Contents

Introduction 5
0.1. Short summary 5
0.2. Introduction 6
1. Preliminaries 13
1.1. Notation 13
1.2. Functions holomorphic in $\mathbb{C}_+$ 13
1.3. Measure theory 13
1.3.1. Vitali's theorem 14
1.3.2. Poisson integral 14
1.3.3. Fatou's theorem 15
1.3.4. Privalov's theorem 15
1.3.5. The set $\Lambda(f)$ 16
1.3.6. De la Vallée Poussin decomposition theorem 16
1.3.7. Standard supports of measures 17
1.4. Bounded operators 18
1.5. Self-adjoint operators 19
1.6. Trace-class and Hilbert–Schmidt operators 20
1.6.1. Schatten ideals 20
1.6.2. Trace-class operators 22
1.6.3. Hilbert–Schmidt operators 23
1.6.4. Fredholm determinant 23
1.6.5. The Birman–Koplienko–Solomyak inequality 24
1.7. Direct integral of Hilbert spaces 24
1.8. Operator-valued holomorphic functions 26
1.8.1. Operator-valued meromorphic functions 28
1.8.2. Analytic Fredholm alternative 28
1.9. The limiting absorption principle 28
2. Framed Hilbert space 30
2.1. Definition 31
2.2. Spectral triple associated with an operator on a framed Hilbert space 33
2.3. Non-compact frames 33
2.4. The set $\Lambda(H_0; F)$ and the matrix $\phi(\lambda)$ 34
2.5. A core of the singular spectrum $\mathbb{R} \setminus \Lambda(H_0; F)$ 35
2.6. The Hilbert spaces $\mathcal{H}_\alpha(F)$ 36
2.6.1. Diamond conjugate 37
2.7. The trace-class matrix $\phi(\lambda + iy)$ 37
2.8. The Hilbert–Schmidt matrix $\eta(\lambda + iy)$ 38
2.9. Eigenvalues $\alpha_j(\lambda + iy)$ of $\eta(\lambda + iy)$ 38
2.10. Zero and non-zero type indices 38
2.11. Vectors $e_j(\lambda + iy)$ 38
2.12. Vectors $\eta_j(\lambda + iy)$ 39

2.13. Unitary matrix $e(\lambda+iy)$ 40
2.14. Vectors $\phi_j(\lambda+iy)$ 40
2.15. The operator $\mathcal{E}_{\lambda+iy}$ 41
2.16. Vectors $b_j(\lambda+iy) \in \mathcal{H}_1$ 43
3. The evaluation operator $\mathcal{E}_\lambda$ 44
3.1. Definition of $\mathcal{E}_\lambda$ 44
3.2. $\mathcal{E}$ is an isometry 48
3.3. $\mathcal{E}$ is unitary 49
3.4. Diagonality of H_0 in $\mathcal{H}$ 51
4. The resonance set $R(\lambda; \{H_r\}, F)$ 52
4.1. Resonance points of a path of operators 52
4.2. Essentially regular points 56
5. Wave matrix $w_\pm(\lambda; H_r, H_0)$ 57
5.1. Operators $\mathfrak{a}_\pm(\lambda; H_r, H_0)$ 58
5.2. Definition of the wave matrix $w_\pm(\lambda; H_r, H_0)$ 60
5.3. Multiplicative property of the wave matrix 61
5.4. The wave operator 65
6. Connection with the time-dependent definition of the wave operator 66
6.1. Time-dependent definition of the wave operator 66
7. The scattering matrix 70
7.1. Definition of the scattering matrix 70
7.2. Stationary formula for the scattering matrix 71
7.3. Infinitesimal scattering matrix 75
8. Absolutely continuous and singular spectral shift functions 77
8.1. Infinitesimal spectral flow 77
8.2. Absolutely continuous and singular spectral shift functions 82
8.3. Non-additivity of the singular spectral shift function 85
9. Pushnitski μ-invariant and singular spectral shift function 87
9.1. Spectral flow for unitary operators 87
9.2. Absolutely continuous part of the Pushnitski μ-invariant 89
9.3. Pushnitski μ-invariant 90
9.4. M-function 90
9.5. Smoothed spectral shift function 92
9.6. Pushnitski formula 93
9.7. Singular part of μ-invariant 94
Appendix. Chronological exponential 97
A.1. Definition and main properties 97
References 99

Abstract

Given a self-adjoint operator H_0, a self-adjoint trace-class operator V and a fixed Hilbert–Schmidt operator F with trivial kernel and cokernel, using the limiting absorption principle an explicit set $\Lambda(H_0; F) \subset \mathbb{R}$ of full Lebesgue measure is defined, such that for all $\lambda \in \Lambda(H_0 + rV; F) \cap \Lambda(H_0; F)$, where $r \in \mathbb{R}$, the wave $w_\pm(\lambda; H_0 + rV, H_0)$ and the scattering matrices $S(\lambda; H_0 + rV, H_0)$ can be defined unambiguously. Many well-known properties of the wave and scattering matrices and operators are proved, including the stationary formula for the scattering matrix. This version of abstract scattering theory allows us, in particular, to prove that

$$\det S(\lambda; H_0 + V, H_0) = e^{-2\pi i \xi^{(a)}(\lambda)}, \qquad \text{a.e. } \lambda \in \mathbb{R},$$

where $\xi^{(a)}(\lambda) = \xi^{(a)}_{H_0+V,H_0}(\lambda)$ is the so called absolutely continuous part of the spectral shift function defined by

$$\xi^{(a)}_{H_0+V,H_0}(\lambda) := \frac{d}{d\lambda} \int_0^1 \operatorname{Tr}(V E^{(a)}_{H_0+rV}(\lambda))\, dr$$

and where $E^{(a)}_H(\lambda) = E^{(a)}_{(-\infty,\lambda)}(H)$ denotes the absolutely continuous part of the spectral projection. Combined with the Birman–Kreĭn formula, this implies that the singular part of the spectral shift function,

$$\xi^{(s)}_{H_0+V,H_0}(\lambda) := \frac{d}{d\lambda} \int_0^1 \operatorname{Tr}(V E^{(s)}_{H_0+rV}(\lambda))\, dr,$$

is an almost everywhere integer-valued function, where $E^{(s)}_H(\lambda) = E^{(s)}_{(-\infty,\lambda)}(H)$ denotes the singular part of the spectral projection.

It is also shown that eigenvalues of the scattering matrix $S(\lambda; H_0 + V, H_0)$ can be connected to 1 in two natural ways, and that the singular spectral shift function measures the difference of the spectral flows of eigenvalues of the scattering matrix.

Acknowledgements. I would like to thank P. G. Dodds for useful discussions, and especially for the proof of Lemma 1.6.5. I also thank D. Zanin for indicating that Theorem 1.3.6 follows from [Sa, Theorem IV.9.6]. I would also like to thank K. A. Makarov and A. B. Pushnitski for useful discussions. Finally, I would like to thank the referee for his/her numerous helpful remarks.

2010 *Mathematics Subject Classification*: Primary 47A40; Secondary 47A70, 81U99.

Key words and phrases: spectral shift function, scattering matrix, absolutely continuous spectral shift function, singular spectral shift function, Birman–Kreĭn formula, Pushnitski μ-invariant, infinitesimal spectral flow, infinitesimal scattering matrix.

Received 28.4.2010; revised version 7.2.2011.

Introduction

0.1. Short summary. In this paper a new approach is given to abstract scattering theory. This approach is constructive and allows us to prove new results in perturbation theory of continuous spectra of self-adjoint operators which the conventional scattering theory is not able to achieve.

Among the results of this paper are: for trace-class perturbations of arbitrary self-adjoint operators:

- A new approach to the spectral theorem for self-adjoint operators (without singular continuous spectrum) via a special constructive representation of the absolutely continuous part (with respect to a fixed self-adjoint operator) of the Hilbert space as a direct integral of fiber Hilbert spaces.
- A new and constructive proof of existence of the wave matrices and of the wave operators.
- A new proof of the multiplicativity property of the wave matrices and of the wave operators.
- A new and constructive proof of the existence of the scattering matrix and of the scattering operator.
- A new proof of the stationary formula for the scattering matrix.
- A new proof of the Kato–Rosenblum theorem.

This paper does not contain only new proofs of existing theorems.

- A new formula (to the best knowledge of the author) for the scattering matrix in terms of chronological exponential.

The main result of this paper is the following

THEOREM. *Let H_0 be a self-adjoint operator and let V be a trace-class self-adjoint operator in a Hilbert space $\mathcal{H}$. Define a generalized function*

$$\xi^{(s)}(\phi) = \int_0^1 \operatorname{Tr}(V\phi(H_r^{(s)}))\,dr, \qquad \phi \in C_c^\infty(\mathbb{R}),$$

where $H_r := H_0 + rV$, and $H_r^{(s)}$ is the singular part of the self-adjoint operator H_r. Then $\xi^{(s)}$ is an absolutely continuous measure and its density $\xi^{(s)}(\lambda)$ (denoted by the same symbol) is a.e. integer-valued.

Note that in the case of operators with compact resolvent this theorem is well known, and the function $\xi^{(s)}(\lambda)$ in this case coincides with the spectral flow [APS, APS_2, Ge,

Ph_1, Ph_2, CP_1, CP_2, ACDS, ACS, Az_8]. Spectral flow is integer-valued just by definition as a total Fredholm index of a path of operators. In the case of operators with compact resolvent instead of $H_r^{(s)}$ one writes H_r, since in this case the continuous spectrum is absent, so that $H_r^{(s)} = H_r$.

The above theorem strongly suggests that the function $\xi^{(s)}(\lambda)$, which I call the singular part of the spectral shift function, calculates the spectral flow of the singular spectrum even in the presence and inside of the absolutely continuous spectrum.

Finally, it is worth stressing that the new approach to abstract scattering theory given in this paper has been invented with the sole purpose to prove the above theorem. Existing versions of scattering theory turned out to be insufficient for this purpose. At the same time, this approach seems to have a value of its own. In particular, I believe that, properly adjusted, this approach may allow one to unify the trace-class and smooth scattering theories, a long-standing problem mentioned in the introduction of D. Yafaev's book [Y].

0.2. Introduction. Let H_0 be a self-adjoint operator, V be a self-adjoint trace-class operator and let $H_1 = H_0 + V$. *The Lifshits–Kreĭn spectral shift function* [L, Kr] is the unique L_1-function $\xi(\cdot) = \xi_{H_1,H_0}(\cdot)$ such that for all $f \in C_c^\infty(\mathbb{R})$ the trace formula

$$\operatorname{Tr}(f(H_1) - f(H_0)) = \int f'(\lambda)\xi_{H_1,H_0}(\lambda)\,d\lambda$$

holds. The *Birman–Solomyak formula* for the spectral shift function [BS_2] asserts that

$$\xi_{H_1,H_0}(\lambda) = \frac{d}{d\lambda}\int_0^1 \operatorname{Tr}(VE_\lambda^{H_r})\,dr, \qquad \text{a.e. } \lambda, \tag{1}$$

where

$$H_r = H_0 + rV,$$

and $E_\lambda^{H_r}$ is the spectral resolution of H_r. This formula was established by V. A. Javrjan in [J] in the case of perturbations of the boundary condition of a Sturm-Liouville operator on $[0,\infty)$, which corresponds to rank-one perturbation of H_0. The Birman–Solomyak formula is also called the *spectral averaging formula.* A simple proof of this formula was found in [S_2]. There is enormous literature on the subject of spectral averaging, cf. e.g. [GM_2, GM_1, Ko] and references therein. A survey on the spectral shift function can be found in [BP].

