] S. Richard. New formulae for the Aharonov-Bohm wave operators. In *Spectral and Scattering Theory for Quantum Magnetic Systems*, 159–168, Contemporary Mathematics 500, AMS, Providence, Rhode Island, 2009.

[90] S. Richard and R. Tiedra de Aldecoa. New formulae for the wave operators for a rank one interaction. *Integral Equations and Operator Theory* 66: 283–292, 2010.

[91] S. Richard and R. Tiedra de Aldecoa. A new formula relating localisation operators to time operators. Submitted and preprint on ArXiv: `0908.2826`.

[92] S. Richard and R. Tiedra de Aldecoa. Time delay is a common feature of quantum scattering theory. Submitted and preprint on ArXiv: `1008.3433`.

[93] S. Richard and R. Tiedra de Aldecoa. A few results on Mourre theory in a two-Hilbert spaces setting. Submitted and preprint on ArXiv: `1104.1665`.

[94] S. Richard and R. Tiedra de Aldecoa. Spectral analysis and time-dependent scattering theory on manifolds with asymptotically cylindrical ends. In preparation.

[95] J. Riss. Eléments de calcul différentiel et théorie des distributions sur les groupes abéliens localement compacts. *Acta Math.* 89: 45–105, 1953.

[96] D. Robert. Relative time-delay for perturbations of elliptic operators and semiclassical asymptotics. *J. Funct. Anal.* 126(1): 36–82, 1994.

[97] D. Robert and X. P. Wang. Existence of time-delay operators for Stark Hamiltonians. *Comm. Partial Differential Equations* 14(1): 63–98, 1989.

[98] D. Robert and X. P. Wang. Time-delay and spectral density for Stark Hamiltonians. II. Asymptotics of trace formulae. *Chinese Ann. Math. Ser. B* 12(3): 358–383, 1991.

[99] M. Rørdam, F. Larsen and N. Laustsen. *An introduction to K-theory for C^*-algebras*, London Mathematical Society Student Texts 49, Cambridge University Press, Cambridge, 2000.

[100] S.N.M. Ruijsenaars. The Aharonov-Bohm effect and scattering theory. *Ann. Physics* 146(1): 1–34, 1983.

[101] J. Sahbani. The conjugate operator method for locally regular Hamiltonians. *J. Operator Theory* 38(2): 297–322, 1997.

[102] J. Sahbani. Spectral theory of certain unbounded Jacobi matrices. *J. Math. Anal. Appl.* 342: 663–681, 2008.

[103] M. Sassoli de Bianchi and P. A. Martin. On the definition of time delay in scattering theory. *Helv. Phys. Acta* 65(8): 1119–1126, 1992.

[104] K. Schmüdgen. On the Heisenberg commutation relation. I. *J. Funct. Anal.* 50(1): 8–49, 1983.

[105] F. T. Smith. Lifetime matrix in collision theory. *Phys. Rev.* 118: 349–356, 1960.

[106] H. Tamura. Magnetic scattering at low energy in two dimensions. *Nagoya Math. J.* 155: 95–151, 1999.

[107] H. Tamura. Norm resolvent convergence to magnetic Schrödinger operators with point interactions. *Rev. Math. Phys.* 13(4): 465–511, 2001.

[108] B. Thaller. *The Dirac Equation*. Springer-Verlag, Berlin, 1992.

[109] R. Tiedra de Aldecoa. Time delay and short-range scattering in quantum waveguides. *Ann. Henri Poincaré* 7(1): 105–124, 2006.

[110] R. Tiedra de Aldecoa. Anisotropic Lavine's formula and symmetrised time delay in scattering theory. *Math. Phys. Anal. Geom.* 11(2): 155–173, 2008.

[111] R. Tiedra de Aldecoa. Time delay for dispersive systems in quantum scattering theory. *Rev. Math. Phys.* 21(5): 675–708, 2009.

[112] X. P. Wang. Phase-space description of time-delay in scattering theory. *Comm. Partial Differential Equations* 13(2): 223–259, 1988.

[113] Z.-Y. Wang and C.-D. Xiong. How to introduce time operator. *Ann. Physics* 322(10): 2304–2314, 2007.

[114] G.N. Watson. *A treatise on the theory of Bessel functions*, second edition, Cambridge University Press, Cambridge, England, 1966.

[115] R. Weder. The Aharonov-Bohm effect and time-dependent inverse scattering theory. *Inverse Problems* 18: 1041–1056, 2002.

[116] J. Weidmann. *Linear operators in Hilbert spaces*. Springer-Verlag, New York, 1980.

[117] E. P. Wigner. Lower limit for the energy derivative of the scattering phase shift. *Phys. Rev. (2)* 98: 145–147, 1955.

[118] D. R. Yafaev. *Mathematical scattering theory*, volume 105 of *Translations of Mathematical Monographs*. American Mathematical Society, Providence, RI, 1992. General theory, Translated from the Russian by J. R. Schulenberger.