Let $S(\lambda; H_1, H_0)$ be the scattering matrix of the pair $H_0, H_1 = H_0 + V$ (cf. [BE], see also [Y]). In [BK] M. Sh. Birman and M. G. Kreĭn established the formula

$$\det S(\lambda; H_1, H_0) = e^{-2\pi i\xi(\lambda)}, \qquad \text{a.e. } \lambda \in \mathbb{R}, \tag{2}$$

for trace-class perturbations $V = H_1 - H_0$ and arbitrary self-adjoint operators H_0. This formula is a generalization of a similar result of V. S. Buslaev and L. D. Fadeev [BF] for Sturm–Liouville operators on $[0,\infty)$.

In [Az_1] I introduced the absolutely continuous and singular spectral shift functions by the formulae

$$\xi^{(a)}_{H_1,H_0}(\lambda) = \frac{d}{d\lambda}\int_0^1 \operatorname{Tr}(VE_\lambda^{H_r}P^{(a)}(H_r))\,dr, \qquad \text{a.e. } \lambda, \tag{3}$$

$$\xi^{(s)}_{H_1,H_0}(\lambda) = \frac{d}{d\lambda}\int_0^1 \operatorname{Tr}(VE^{H_r}_\lambda P^{(s)}(H_r))\,dr, \qquad \text{a.e. } \lambda, \tag{4}$$

where $P^{(a)}(H_r)$ (respectively, $P^{(s)}(H_r)$) is the projection onto the absolutely continuous (respectively, singular) subspace of H_r. These formulae are obvious modifications of the Birman–Solomyak spectral averaging formula, and one can see that

$$\xi = \xi^{(s)} + \xi^{(a)}.$$

In [Az$_1$] it was observed that for n-dimensional Schrödinger operators $H_r = -\Delta + rV$ with quickly decreasing potentials V the scattering matrix $S(\lambda; H_r, H_0)$ is a continuous operator-valued function of r and it was shown that

$$-2\pi i\xi^{(a)}_{H_r,H_0}(\lambda) = \log\det S(\lambda; H_r, H_0), \tag{5}$$

where the logarithm is defined in such a way that the function

$$[0, r] \ni s \mapsto \log\det S(\lambda; H_s, H_0)$$

is continuous. It was natural to conjecture that some variant of this formula should hold in the general case. In particular, this formula, compared with the Birman–Kreĭn formula (2), has naturally led to a conjecture that the singular part of the spectral shift function is an a.e. integer-valued function. In the case of n-dimensional Schrödinger operators with quickly decreasing potentials this is an obvious result, since these operators do not have singular spectrum on the positive semi-axis. In [Az$_2$] it was observed that even in the case of operators which admit embedded eigenvalues the singular part of the spectral shift function is also either equal to zero on the positive semi-axis or in any case it is integer-valued.

In this paper I give a positive solution of this conjecture for trace-class perturbations of arbitrary self-adjoint operators.

The proof of (5) is based on the following formula for the scattering matrix:

$$S(\lambda; H_r, H_0) = \operatorname{Texp}\left(-2\pi i\int_0^r w_+(\lambda; H_0, H_s)\Pi_{H_s}(V)(\lambda)w_+(\lambda; H_s, H_0)\,ds\right), \tag{6}$$

where $\Pi_{H_s}(V)(\lambda)$ is the so-called infinitesimal scattering matrix (see (7.11)). If λ is fixed, then for this formula to make sense, the wave matrix $w_+(\lambda; H_s, H_0)$ has to be defined for all $s \in [0, r]$, except possibly a discrete set. In the case of Schrödinger operators

$$H = -\Delta + V$$

in $\mathbb{R}^n$ with short range potentials (in the sense of [Ag]), the wave matrices $w_\pm(\lambda; H_s, H_0)$ are well-defined, since there are explicit formulae for them (cf. e.g. [Ag, BY, Ku$_1$, Ku$_2$, Ku$_3$]). For example, if λ does not belong to the discrete set $e_+(H)$ of embedded eigenvalues of H, then the scattering matrix $S(\lambda)$ exists as an operator from $L_2(\Sigma)$ to $L_2(\Sigma)$, where $\Sigma = \{\omega \in \mathbb{R}^n : |\omega| = 1\}$ (cf. e.g. [Ag, Theorem 7.2]).

The situation is quite different in the case of the main setting of abstract scattering theory [BW, BE, RS$_3$, Y], which considers trace-class perturbations of arbitrary self-adjoint operators. A careful reading of proofs in [BE, Y] shows that one takes an arbitrary core of the spectrum of the initial operator H_0 and during the proofs one removes from the core several finite and even countable families of null sets. Furthermore, the nature of the initial core and of the null sets being removed is not clarified. They depend on arbitrarily chosen objects. This is in sharp contrast with potential scattering theory, where non-existence of the wave matrix or the scattering matrix at some point λ of the absolutely continuous spectrum means that λ is an embedded eigenvalue (cf. e.g. [Ag]).

So, in the case of trace-class perturbations of arbitrary self-adjoint operators, given a fixed λ (from some predefined full measure set Λ) the existence of the wave matrix for all $r \in [0,1]$, except possibly a discrete set, cannot be established by usual means. In order to make the argument of the proof of (6), given in [Az_1], work for trace-class (to begin with) perturbations of arbitrary self-adjoint operators, one at least needs to give an explicit set Λ of full measure, such that for all λ from Λ all the necessary ingredients of scattering theory, such as $w_\pm(\lambda; H_r, H_0)$, $S(\lambda; H_r, H_0)$ and $Z(\lambda; G)$, exist. One of the difficulties here is that the spectrum of an arbitrary self-adjoint operator, unlike the spectrum of Schrödinger operators, can be very bad: it can, say, have everywhere dense pure point spectrum, or a singular continuous spectrum, or even both.

To the best knowledge of the author, abstract scattering theory in its present form (cf. [BW, BE, RS_3, Y]) does not allow one to resolve this problem. In the present paper a new abstract scattering theory is developed.

In this theory, given a self-adjoint operator H_0 on a Hilbert space $\mathcal{H}$ with the so-called frame F and a trace-class perturbation V, an explicit set $\Lambda(H_0; F)$ of full measure is defined in a canonical (constructive) way via the data (H_0, F), such that for all $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_r; F)$ the wave matrices $w_\pm(\lambda; H_r, H_0)$ exist, and moreover, explicitly constructed.

Definition 0.2.1. A *frame* F in a Hilbert space $\mathcal{H}$ is a sequence

$$((\phi_1, \kappa_1), (\phi_2, \kappa_2), \ldots),$$

where $(\kappa_j)_{j=1}^\infty$ is an ℓ_2-sequence of positive numbers, and $(\phi_j)_{j=1}^\infty$ is an orthonormal basis of $\mathcal{H}$.

In other words, a frame is a fixed orthonormal basis such that the norms of the basis vectors form an ℓ_2-sequence. It is convenient to encode the information about a frame in a Hilbert–Schmidt operator with trivial kernel and cokernel

$$F\colon \mathcal{H} \to \mathcal{K}, \qquad F = \sum_{j=1}^\infty \kappa_j \langle \phi_j, \cdot \rangle \psi_j,$$

where $\mathcal{K}$ is another Hilbert space and $(\psi_j)_{j=1}^\infty$ is an orthonormal basis in $\mathcal{K}$. The nature of the Hilbert space $\mathcal{K}$ and of the basis $(\psi_j)_{j=1}^\infty$ is immaterial, so that one can actually take $\mathcal{K} = \mathcal{H}$ and $(\psi_j)_{j=1}^\infty = (\phi_j)_{j=1}^\infty$.

Once a frame (operator) F is fixed in $\mathcal{H}$, given a self-adjoint operator H_0 on $\mathcal{H}$, the frame enables to construct explicitly:

1. an explicit set $\Lambda(H_0; F)$ of full measure, which depends only on H_0 and F;
2. for every $\lambda \in \Lambda(H_0; F)$, an explicit (to be fiber) Hilbert space $\mathfrak{h}_\lambda \subset \ell_2$;
3. a measurability base $\{\phi_j(\cdot)\}$, $j = 1, 2, \ldots$, where all functions $\phi_j(\lambda) \in \mathfrak{h}_\lambda$, $j = 1, 2, \ldots$, are explicitly defined for *all* $\lambda \in \Lambda(H_0; F)$;

4. (as a consequence) a direct integral of Hilbert spaces
$$\mathcal{H} := \int^{\oplus}_{\Lambda(H_0;F)} \mathfrak{h}_\lambda \, d\lambda,$$
where the case of $\dim \mathfrak{h}_\lambda = 0$ is *not excluded.*
5. Further, considered as a rigging, a frame F generates a triple of Hilbert spaces $\mathcal{H}_1 \subset \mathcal{H} = \mathcal{H}_0 \subset \mathcal{H}_{-1}$ with scalar products
$$\langle f, g\rangle_{\mathcal{H}_\alpha} = \langle |F|^{-\alpha} f, |F|^{-\alpha} g\rangle, \qquad \alpha = -1, 0, 1,$$
and natural isomorphisms
$$\mathcal{H}_{-1} \xrightarrow{|F|} \mathcal{H} \xrightarrow{|F|} \mathcal{H}_1.$$
6. For any $\lambda \in \Lambda(H_0; F)$ we have an *evaluation* operator
$$\mathcal{E}_\lambda = \mathcal{E}_{\lambda+i0} \colon \mathcal{H}_1 \to \mathfrak{h}_\lambda; \qquad \mathcal{E} \colon \mathcal{H}_1 \to \mathcal{H}.$$
The operator $\mathcal{E}_\lambda \colon \mathcal{H}_1 \to \mathfrak{h}_\lambda$ is a Hilbert–Schmidt operator, and the operator $\mathcal{E}$, considered as an operator $\mathcal{H} \to \mathcal{H}$, extends continuously to a *unitary isomorphism* of the absolutely continuous part (with respect to H_0) of $\mathcal{H}$ to $\mathcal{H}$, and, moreover, the operator $\mathcal{E}$ *diagonalizes* the absolutely continuous part of H_0.

Here is a quick description of this construction.

Definition 0.2.2. A point $\lambda \in \mathbb{R}$ belongs to $\Lambda(H_0; F)$ if and only if

(i) the operator $F R_{\lambda+iy}(H_0) F^*$ has a limit in the uniform (norm) topology as $y \to 0^+$, and
(ii) the operator $F \operatorname{Im} R_{\lambda+iy}(H_0) F^*$ has a limit in the trace-class norm as $y \to 0^+$.

It follows from the limiting absorption principle (cf. [B, BE] and [Y, Theorems 6.1.5, 6.1.9]) that $\Lambda(H_0; F)$ has full Lebesgue measure, and that for all $\lambda \in \Lambda(H_0; F)$ the matrix
$$\phi(\lambda) := (\phi_{ij}(\lambda)) = \frac{1}{\pi} (\kappa_i \kappa_j \langle \phi_i, \operatorname{Im} R_{\lambda+i0}(H_0) \phi_j\rangle)$$
exists and is a non-negative trace-class operator on ℓ_2 (Proposition 2.4.3). The value $\phi_j(\lambda)$ of the vector ϕ_j at $\lambda \in \Lambda(H_0; F)$ is defined as the jth column $\eta_j(\lambda)$ of the Hilbert–Schmidt operator $\sqrt{\phi(\lambda)}$ over the weight κ_j of ϕ_j:
$$\phi_j(\lambda) = \kappa_j^{-1} \eta_j(\lambda).$$
It is not difficult to see that if $f \in \mathcal{H}_1(F)$, so that
$$f = \sum_{j=1}^\infty \kappa_j \beta_j \phi_j,$$
where $(\beta_j) \in \ell_2$, then the series
$$f(\lambda) := \sum_{j=1}^\infty \kappa_j \beta_j \phi_j(\lambda) = \sum_{j=1}^\infty \beta_j \eta_j(\lambda)$$
absolutely converges in ℓ_2. The fiber Hilbert space $\mathfrak{h}_\lambda$ is by definition the closure of the image of $\mathcal{H}_1$ under the map
$$\mathcal{E}_\lambda \colon \mathcal{H}_1 \ni f \mapsto f(\lambda) \in \ell_2.$$

The image of the set of frame vectors ϕ_j under the map $\mathcal{E}$ forms a measurability base of a direct integral of Hilbert spaces

$$\mathfrak{H} := \int_{\Lambda(H_0;F)}^{\oplus} \mathfrak{h}_\lambda \, d\lambda,$$

and the operator

$$\mathcal{E} \colon \mathcal{H}_1 \to \mathfrak{H}$$

is bounded as an operator from $\mathcal{H}$ to $\mathfrak{H}$, vanishes on the singular subspace $\mathcal{H}^{(s)}(H_0)$ of H_0, is isometric on the absolutely continuous subspace $\mathcal{H}^{(a)}(H_0)$ of H_0 with the range $\mathfrak{H}$ (Propositions 3.2.1, 3.3.5) and is diagonalizing for H_0 (Theorem 3.4.2), that is,

$$\mathcal{E}_\lambda(H_0 f) = \lambda \mathcal{E}_\lambda f \quad \text{for all } \lambda \in \Lambda(H_0; F).$$

***

So far, we have had one self-adjoint operator H_0 acting in $\mathcal{H}$. Let V be a self-adjoint trace-class operator. Let a frame F be such that $V = F^* J F$, where $J \colon \mathcal{K} \to \mathcal{K}$ is a self-adjoint bounded operator. Clearly, for any trace-class operator such a frame exists. This means that the operator V can be considered as a bounded operator

$$V \colon \mathcal{H}_{-1} \to \mathcal{H}_1.$$

By definition, if $\lambda \in \Lambda(H_0; F)$, then the limit

$$R_{\lambda+i0}(H_0) \colon \mathcal{H}_1 \to \mathcal{H}_{-1}$$

exists in the uniform norm and the limit

$$\operatorname{Im} R_{\lambda+i0}(H_0) \colon \mathcal{H}_1 \to \mathcal{H}_{-1}$$

exists in the trace-class norm. So, if $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_1; F)$, then the following operator is a well-defined trace-class operator (from $\mathcal{H}_1$ to $\mathcal{H}_{-1}$):

$$\mathfrak{a}_\pm(\lambda; H_1, H_0) := [1 - R_{\lambda \mp i0}(H_1) V] \cdot \frac{1}{\pi} \operatorname{Im} R_{\lambda+i0}(H_0).$$

Let $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_1; F)$, where $H_1 = H_0 + V$, so that both fiber Hilbert spaces $\mathfrak{h}_\lambda^{(0)}$ and $\mathfrak{h}_\lambda^{(1)}$ are well-defined. Then there exists a unique (for each sign $\pm$) operator

$$w_\pm(\lambda; H_1, H_0) \colon \mathfrak{h}_\lambda^{(0)} \to \mathfrak{h}_\lambda^{(1)}$$

such that for any $f, g \in \mathcal{H}_1$ the equality

$$\langle \mathcal{E}_\lambda(H_1) f, w_\pm(\lambda; H_1, H_0) \mathcal{E}_\lambda(H_0) g \rangle = \langle f, \mathfrak{a}_\pm(\lambda; H_1, H_0) g \rangle_{1,-1}$$

holds, where $\langle \cdot, \cdot \rangle_{1,-1}$ is the pairing of the rigged Hilbert space $(\mathcal{H}_1, \mathcal{H}, \mathcal{H}_{-1})$. The operator

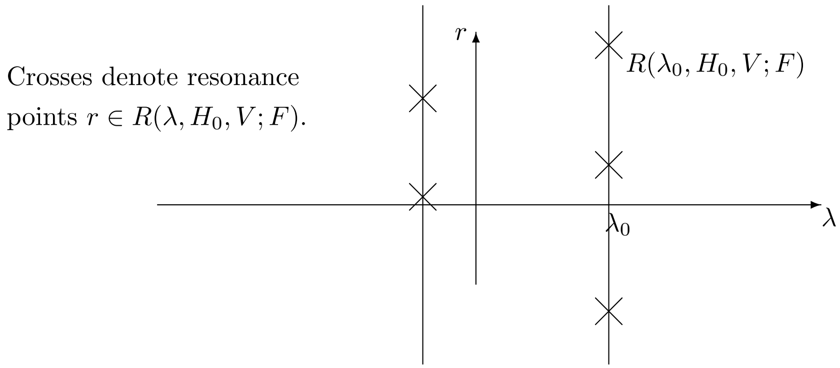
$$w_\pm(\lambda; H_1, H_0)$$

is correctly defined, and, moreover, it is unitary and has the multiplicative property. The operator $w_\pm(\lambda; H_1, H_0)$ is actually the wave matrix, which is thus explicitly constructed for *all* λ from the set $\Lambda(H_0; F) \cap \Lambda(H_1; F)$ of full Lebesgue measure.

So far we have considered a pair of operators H_0 and H_1. But if the aim is to prove the formula (6), then one needs to make sure that the wave matrix $w_\pm(\lambda; H_r, H_0)$ exists for all values of $r \in [0, 1]$, with a possible exception of some small set. It turns out that, indeed, the wave matrix $w_\pm(\lambda; H_r, H_0)$ is defined for all r except a discrete set, as follows from the following simple but important property of $\Lambda(H_0; F)$ (Theorem 4.1.9):

$$\text{if } \lambda \in \Lambda(H_0; F), \quad \text{then } \lambda \in \Lambda(H_r; F) \quad \text{for all } r \notin R(\lambda, H_0, V; F),$$

where $R(\lambda, H_0, V; F)$ is a discrete set of special importance called the resonance set (see the picture below).



If λ is an eigenvalue of $H_r = H_0 + rV$, then $r \in R(\lambda, H_0, V; F)$ for any F. But $R(\lambda, H_0, V; F)$ may contain other points as well, which may depend on F. This partly justifies the terminology "resonance points" and gives a basis for classification of resonance points into two different types.

So, the set $\{(\lambda, r) : \lambda \in \Lambda(H_r; F)\}$ behaves very regularly with respect to r, but it does not do so with respect to λ: while for fixed $r_0 \in \mathbb{R}$ and $\lambda_0 \in \mathbb{R}$ the set $\{\lambda \in \mathbb{R} : \lambda \notin \Lambda(H_{r_0}; F)\}$ can be a more or less arbitrary null set, the set $\{r \in \mathbb{R} : \lambda_0 \notin \Lambda(H_r; F)\}$ is a discrete set, i.e. a set with no finite accumulation points.

Further, the multiplicative property of the wave matrix

$$w_\pm(\lambda; H_{r_2}, H_{r_0}) = w_\pm(\lambda; H_{r_2}, H_{r_1}) w_\pm(\lambda; H_{r_1}, H_{r_0})$$

is proved (Theorem 5.3.7), where r_2, r_1, r_0 do not belong to the above mentioned discrete resonance set $R(\lambda, H_0, V; F)$. As is known (cf. [Y, Subsection 2.7.3]), the proof of this property for the wave operator $W_\pm(H_1, H_0)$ is the main difficulty of the stationary approach to the abstract scattering theory. A bulk of this paper is devoted to the definition of $w_\pm(\lambda; H_r, H_0)$ for all $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$ and to the proof of the multiplicative property. This is the main feature of the new scattering theory given in this paper. Further, for all $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$ the scattering matrix $S(\lambda; H_r, H_0)$ is *defined* as an operator from $\mathfrak{h}_\lambda^{(0)}$ to $\mathfrak{h}_\lambda^{(0)}$ by the formula

$$S(\lambda; H_r, H_0) = w_+^*(\lambda; H_r, H_0) w_-(\lambda; H_r, H_0).$$

The scattering operator $\mathbf{S}(H_r, H_0) \colon \mathcal{H}^{(a)}(H_0) \to \mathcal{H}^{(a)}(H_0)$ is defined as the direct integral of scattering matrices:

$$\mathbf{S}(H_r, H_0) := \int_{\Lambda(H_0;F)\cap\Lambda(H_r;F)} S(\lambda; H_r, H_0)\, d\lambda.$$

For all $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$ the stationary formula for the scattering matrix

$$S(\lambda; H_r, H_0) = 1_\lambda - 2\pi i \mathcal{E}_\lambda r V (1 + rR_{\lambda+i0}(H_0)V)^{-1} \mathcal{E}_\lambda^\diamondsuit$$

is proved (Theorem 7.2.2). Though the scattering matrix $S(\lambda; H_r, H_0)$ does not exist for resonance points $r \in R(\lambda, H_0, V; F)$, a simple but important property of the scattering matrix is that it admits analytic continuation to the resonance points (Proposition 7.2.5). The stationary formula enables us to show that for all $\lambda \in \Lambda(H_0; F)$ and all r not in the resonance set $R(\lambda, H_0, V; F)$, the formula (6) holds (Theorem 7.3.4), where for all non-resonance points r the infinitesimal scattering matrix is defined as

$$\Pi_{H_r}(V)(\lambda) = \mathcal{E}_\lambda(H_r) V \mathcal{E}_\lambda^\diamondsuit(H_r) \colon \mathfrak{h}_\lambda^{(r)} \to \mathfrak{h}_\lambda^{(r)}$$

and where $\mathcal{E}_\lambda^\diamondsuit = |F|^{-2}\mathcal{E}_\lambda^*$.

The main object of the abstract scattering theory given in [BE, Y], the wave operator $W_\pm(H_r, H_0)$, is defined as the direct integral of the wave matrices

$$W_\pm(H_r, H_0) = \int^\oplus_{\Lambda(H_r;F)\cap\Lambda(H_0;F)} w_\pm(\lambda; H_r, H_0)\, d\lambda.$$

The usual definition

$$W_\pm(H_r, H_0) = \text{s-}\lim_{t\to\pm\infty} e^{itH_r} e^{-itH_0} P_0^{(a)}$$

of the wave operator becomes a theorem (Theorem 6.1.4). The formula

$$\mathbf{S}(H_r, H_0) = W_+^*(H_r, H_0) W_-(H_r, H_0),$$

which is usually considered as definition of the scattering operator, obviously holds.

This new scattering theory has allowed us to prove (5) for all $\lambda \in \Lambda(H_0; F)$ (Theorem 8.2.4). Combined with the Birman–Kreĭn formula (2), this implies that the singular part of the spectral shift function is an a.e. integer-valued function for arbitrary trace-class perturbations of arbitrary self-adjoint operators (Theorem 8.2.6):

$$\xi^{(s)}_{H_1,H_0}(\lambda) \in \mathbb{Z} \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Theorem 8.2.6 is the main result of this paper. This result is to be considered as unexpected, since the definition (4) of the singular part of the spectral shift function does not suggest anything like this.

In Section 9 another proof of Theorem 8.2.6 is given which does not use the Birman–Kreĭn formula (2), so that the formula itself becomes a corollary of Theorem 8.2.6 and (5). This proof uses the so-called μ-invariant introduced by Alexander Pushnitski [Pu]. Pushnitski's μ-invariant measures spectral flow of scattering phases (eigenvalues of the scattering matrix) through a given point $e^{i\theta}$ on the unit circle $\mathbb{T}$. In Section 9 it is shown that there is another natural way to measure the spectral flow of scattering phases. It is shown that the difference of these two μ-invariants does not depend on the angle variable θ and is equal (up to a sign) to the singular part of the spectral shift function.

I would like to stress that even though the scattering theory presented in this paper is different in its nature from the conventional scattering theory given in [BE, Y], many essential ideas are taken from [BE, Y] (cf. also [BW, RS_3]), and essentially no new results appear until Subsection 7.3, though most of the proofs are original (to the best of the author's knowledge). At the same time, this new approach to abstract scattering theory is simpler than that given in [Y], and it is this new approach that allows one to prove the main results of this paper.

1. Preliminaries

In these preliminaries I follow mainly [GK, RS_1, S_1, Y]. Details and (omitted) proofs can be found in these references. A partial purpose of these preliminaries is to fix notation and terminology.

1.1. Notation. $\mathbb{R}$ is the set of real numbers. $\mathbb{C}$ is the set of complex numbers. $\mathbb{C}_+$ is the open upper half-plane of the complex plane $\mathbb{C}$.

1.2. Functions holomorphic in $\mathbb{C}_+$. Proof of the following theorem can be found in [Pr] (see also [Y, §1.2]).

Theorem 1.2.1.

(a) *If $f\colon \mathbb{C}_+ \to \mathbb{C}$ is a bounded holomorphic function, then for a.e. $\lambda \in \mathbb{R}$ the angular limit $f(\lambda + i0)$ exists.*
(b) *If the function $f(\lambda + i0)$ is equal to zero on a set of positive Lebesgue measure then $f = 0$.*

This theorem has a much stronger version, but the above is all we need.

1.3. Measure theory. Here we collect some definitions from measure theory. Details can be found in D. Yafaev's book [Y].

The σ-algebra $B(\mathbb{R})$ of Borel sets is generated by open subsets of $\mathbb{R}$. By a measure on $\mathbb{R}$ we mean a locally-finite non-negative countably additive function m defined on the σ-algebra of Borel sets. Locally-finite means that the measure of any compact set is finite. By a *Borel support* of a measure m we mean any Borel set X whose complement has zero m-measure: $m(\mathbb{R} \setminus X) = 0$. By the *closed support* of a measure m we mean the smallest closed Borel support of m. The closed support exists and is unique.

By $|X|$ we denote the Lebesgue measure of a Borel set X. A Borel set Z is called a *null set* if it has zero Lebesgue measure: $|Z| = 0$. A Borel set Λ is called a *full set* if the complement of X is a null set: $|\mathbb{R} \setminus \Lambda| = 0$. Full sets will usually be denoted by Λ, with indices and arguments, if necessary.

A Borel support X of a measure m is called *minimal* if $|X \setminus X'| = 0$ for any other Borel support X'. Note that the closed support of a measure is not necessarily minimal. A minimal Borel support exists, but it is not unique. Two minimal supports can differ by not more than a null set.

A measure m is called *absolutely continuous* if $m(Z) = 0$ for any null set Z. The Radon–Nikodym theorem asserts that a measure m is absolutely continuous if and only if there exists a locally summable non-negative function f such that for any Borel set X,

$$m(X) = \int_X f(\lambda)\, d\lambda.$$

A measure m is called *singular* if there exists a null Borel support of m, that is, a Borel support of zero Lebesgue measure. Any measure m admits a unique decomposition

$$m = m^{(a)} + m^{(s)}$$

into the sum of an absolutely continuous measure $m^{(a)}$ and a singular measure $m^{(s)}$.

Two measures m_1 and m_2 *have the same spectral type* if they are absolutely continuous with respect to each other, that is, if $m_1(X) = 0$ for some Borel set X, then $m_2(X) = 0$, and vice versa.

The abbreviation a.e. will always refer to the Lebesgue measure.

Two measures are *mutually singular* if they have non-intersecting Borel supports.

A *signed measure* is a locally finite countably additive function m defined on bounded Borel sets. Every signed measure m admits a unique *Hahn decomposition*

$$m = m_+ - m_-,$$

where the non-negative measures m_- and m_+ are mutually singular. The measure $|m| := m_+ + m_-$ is called the *total variation* of m.

1.3.1. Vitali's theorem. Apart from Lebesgue's dominated convergence theorem, we shall need Vitali's theorem (for a proof see [Nat]):

THEOREM 1.3.1. *Let X be a Borel subset of $\mathbb{R}$. Suppose for functions $f_y \in L_1(\mathbb{R})$, $y > 0$, the integrals*

$$\int_X f_y(\lambda)\, d\lambda$$

tend to zero uniformly with respect to y as $|X| \to 0$. Suppose also the same for $X = (-\infty, -N) \cup (N, \infty)$ as $N \to \infty$. If for a.e. $\lambda \in \mathbb{R}$,

$$\lim_{y \to 0} f_y(\lambda) = f(\lambda),$$

then the function f is summable and

$$\lim_{y \to 0} \int_{-\infty}^{\infty} f_y(\lambda)\, d\lambda = \int_{-\infty}^{\infty} f(\lambda)\, d\lambda.$$

1.3.2. Poisson integral. Let F be a function of bounded variation on $\mathbb{R}$. The *Poisson integral* $\mathcal{P}_F$ of F is the following function of two variables:

$$\mathcal{P}_F(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{dF(t)}{(x - t)^2 + y^2}.$$

The function

$$P_y(x) = \frac{1}{\pi} \frac{y}{x^2 + y^2} \tag{1.1}$$

is the kernel of the Poisson integral and

$$\mathcal{P}_F(x, y) = P_y * dF(x).$$

The family $\{P_y(x) : y > 0\}$ is an approximate unit for the delta function, that is, all these functions are non-negative, an integral of each of the functions P_y is equal to 1 and P_y converges in the sense of distributions to Dirac's delta function δ.

When F is the distribution function of a summable function $f \in L_1(\mathbb{R})$, allowing an abuse of terminology, we also say that $P_y * f(x)$ is the Poisson integral of f.

Lemma 1.3.2. *Let $g \in L_1(\mathbb{R})$ and let g_y be the Poisson integral of g. If X is a Borel set, then the integral*

$$\int_X |g_y(\lambda)|\, d\lambda$$

converges to zero as $|X| \to 0$ and as $N \to \infty$ in $X = (-\infty, -N) \cup (N, \infty)$ uniformly with respect to $y \in (0,1)$.

1.3.3. Fatou's theorem. The following Fatou's theorem plays an important role in this paper. For a discussion of this theorem see [Y].

Theorem 1.3.3. *Let F be a function of bounded variation on $\mathbb{R}$. If at some point $x_0 \in \mathbb{R}$ the function F has the symmetric derivative*

$$F'_{\mathrm{sym}}(x_0) := \lim_{h \to 0^+} \frac{F(x_0 + h) - F(x_0 - h)}{2h},$$

then the limit of the Poisson integral of F,

$$\lim_{y \to 0^+} \mathcal{P}_F(x_0, y),$$

exists and is equal to $F'_{\mathrm{sym}}(x_0)$. In particular, the limit exists for a.e. x_0.

1.3.4. Privalov's theorem. Let $F\colon \mathbb{R} \to \mathbb{C}$ be a function of bounded variation. The Cauchy–Stieltjes transform of F is a function holomorphic in both the upper and the lower complex half-planes $\mathbb{C}_\pm$; this function is defined by the formula

$$\mathcal{C}_F(z) = \int_{-\infty}^{\infty} (x - z)^{-1}\, dF(x).$$

The following theorem is known as *Privalov's theorem* (cf. [Pr], [Y, Theorem 1.2.5]). This theorem can be formulated for an upper half-plane or, equivalently, for a unit disk. Its proof can also be found in [AhG, Chapter VI, §59, Theorem 1].

Theorem 1.3.4. *Let $F\colon \mathbb{R} \to \mathbb{C}$ be a function of bounded variation. The limit values*

$$\mathcal{C}_F(\lambda \pm i0) := \lim_{y \to 0^+} \mathcal{C}_F(\lambda \pm iy)$$

of the Cauchy–Stieltjes transform $\mathcal{C}_F(z)$ of F exist for a.e. $\lambda \in \mathbb{R}$, and for a.e. $\lambda \in \mathbb{R}$ the equality

$$\mathcal{C}_F(\lambda \pm i0) = \pm \pi i \frac{dF(\lambda)}{d\lambda} + \text{p.v.} \int_{-\infty}^{\infty} (\mu - \lambda)^{-1}\, dF(\mu) \tag{1.2}$$

holds, where the principal value integral on the right hand side also exists for a.e. $\lambda \in \mathbb{R}$.

Since the imaginary part of the Cauchy–Stieltjes transform of F is the Poisson integral of F:

$$\frac{1}{\pi} \operatorname{Im} \mathcal{C}_F(\lambda + iy) = \mathcal{P}_F(\lambda, y), \tag{1.3}$$

the convergence of $\frac{1}{\pi} \operatorname{Im} \mathcal{C}_F(\lambda \pm iy)$ to $\pm F'(\lambda)$ for a.e. λ follows from Fatou's theorem 1.3.3.

1.3.5. The set $\Lambda(f)$. It is customary to consider a summable function $f \in L_1(\mathbb{R})$ as a class of equivalent functions, where two functions are considered to be equivalent if they coincide everywhere except on a null set. So, a summable function is defined up to a set of Lebesgue measure zero. In this way, in general one cannot ask what is the value of a summable function f at, say, $\sqrt{2}$. In this paper we take a different approach. By a summable function we mean a complex-valued summable function f which is *explicitly* defined on some explicit set of full Lebesgue measure.

Given a summable function $f \in L_1(\mathbb{R})$ there are two (among many other) natural ways to assign to the function a canonical set Λ of full Lebesgue measure, so that f is in some natural way defined at *every* point of Λ (see the first paragraph of [AD, p. 384]).

The first way is this. If $f \in L_1(\mathbb{R})$, then one can define a set $\Lambda'(f)$ of full Lebesgue measure as the set of all those numbers x at which the function

$$\int_0^x f(t)\,dt$$

is differentiable. Lebesgue's differentiation theorem says this set has full measure. If $x \in \Lambda'(f)$, then one can define $f(x)$ by the formula

$$f(\lambda) := \frac{d}{d\lambda}\int_0^\lambda f(x)\,dx.$$

However, there is another canonical set of full Lebesgue measure, associated with f:

$$\Lambda(f) := \Big\{\lambda \in \mathbb{R} : \lim_{y\to 0^+} \operatorname{Im} \mathcal{C}_F(\lambda + iy) \text{ exists}\Big\},$$

where $F(\lambda) = \int_0^\lambda f(x)\,dx$ and $\mathcal{C}_F(z)$ is the Cauchy–Stieltjes transform of F. That $\Lambda(f)$ is a full set follows from Theorem 1.3.3. For any $\lambda \in \Lambda(f)$ one can define

$$f(\lambda) := \frac{1}{\pi}\operatorname{Im}\mathcal{C}_F(\lambda + i0) := \frac{1}{\pi}\lim_{y\to 0^+}\operatorname{Im}\mathcal{C}_F(\lambda+iy) = \lim_{y\to 0^+} f * P_y(\lambda). \tag{1.4}$$

Since $\frac{1}{\pi}\operatorname{Im}\mathcal{C}_F(\lambda+iy)$ is the Poisson integral of F (see (1.3)), it follows from Theorem 1.3.3 that the two explicit summable functions defined in this way are equivalent.

It is clear that two elements f and g of $L_1(\mathbb{R})$ (as equivalence classes) coincide if and only if $\Lambda(f) = \Lambda(g)$ and $f(\lambda) = g(\lambda)$ for all $\lambda \in \Lambda(f)$.

So, from now on, all summable functions f are understood in this sense (if not stated otherwise): f is a function on the full set $\Lambda(f)$ defined by (1.4). Probably, it is worth stressing again that in this definition by a function we mean a "genuine" function.

1.3.6. De la Vallée Poussin decomposition theorem. This is the following theorem (see e.g. [Sa, Theorem IV.9.6], [Ru]):

THEOREM 1.3.5. *Let m be a finite signed measure. Let $|m|$ be the total variation of m. Let $E_{-\infty}$ (respectively, $E_{+\infty}$) be the set where the derivative of the distribution function F_m of m is $-\infty$ (respectively, $+\infty$). If X is a Borel subset of $\mathbb{R}$, then*

$$m(X) = m(X\cap E_{-\infty}) + m(X \cap E_{+\infty}) + \int_X F_m'(t)\,dt$$

and

$$|m|(X) = |m(X\cap E_{-\infty})| + m(X \cap E_{+\infty}) + \int_X |F_m'(t)|\,dt.$$

REMARK. The formulation of [Sa, Theorem IV.9.6] contains an additional condition that F_m is continuous at every point of X. This condition is obviously redundant.

1.3.7. Standard supports of measures. If m is a finite signed measure, then its Cauchy–Stieltjes transform $\mathcal{C}_m(z)$ is defined as the Cauchy–Stieltjes transform of its distribution function

$$F_m(x) = m((-\infty, x)).$$

That is,

$$\mathcal{C}_m(z) := \int_{-\infty}^{\infty} \frac{m(dx)}{x-z}.$$

A finite signed measure has a natural decomposition

$$m = m^{(a)} + m^{(s)}$$

into the sum of an absolutely continuous measure $m^{(a)}$ and a singular measure $m^{(s)}$. The signed measures $m^{(a)}$ and $m^{(s)}$ are mutually singular. It is desirable to split the set of real numbers $\mathbb{R}$ in some natural way, so that the first set is a Borel support of the absolutely continuous part $m^{(a)}$, while the second set is a Borel support of the singular part $m^{(s)}$ of the measure m.

It is possible to do so in several ways. The choice which best suits our needs is the following. To every finite signed measure m we assign the set

$$\Lambda(m) := \{\lambda \in \mathbb{R} : \text{a finite limit } \operatorname{Im} \mathcal{C}_m(\lambda + i0) \in \mathbb{R} \text{ exists}\}.$$

This set was introduced by Aronszajn in [Ar].

The following theorem is due Aronszajn [Ar].

THEOREM 1.3.6. *Let m be a finite signed measure. The set $\Lambda(m)$ is a full set. The complement of $\Lambda(m)$ is a minimal Borel support of the singular part of m.*

The main point of this theorem is that it gives a natural splitting of the set of real numbers $\mathbb{R}$ into two parts such that the first part supports $m^{(a)}$ and the second part supports $m^{(s)}$. Actually, the support of the singular part $\mathbb{R} \setminus \Lambda(m)$ can be made smaller. Namely, the set of all points $\lambda \in \mathbb{R}$ for which $\operatorname{Im} \mathcal{C}_m(\lambda + i0)$ equals $+\infty$ or $-\infty$ is a Borel support of the singular part of m.

The function $\operatorname{Im} \mathcal{C}_m(\lambda + iy)$ cannot grow to infinity faster than C/y. If it grows as C/y, then the point λ has a non-zero measure equal to C. The set of points where $\operatorname{Im} \mathcal{C}_m(\lambda + iy)$ grows as C/y is a Borel support of the discrete part of m. The set of points where $\operatorname{Im} \mathcal{C}_m(\lambda + iy)$ grows to infinity slower than C/y is a Borel support of the singular continuous part of m. These Borel supports were also introduced in [Ar]. Though these supports of the singular part(s) of m are more natural and finer than $\mathbb{R} \setminus \Lambda(m)$, for the purposes of this paper the last support suffices.

Also, imposing different growth conditions on $\operatorname{Im} \mathcal{C}_m(\lambda + iy)$, such as $\operatorname{Im} \mathcal{C}_m(\lambda + iy) \sim C/y^\rho$, where $\rho \in (0, 1)$, one can get a further finer classification of the singular continuous spectrum; see [Ro] for details.

The set $\Lambda(m)$ is not a minimal Borel support of $m^{(a)}$, but it is not difficult to indicate a natural minimal Borel support of $m^{(a)}$ (see [Ar]):

$$\mathcal{A}(m) = \{\lambda \in \Lambda(m) : \operatorname{Im} \mathcal{C}_m(\lambda + i0) \neq 0\}. \tag{1.5}$$

This follows from the fact that for a.e. $\lambda \in \Lambda(m)$,

$$F'_m(\lambda) = \frac{1}{\pi} \operatorname{Im} \mathcal{C}_m(\lambda + i0),$$

and from the fact that the function $\lambda \mapsto F'_m(\lambda)$ is a density of the absolutely continuous part of m. The number $F'_m(\lambda)$ will be considered as a standard value of the density function at points of $\Lambda(m)$.

Corollary 1.3.7. *Let F be a function of bounded variation on $\mathbb{R}$ and let m be the corresponding (signed) measure. For any Borel subset Δ of $\Lambda(m)$,*

$$\int_\Delta dF(\lambda) = \int_\Delta F'(\lambda)\, d\lambda = \frac{1}{\pi} \int_\Delta \operatorname{Im} \mathcal{C}_F(\lambda + i0)\, d\lambda = \frac{1}{\pi} \int_\Delta \operatorname{Im} \mathcal{C}_{F^{(a)}}(\lambda + i0)\, d\lambda.$$

There is another canonical full set associated with a function of bounded variation, namely, the Lebesgue set of all points where F is differentiable. But the set $\Lambda(F)$ is easier to deal with, and it seems to be more natural in the context of scattering theory.

1.4. Bounded operators. Let $\mathcal{H}$ be a separable Hilbert space with scalar product $\langle \cdot, \cdot \rangle$, anti-linear in the first variable (all Hilbert spaces in this paper are complex and separable). Let T be a bounded operator on $\mathcal{H}$. The (uniform) norm $\|T\|$ of a bounded operator T is defined as

$$\|T\| = \sup_{f \in \mathcal{H},\, \|f\|=1} \|Tf\|.$$

A bounded operator T in $\mathcal{H}$ is *non-negative* if $\langle Tf, f \rangle \geq 0$ for any $f \in \mathcal{H}$.

The algebra of all bounded operators in $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$. Let α run through some net I of indices.

A net of operators $T_\alpha \in \mathcal{B}(\mathcal{H})$ converges to $T \in \mathcal{B}(\mathcal{H})$ in the *strong operator topology* if for any $f \in \mathcal{H}$ the net of vectors $T_\alpha f$ converges to Tf. In other words, the strong operator topology is generated by the seminorms $T \mapsto \|Tf\|$, where $f \in \mathcal{H}$.

A net of operators $T_\alpha \in \mathcal{B}(\mathcal{H})$ converges to $T \in \mathcal{B}(\mathcal{H})$ in the *weak operator topology* if for any $f, g \in \mathcal{H}$ the net $\langle f, T_\alpha g \rangle$ converges to $\langle f, Tg \rangle$. In other words, the weak operator topology is generated by the seminorms $T \mapsto |\langle f, Tg \rangle|$, where $f, g \in \mathcal{H}$.

The *adjoint* T^* of a bounded operator T is the unique operator which for all $f, g \in \mathcal{H}$ satisfies the equality $\langle T^* f, g \rangle = \langle f, Tg \rangle$. A bounded operator T is *self-adjoint* if $T^* = T$.

If T is a bounded self-adjoint operator, then for any bounded Borel function f there is a bounded self-adjoint operator $f(T)$ (the Spectral Theorem), such that, in particular, the map $f \mapsto f(T)$ is a homomorphism.

The real $\operatorname{Re}(T)$ and the imaginary $\operatorname{Im}(T)$ parts of an operator $T \in \mathcal{B}(\mathcal{H})$ are defined by

$$\operatorname{Re}(T) = \frac{T + T^*}{2} \quad \text{and} \quad \operatorname{Im}(T) = \frac{T - T^*}{2i}.$$

The real and imaginary parts are self-adjoint operators.

The absolute value $|T|$ of a bounded operator T is the operator

$$|T| = \sqrt{T^*T}.$$

An operator $T \in \mathcal{B}(\mathcal{H})$ is *Fredholm* if (1) its kernel

$$\ker(T) := \{f \in \mathcal{H} : Tf = 0\}$$

is finite-dimensional, (2) its image

$$\operatorname{im}(T) := \{f \in \mathcal{H} : \exists g \in \mathcal{H}\ f = Tg\}$$

is closed and (3) the orthogonal complement (that is, the *cokernel* $\operatorname{coker}(T)$) of $\operatorname{im}(T)$ is finite-dimensional. If T is Fredholm, then the *index* $\operatorname{ind}(T)$ of T is the number

$$\operatorname{ind}(T) := \dim\ker(T) - \dim\operatorname{coker}(T) = \dim\ker(T) - \dim\ker(T^*).$$

THEOREM 1.4.1 (Fredholm alternative). *If K is a compact operator, then $1 + K$ is Fredholm and* $\operatorname{ind}(1 + K) = 0$.

In particular, if K is compact and if $1 + K$ has trivial kernel, then $1 + K$ is invertible.

1.5. Self-adjoint operators. For details regarding the material of this subsection see [RS$_1$].

Let $\mathcal{H}$ be a separable Hilbert space with scalar product $\langle\cdot,\cdot\rangle$, anti-linear in the first variable.

By a linear operator T on $\mathcal{H}$ one means a linear operator from some linear manifold $\mathcal{D}(T) \subset \mathcal{H}$ to $\mathcal{H}$. The set $\mathcal{D}(T)$ is called the *domain* of T. A linear operator T is *symmetric* if its domain $\mathcal{D}(T)$ is dense and if $\langle Tf, g\rangle = \langle f, Tg\rangle$ for any $f, g \in \mathcal{D}(T)$. A linear operator S is an *extension* of a linear operator T if $\mathcal{D}(T) \subset \mathcal{D}(S)$ and $Sf = Tf$ for all $f \in \mathcal{D}(T)$. In this case one also writes $T \subset S$ (this inclusion can be considered as inclusion of sets, if one identifies an operator with its graph). A linear operator T is *closed* if $f_1, f_2, \ldots \in \mathcal{D}(T)$, $f_n \to f$ and $Tf_n \to g$ as $n \to \infty$ imply that $f \in \mathcal{D}(T)$ and $Tf = g$. An operator T is *closable* if it has a closed extension. For every closable operator T there exists a minimal (with respect to $\subset$) closed extension $\overline{T}$. The *adjoint* T^* of a densely defined operator T is a linear operator with domain

$$\mathcal{D}(T^*) := \{g \in \mathcal{H} : \exists h \in \mathcal{H}\ \forall f \in \mathcal{D}(T)\ \langle g, Tf\rangle = \langle h, f\rangle\};$$

such a vector h is unique and by definition $T^*g = h$. For every densely defined closable operator T its adjoint T^* is closed. For every densely defined operator T the inclusion $\overline{T} \subset T^{**}$ holds. A symmetric operator T satisfies $\overline{T} \subset T^*$. A symmetric operator T is called *self-adjoint* if $T = T^*$. So, self-adjoint operator is automatically closed.

The *resolvent set* $\rho(H)$ of an operator H in $\mathcal{H}$ consists of all those complex numbers $z \in \mathbb{C}$ for which the operator $H - z$ has a bounded inverse with domain dense in $\mathcal{H}$. The *resolvent* of an operator H is the operator

$$R_z(H) = (H - z)^{-1}, \quad z \in \rho(H).$$

The *spectrum* $\sigma(H)$ of H is the complement of the resolvent set $\rho(H)$, i.e.

$$\sigma(H) = \mathbb{C} \setminus \rho(H).$$

A closed symmetric operator H is self-adjoint if and only if $\ker(H - z) = \{0\}$ for any non-real $z \in \mathbb{C}$. The spectrum of a self-adjoint operator is a subset of $\mathbb{R}$.

Let H_0 be a self-adjoint operator with domain $\mathcal{D}(H_0)$ in $\mathcal{H}$. By $E_X = E_X^{H_0}$ we denote the spectral projection of the operator H_0, corresponding to a Borel set $X \subset \mathbb{R}$ (cf. [RS$_1$]). Usually, dependence on the operator H_0 will be omitted in the notation of the spectral projection. If $X = (-\infty, \lambda)$, then we also write $E_\lambda = E_{(-\infty,\lambda)}$.

By a subspace of a Hilbert space $\mathcal{H}$ we mean a closed linear subspace of $\mathcal{H}$.

If $f, g \in \mathcal{H}$, then the *spectral measure* associated with f and g is the (signed) measure

$$m_{f,g}(X) = \langle f, E_X g\rangle.$$

We also write $m_f = m_{f,f}$.

A vector f is called *absolutely continuous* (respectively, *singular*) with respect to H_0 if the spectral measure $m_f(X) = \langle f, E_X f\rangle$ is absolutely continuous (respectively, singular). The set of all vectors absolutely continuous with respect to H_0 is a (closed) subspace of $\mathcal{H}$, denoted by $\mathcal{H}^{(a)}(H_0)$. The subspace $\mathcal{H}^{(a)}(H_0)$ is called the *absolutely continuous subspace* (with respect to H_0). Similarly, the set of all vectors singular with respect to H_0 is a subspace of $\mathcal{H}$, denoted by $\mathcal{H}^{(s)}(H_0)$. The subspace $\mathcal{H}^{(s)}(H_0)$ is called the *singular subspace* (with respect to H_0). If there is no danger of confusion, dependence on the self-adjoint operator H_0 is usually omitted.

The absolutely continuous and singular subspaces of H_0 are invariant subspaces of H_0. That is, if $f \in \mathcal{H}^{(a)}(H_0) \cap \mathcal{D}(H_0)$ then $H_0 f \in \mathcal{H}^{(a)}(H_0)$; similarly, if $f \in \mathcal{H}^{(s)}(H_0) \cap \mathcal{D}(H_0)$ then $H_0 f \in \mathcal{H}^{(s)}(H_0)$. Also, $\mathcal{H}^{(a)}(H_0)$ and $\mathcal{H}^{(s)}(H_0)$ are orthogonal, and their direct sum is the whole $\mathcal{H}$:

$$\mathcal{H}^{(a)} \perp \mathcal{H}^{(s)} \quad \text{and} \quad \mathcal{H}^{(a)} \oplus \mathcal{H}^{(s)} = \mathcal{H}.$$

The *absolutely continuous* (respectively, *singular*) *spectrum* $\sigma^{(a)}(H_0)$ (respectively, $\sigma^{(s)}(H_0)$) of H_0 is the spectrum of the restriction of H_0 to $\mathcal{H}^{(a)}(H_0)$ (respectively, to $\mathcal{H}^{(s)}(H_0)$).

By $P^{(a)}(H_0)$ we denote the orthogonal projection onto the absolutely continuous subspace of H_0. If $f \in \mathcal{H}$, then by $f^{(a)}$ we denote the absolutely continuous part of f with respect to H_0, i.e. $f^{(a)} = P^{(a)} f$.

The set of all densely defined closed operators on $\mathcal{H}$ will be denoted by $\mathcal{C}(\mathcal{H})$.

1.6. Trace-class and Hilbert–Schmidt operators

1.6.1. Schatten ideals. Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces. A bounded operator $T\colon \mathcal{H} \to \mathcal{K}$ is *finite-dimensional* if its image $\operatorname{im}(T)$ is finite-dimensional. A bounded operator T : $\mathcal{H} \to \mathcal{K}$ is *compact* if one of the following equivalent conditions holds: (1) T is the uniform limit of a sequence of finite-dimensional operators; (2) the closure of the image $T(B_1)$ of the unit ball $B_1 := \{f \in \mathcal{H} : \|f\| \le 1\}$ is compact in $\mathcal{K}$.

By $\mathcal{L}_\infty(\mathcal{H}, \mathcal{K})$ we denote the set of all compact operators from a Hilbert space $\mathcal{H}$ to a possibly another Hilbert space $\mathcal{K}$. If $\mathcal{K} = \mathcal{H}$, then we write $\mathcal{L}_\infty(\mathcal{H})$. The same convention is used in relation to other classes of operators.

The set $\mathcal{L}_\infty(\mathcal{H})$ of compact operators is an involutive norm-closed two-sided ideal of the algebra $\mathcal{B}(\mathcal{H})$.

Let T be a compact operator in $\mathcal{H}$. If $\lambda \in \mathbb{C}$ is an eigenvalue of T, then the *root space* of this eigenvalue is the vector space of all those vectors f for which there exists an integer $k = 1, 2, \ldots$ such that $(T - \lambda)^k f = 0$. The root space of any non-zero eigenvalue of a compact operator is finite-dimensional. The dimension of this root space is called the (algebraic) *multiplicity* of the corresponding eigenvalue. The *spectral measure* ν_T of a compact operator T is a measure in $\mathbb{C} \setminus \{0\}$ which to every subset X of $\mathbb{C} \setminus \{0\}$ assigns the sum of the algebraic multiplicities of all eigenvalues λ from the set X. If two bounded operators $A\colon \mathcal{H} \to \mathcal{K}$ and $B\colon \mathcal{K} \to \mathcal{H}$ are such that the operators AB and BA are compact, then

$$\nu_{AB} = \nu_{BA}. \tag{1.6}$$

Also,

$$\nu_{T^*} = \bar{\nu}_T. \tag{1.7}$$

Let T be a compact operator from $\mathcal{H}$ to $\mathcal{K}$. The absolute value of T is the self-adjoint compact operator

$$|T| := \sqrt{T^*T}.$$

The *singular numbers* (or s-numbers)

$$s_1(T), s_2(T), s_3(T), \ldots$$

of the operator T are the eigenvalues of $|T|$, listed as a non-increasing sequence, and such that each eigenvalue is repeated according to its multiplicity. Every compact operator $T \in \mathcal{L}_\infty(\mathcal{H}, \mathcal{K})$ can be written in the Schmidt representation:

$$T = \sum_{n=1}^{\infty} s_n(T) \langle \phi_n, \cdot \rangle \psi_n,$$

where (ϕ_n) is an orthonormal basis in $\mathcal{H}$, and (ψ_n) is an orthonormal basis in $\mathcal{K}$.

The singular numbers of a compact operator T have the following property: for any $A, B \in \mathcal{B}(\mathcal{H})$,

$$s_n(ATB) \leq \|A\| \, \|B\| s_n(T). \tag{1.8}$$

Also, $s_n(A) = s_n(A^*)$.

Let $p \in [1, \infty)$. By $\mathcal{L}_p(\mathcal{H})$ we denote the set of all compact operators T in $\mathcal{H}$ such that

$$\|T\|_p := \Big(\sum_{n=1}^{\infty} s_n^p(T) \Big)^{1/p} < \infty.$$

The space $(\mathcal{L}_p(\mathcal{H}), \|\cdot\|_p)$ is an *invariant operator ideal*; this means that

1. $\mathcal{L}_p(\mathcal{H})$ is a Banach space,
2. $\mathcal{L}_p(\mathcal{H})$ is a $*$-ideal, that is, if $T \in \mathcal{L}_p(\mathcal{H})$ and $A \in \mathcal{B}(\mathcal{H})$, then $T^*, AT, TA \in \mathcal{L}_p(\mathcal{H})$,
3. for any $T \in \mathcal{L}_p(\mathcal{H})$ and $A, B \in \mathcal{B}(\mathcal{H})$,

$$\|T\|_p \geq \|T\|, \qquad \|T^*\|_p = \|T\|_p \quad \text{and} \quad \|ATB\|_p \leq \|A\| \, \|T\|_p \|B\|.$$

A norm which satisfies the above three conditions is called a unitarily invariant norm. The ideal $\mathcal{L}_p(\mathcal{H})$ is called the *Schatten ideal of p-summable operators*.

Note that for the definition of the singular numbers $s_1(T), s_2(T), \dots$ of an operator T it is immaterial whether T acts from $\mathcal{H}$ to $\mathcal{H}$, or maybe from $\mathcal{H}$ to another Hilbert space $\mathcal{K}$. In the latter case we write $T \in \mathcal{L}_p(\mathcal{H}, \mathcal{K})$.

Proofs of the following lemmas can be found in [Y, §6.1].

LEMMA 1.6.1. *If $A \in \mathcal{L}_p(\mathcal{H})$, then $A = BT$ (or $A = TB$) for some $B \in \mathcal{L}_p(\mathcal{H})$ and some compact operator T.*

LEMMA 1.6.2. *Let $A_1, A_2, \dots$ be a sequence of bounded operators converging to A in the strong operator topology and let $p \in [1, \infty]$. If $V \in \mathcal{L}_p(\mathcal{H})$, then $A_n V \to AV$ and $VA_n \to VA$ in $\mathcal{L}_p(\mathcal{H})$.*

LEMMA 1.6.3. *Let $A_1, A_2, \dots$ be a sequence of operators from $\mathcal{L}_p(\mathcal{H})$ converging to A in the weak operator topology and such that $\|A_n\|_p \le C < \infty$. Then $A \in \mathcal{L}_p(\mathcal{H})$ and for any compact operators T, Y,*

$$\lim_{n\to\infty} \|T(A_n - A)Y\|_p = 0.$$

1.6.2. Trace-class operators. Operators from $\mathcal{L}_1(\mathcal{H})$ are called *trace-class operators.* For a trace-class operator T one defines the trace $\mathrm{Tr}(T)$ by the formula

$$\mathrm{Tr}(T) = \sum_{j=1}^{\infty} \langle T\phi_j, \phi_j \rangle, \tag{1.9}$$

where $\{\phi_j\}_{j=1}^{\infty}$ is an arbitrary orthonormal basis of $\mathcal{H}$. Sometimes we write $\mathrm{Tr}_{\mathcal{H}}(T)$ instead of $\mathrm{Tr}(T)$ to indicate the Hilbert space which T acts on. For a trace-class operator T the series above is absolutely convergent and is independent of the choice of the basis $\{\phi_j\}_{j=1}^{\infty}$. The trace $\mathrm{Tr}\colon \mathcal{L}_1(\mathcal{H}) \to \mathbb{C}$ is a continuous linear functional, which satisfies the equality

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$$

whenever both products AB and BA are trace-class. In particular, the above equality holds if A is trace-class and B is a bounded operator.

The norm $\|\cdot\|_1$ is called the *trace-class norm.* For any trace-class operator T,

$$\|T\|_1 = \mathrm{Tr}(|T|).$$

More generally,

$$\|T\|_p = (\mathrm{Tr}(|T|^p))^{1/p}.$$

The Lidskii theorem asserts that for any trace-class operator T,

$$\mathrm{Tr}(T) = \sum_{j=1}^{\infty} \lambda_j, \tag{1.10}$$

where $\lambda_1, \lambda_2, \dots$ is the list of eigenvalues of T counting multiplicities ([1]).

The dual of the Banach space $\mathcal{L}_1(\mathcal{H})$ is the algebra $\mathcal{B}(\mathcal{H})$ of all bounded operators with the uniform norm $\|\cdot\|$: every continuous linear functional on $\mathcal{L}_1(\mathcal{H})$ has the form

$$T \mapsto \mathrm{Tr}(AT)$$

([1]) By multiplicity of an eigenvalue λ_j of T we always mean its algebraic multiplicity; that is, the dimension of the vector space $\{f \in \mathcal{H} : \exists\, k = 1, 2, \dots\ (T - \lambda_j)^k f = 0\}$.

for some bounded operator $A \in \mathcal{B}(\mathcal{H})$, and, vice versa, any functional of this form is continuous.

1.6.3. Hilbert–Schmidt operators. Operators from $\mathcal{L}_2(\mathcal{H})$ are called *Hilbert–Schmidt operators.* The norm

$$\|T\|_2 = \sqrt{\mathrm{Tr}(|T|^2)}$$

is also called the *Hilbert–Schmidt norm.* For $T \in \mathcal{L}_2(\mathcal{H})$ and any orthonormal basis (ϕ_j) of $\mathcal{H}$,

$$\|T\|_2^2 = \sum_{j=1}^{\infty} \|T\phi_j\|^2. \tag{1.11}$$

If S, T are Hilbert–Schmidt operators, then the product ST is trace-class and

$$\|ST\|_1 \le \|S\|_2 \|T\|_2. \tag{1.12}$$

This is a particular case of a more general Hölder inequality: Let $p, q \in [1, +\infty]$ with $1/p + 1/q = 1$. If $S \in \mathcal{L}_p(\mathcal{H})$ and $T \in \mathcal{L}_q(\mathcal{H})$, then ST is trace-class and

$$\|ST\|_1 \le \|S\|_p \|T\|_q,$$

where $\|\cdot\|_\infty$ means the usual operator norm. This inequality implies that

$$\text{if } \|S_n - S\|_p \to 0 \text{ and } \|T_n - T\|_q \to 0 \text{ then } \|S_nT_n - ST\|_1 \to 0. \tag{1.13}$$

The ideal $\mathcal{L}_2(\mathcal{H})$ is actually a Hilbert space with the scalar product

$$\langle S, T\rangle = \mathrm{Tr}(S^*T).$$

So, the dual of $\mathcal{L}_2(\mathcal{H})$ is $\mathcal{L}_2(\mathcal{H})$ itself.

1.6.4. Fredholm determinant. Let (ϕ_j) be an orthonormal basis in $\mathcal{H}$. If T is a trace-class operator, then one can define the *determinant* $\det(1+T)$ of $1+T$ by the formula

$$\det(1+T) = \lim_{n\to\infty} \det(\langle \phi_i, (1+T)\phi_j\rangle)_{i,j=1}^n,$$

where the determinant on the right hand side is the usual finite-dimensional determinant. For any trace-class operator T the limit on the right hand side exists and it does not depend on the choice of the orthonormal basis (ϕ_j).

We list some properties of the determinant.

The determinant has the product property: for any trace-class operators S, T,

$$\det((1+S)(1+T)) = \det(1+S)\det(1+T). \tag{1.14}$$

If $0 \le S \le T \in \mathcal{L}_1(\mathcal{H})$, then

$$\det(1+S) \le \det(1+T). \tag{1.15}$$

Also,

$$\det(1+T^*) = \overline{\det(1+T)}. \tag{1.16}$$

If $0 \le T \in \mathcal{L}_1(\mathcal{H})$, then

$$\mathrm{Tr}(T) \le \det(1+T). \tag{1.17}$$

The non-linear functional

$$\mathcal{L}_1(\mathcal{H}) \ni T \mapsto \det(1+T) \quad \text{ is continuous.} \tag{1.18}$$

The following Lidskii formula holds:

$$\det(1+T) = \prod_{j=1}^{\infty}(1+\lambda_j), \tag{1.19}$$

where $\lambda_1, \lambda_2, \ldots$ is the list of eigenvalues of T counting multiplicities.

1.6.5. The Birman–Koplienko–Solomyak inequality. The following assertion is called the *Birman–Koplienko–Solomyak inequality* ([2]) (cf. [BKS]).

THEOREM 1.6.4. *If A and B are two non-negative trace-class operators, then*

$$\big\|\sqrt{A} - \sqrt{B}\big\|_2 \le \big\|\sqrt{|A-B|}\big\|_2.$$

In [BKS] a more general inequality is proved:

$$\|A^p - B^p\|_{\mathfrak{S}} \le \||A-B|^p\|_{\mathfrak{S}},$$

where $p \in (0,1]$ and $\|\cdot\|_{\mathfrak{S}}$ is any unitarily invariant norm.

In [An], T. Ando (who was not aware of the paper [BKS] at the time of writing [An]) proved the inequality

$$\|f(A) - f(B)\|_{\mathfrak{S}} \le \|f(|A-B|)\|_{\mathfrak{S}},$$

where $f\colon [0,\infty) \to [0,\infty)$ is any operator-monotone function, that is, a function with the property: if $A \ge B \ge 0$, then $f(A) \ge f(B) \ge 0$. Ando's inequality implies the Birman–Koplienko–Solomyak inequality, since $f(x) = x^p$ with $p \in (0,1]$ is operator-monotone. Ando's inequality was generalized to the setting of semifinite von Neumann algebras in [DD].

LEMMA 1.6.5. *If $A_n \ge 0$, $A_n \in \mathcal{L}_1$ for all $n = 1, 2, \ldots$, and if $A_n \to A$ in $\mathcal{L}_1$, then $\sqrt{A_n} \to \sqrt{A}$ in $\mathcal{L}_2$.*

Proof. It follows from Theorem 1.6.4, that

$$\big\|\sqrt{A_n} - \sqrt{A}\big\|_2 \le \big\|\sqrt{|A_n - A|}\big\|_2 = \sqrt{\|A_n - A\|_1} \to 0$$

as $n \to \infty$. The proof is complete. ■

1.7. Direct integral of Hilbert spaces. In this subsection I follow [BS_1, Chapter 7]. Let Λ be a Borel subset of $\mathbb{R}$ with a Borel measure ρ (we do not need more general measure spaces here), and let $\{\mathfrak{h}_\lambda : \lambda \in \Lambda\}$ be a family of Hilbert spaces such that the dimension function

$$\Lambda \ni \lambda \mapsto \dim \mathfrak{h}_\lambda \in \{0, 1, \ldots, \infty\}$$

is measurable. Let Ω_0 be a countable family of vector-functions (or sections) $f_1, f_2, \ldots$ such that to each $\lambda \in \Lambda$, f_j assigns a vector $f_j(\lambda) \in \mathfrak{h}_\lambda$.

DEFINITION 1.7.1. A family $\Omega_0 = \{f_1, f_2, \ldots\}$ of vector-functions is called a *measurability base* if it satisfies the following two conditions:

1. for a.e. $\lambda \in \Lambda$ the set $\{f_j(\lambda) : j \in \mathbb{N}\}$ generates the Hilbert space $\mathfrak{h}_\lambda$;
2. the scalar product $\langle f_i(\lambda), f_j(\lambda)\rangle$ is ρ-measurable for all $i, j = 1, 2, \ldots$.

([2]) I thank Prof. P. G. Dodds for pointing out this inequality.

A vector-function $\Lambda \ni \lambda \mapsto f(\lambda) \in \mathfrak{h}_\lambda$ is called *measurable* if $\langle f(\lambda), f_j(\lambda)\rangle$ is measurable for all $j = 1, 2, \dots$. The set of all measurable vector-functions is denoted by $\hat{\Omega}_0$.

A measurability base $\{e_j(\cdot)\}$ is called *orthonormal* if for ρ-a.e. λ the system $\{e_j(\lambda)\}$—after removing zero vectors—is an orthonormal basis of the fiber Hilbert space $\mathfrak{h}_\lambda$. (This definition of an orthonormal measurability base slightly differs from the one given in [BS_1]).

If we have a sequence $f_1, f_2, \dots$ of vectors in a Hilbert space, then by Gram–Schmidt orthogonalization process we mean the following procedure: for $n = 1, 2, \dots$ we replace the function f_n by the zero vector if f_n is a linear combination (in particular, if $f_n = 0$) of $f_1, \dots, f_{n-1}$, otherwise, we replace f_n by the unit vector e_n which is a linear combination of $f_1, \dots, f_n$, which is orthogonal to all $f_1, \dots, f_{n-1}$ and which satisfies the inequality $\langle e_n, f_n\rangle > 0$. Obviously, the systems $\{f_j\}$ and $\{e_j\}$ generate the same linear subspace of the Hilbert space.

Lemma 1.7.2 ([BS_1, Lemma 7.1.1]). *If Ω_0 is a measurability base, then there exists an orthonormal measurability base Ω_1 such that $\hat{\Omega}_0 = \hat{\Omega}_1$, that is, the sets of measurable vector-functions generated by Ω_0 and Ω_1 coincide.*

Lemma 1.7.3 ([BS_1, Corollary 7.1.2]).

(i) *If $f(\cdot)$ and $g(\cdot)$ are measurable vector-functions, then $\Lambda \ni \lambda \mapsto \langle f(\lambda), g(\lambda)\rangle_{\mathfrak{h}_\lambda}$ is also measurable.*
(ii) *If $f(\cdot)$ is a measurable vector-function, then $\Lambda \ni \lambda \mapsto \|f(\lambda)\|_{\mathfrak{h}_\lambda}$ is measurable.*

Two measurable functions are *equivalent* if they coincide for ρ-a.e. $\lambda \in \Lambda$. The direct integral of Hilbert spaces

$$\mathcal{H} = \int_\Lambda^\oplus \mathfrak{h}_\lambda\, \rho(d\lambda) \tag{1.20}$$

consists of all (equivalence classes of) measurable vector-functions $f(\lambda)$ such that

$$\|f\|^2_{\mathcal{H}} := \int_\Lambda \|f(\lambda)\|^2_{\mathfrak{h}_\lambda}\, \rho(d\lambda) < \infty.$$

The scalar product of $f, g \in \mathcal{H}$ is given by the formula

$$\langle f, g\rangle_{\mathcal{H}} = \int_\Lambda \langle f(\lambda), g(\lambda)\rangle_{\mathfrak{h}_\lambda}\, \rho(d\lambda).$$

The set of square summable vector-functions with this scalar product is a Hilbert space.

Lemma 1.7.4 ([BS_1, Lemma 7.1.5]). *Let $\{\mathfrak{h}_\lambda : \lambda \in \Lambda\}$ be a family of Hilbert spaces with an orthogonal measurability base $\{e_j(\cdot)\}$, and let $f_0 \in L_2(\Lambda, d\rho)$ be a fixed function such that $f_0 \neq 0$ for ρ-a.e. λ. Then the linear span of the set of functions*

$$\{f_0(\lambda)\chi_\Delta(\lambda)e_j(\lambda) : j = 1, 2, \dots,\ \Delta \text{ is a Borel subset of } \Lambda\}$$

is dense in the Hilbert space (1.20).

There is an example of the direct integral of Hilbert spaces relevant to this paper (cf. e.g. [BS_1, Chapter 7]). Let $\mathfrak{h}$ be a fixed Hilbert space, let $\{\mathfrak{h}_\lambda : \lambda \in \Lambda\}$ be a family of subspaces of $\mathfrak{h}$ and let P_λ be the orthogonal projection onto $\mathfrak{h}_\lambda$. Let the operator-function P_λ, $\lambda \in \Lambda$, be weakly measurable. Let (ω_j) be an orthonormal basis in $\mathfrak{h}$. The family of vector-functions $f_j(\lambda) = \{P_\lambda \omega_j\}$ is a measurability base for the family of Hilbert spaces $\{\mathfrak{h}_\lambda : \lambda \in \Lambda\}$. The direct integral of Hilbert spaces (1.20) corresponding to this family is naturally isomorphic (in an obvious way) to the subspace of $L_2(\Lambda, \mathfrak{h})$ which consists of all measurable square integrable vector-functions $f(\cdot)$ such that $f(\lambda) \in \mathfrak{h}_\lambda$ for a.e. $\lambda \in \Lambda$ [BS_1, Chapter 7].

One of the versions of the Spectral Theorem says that for any self-adjoint operator H in $\mathcal{H}$ there exists a direct integral of Hilbert spaces (1.20) and an isomorphism

$$\mathcal{F} \colon \mathcal{H} \to \mathfrak{H}$$

such that H_0 is diagonalized in this representation:

$$\mathcal{F}(Hf)(\lambda) = \lambda \mathcal{F}(f)(\lambda), \qquad f \in \operatorname{dom}(H),$$

for ρ-a.e. $\lambda \in \Lambda$.

1.8. Operator-valued holomorphic functions. In this subsection I follow mainly Kato's book [Ka_2]. Proofs and details can be found there. See also [HPh, Chapter III].

Let X be a Banach space. Let G be a region (open connected subset) of the complex plane $\mathbb{C}$. A vector-function $f \colon G \to X$ is called *holomorphic* (or strongly holomorphic) if for every $z \in G$ the limit

$$f'(z) := \lim_{h \to 0} \frac{f(z+h) - f(z)}{h}$$

exists. A vector-function $f \colon G \to X$ is holomorphic if and only if it is weakly holomorphic, that is, if for any continuous linear functional l on X the function $l(f(z))$ is holomorphic in G. The proof can be found in [Ka_2, Theorem III.1.37] (see also [Ka_2, Theorem III.3.12], [RS_1]).

A vector-function $f \colon G \to X$ is holomorphic at $z_0 \in G$ if and only if f is analytic at z_0, that is, f admits a power series representation

$$f(z) = f_0 + (z - z_0) f_1 + (z - z_0)^2 f_2 + \cdots$$

with a non-zero radius of convergence, where $f_0, f_1, \ldots \in X$.

In this paper we consider only holomorphic families of compact operators on a Hilbert space. On one occasion we also consider a holomorphic family of operators of the form $1 + T(z)$, where $T(z)$ is a holomorphic family of compact operators.

Let $T \colon G \to \mathcal{L}_\infty(\mathcal{H})$ be a holomorphic family of compact operators. Let $z \in G$ and let Γ be a piecewise smooth contour in the resolvent set $\rho(T(z))$ of $T(z)$. Assume that there are only a finite number of eigenvalues (counting multiplicities) $\lambda_1(z), \ldots, \lambda_h(z)$ of $T(z)$ inside of Γ. The operator

$$P(z) = \frac{1}{2\pi i} \int_\Gamma (\zeta - T(z))^{-1} \, d\zeta \tag{1.21}$$

is an idempotent operator (3) (an *idempotent operator* is a bounded operator E which satisfies the equality $E^2 = E$), corresponding to the set of eigenvalues $\lambda_1(z), \ldots, \lambda_h(z)$. The idempotent $P(z)$ is called the *Riesz idempotent operator*. By the Cauchy theorem,

(3) We do not use the word projection here, since by projection we mean an orthogonal idempotent.

$P(z)$ does not change if Γ is changed continuously inside the resolvent set of T. The range of $P(z)$ is the direct sum of the root spaces of the eigenvalues $\lambda_1(z), \dots, \lambda_h(z)$.

Let $z \in G$. If $\lambda_j(z)$ is a simple (that is, of algebraic multiplicity 1) non-zero eigenvalue of $T(z)$, then in some neighbourhood of z it depends holomorphically on z and remains simple. Also the idempotent operator $P_j(z)$ associated with the eigenvalue $\lambda_j(z)$ is holomorphic in z. In particular, the eigenvector $v_j(z)$, corresponding to $\lambda_j(z)$, is also a holomorphic function in a neighbourhood of z.

The situation is not so simple if the eigenvalue $\lambda_j(z)$ is not simple at some $z_0 \in G$. In this case in a neighbourhood of z_0 the eigenvalue $\lambda_j(z)$ splits (more exactly, may split and most likely does split) into several different eigenvalues $\lambda_{z_0,1}(z), \dots, \lambda_{z_0,p}(z)$, where p is the multiplicity of $\lambda_j(z_0)$. The functions $\lambda_{z_0,1}(z), \dots, \lambda_{z_0,p}(z)$ represent branches of a multi-valued holomorphic function with branch point z_0. So, they can have an algebraic singularity at z_0, though they are still continuous at z_0. The idempotent of the whole set of eigenvalues $\lambda_{z_0,1}(z), \dots, \lambda_{z_0,p}(z)$ is holomorphic in a neighbourhood of z_0; but the idempotent of a subset firstly is not defined at z_0 and secondly as $z \to z_0$ it (more exactly, its norm) may go to infinity—that is, it can have a pole at z_0 (see e.g. [Ka$_2$, Theorem II.1.9]). Note that this is possible since an idempotent is not necessarily self-adjoint.

All these potentially "horrible" things cannot happen if the holomorphic family of operators $T(z)$ is *symmetric*. This means that the region G has a non-empty intersection with the real-axis $\mathbb{R}$ and for $\operatorname{Im} z = 0$ the operator $T(z)$ is self-adjoint, or—at the very least—normal. Fortunately, in this paper we shall deal only with such symmetric families of holomorphic functions. Namely, if the family $T(z)$ is symmetric, then (1) the eigenvalues $\lambda_1(z), \lambda_2(z), \dots$ of $T(z)$ are analytic functions for real values of z (more exactly, they can be enumerated at every point z in such a way that they become analytic), (2) the eigenvectors $v_1(z), v_2(z), \dots$ of $T(z)$ corresponding to those eigenvalues are analytic as well. The eigenvectors admit analytic continuation to any real point z_0, where some eigenvalue is not simple, since in this case all Riesz idempotents of the set of isolated eigenvalues are orthogonal, and—as a consequence—bounded. So, the Riesz idempotents cannot have a singularity at z_0 and thus are analytic at z_0. It follows that the eigenvalues are also analytic.

For details see Kato's book.

LEMMA 1.8.1. *Let* $A\colon [0,1) \ni y \mapsto A_y \in \mathcal{L}_1(\mathcal{H})$, $A_y \geq 0$.

(i) *If* A_y *is a real-analytic function for* $y > 0$ *with values in* $\mathcal{L}_1$, *then* $\sqrt{A_y}$ *is a real-analytic function for* $y > 0$ *with values in* $\mathcal{L}_2$.
(ii) *If, moreover,* A_y *is continuous at* $y = 0$ *in* $\mathcal{L}_1$, *then* $\sqrt{A_y}$ *is continuous at* $y = 0$ *in* $\mathcal{L}_2$.

THEOREM 1.8.2. *Let* A_y, $y \in [0,1)$, *be a family of non-negative Hilbert–Schmidt* (*respectively, compact*) *operators, real-analytic in* $\mathcal{L}_2$ (*respectively, in* $\|\cdot\|$) *for* $y > 0$. *Then there exists a family* $\{e_j(y)\}$ *of orthonormal bases, consisting of eigenvectors of* A_y, *such that all vector-functions* $(0,1) \ni y \mapsto e_j(y)$, $j = 1, 2, \dots$, *are real-analytic functions, as also are the corresponding eigenvalue functions* $\alpha_j(y)$. *Moreover, if* A_y *is continuous at* $y = 0$ *in the Hilbert–Schmidt norm, then all eigenvalue functions* $\alpha_j(y)$ *are also continuous at*

$y = 0$, and if $\alpha_j(0) > 0$, then the corresponding eigenvector function $e_j(y)$ can also be chosen to be continuous at $y = 0$.

1.8.1. Operator-valued meromorphic functions. Let G be a region in $\mathbb{C}$. Let $z_0 \in G$ and let $T\colon G \setminus \{z_0\} \to \mathcal{B}(\mathcal{H})$ be a holomorphic family of bounded operators in a deleted neighbourhood of z_0. Then T admits a Laurent expansion

$$T(z) = \sum_{n=-\infty}^{\infty} (z - z_0)^n T_n,$$

where T_n are bounded operators.

Let $N = \min\{n : T_n \neq 0\}$. If $0 > N > -\infty$, then $T(z)$ is said to have a pole of order N at z_0.

1.8.2. Analytic Fredholm alternative. This is the following theorem (see e.g. [RS_1, Theorem VI.14], [Y, Theorem 1.8.2]).

THEOREM 1.8.3. *Let G be an open connected subset of $\mathbb{C}$. Let $T\colon G \to \mathcal{L}_\infty(\mathcal{H})$ be a holomorphic family of compact operators in G. If the family of operators $1 + T(z)$ is invertible at some point $z_1 \in G$, then it is invertible at all points of G except the discrete set*

$$\mathcal{N} := \{z \in G : 1 \in \sigma(T(z))\}.$$

Further, the operator-function $F(z) := (1 + T(z))^{-1}$ is meromorphic and the set of its poles is $\mathcal{N}$. Moreover, in the expansion of $F(z)$ in a Laurent series in a neighbourhood of any point $z_0 \in \mathcal{N}$ the coefficients of negative powers of $z - z_0$ are finite-dimensional operators.

1.9. The limiting absorption principle. We recall two theorems from [Y] (cf. also [BW]), which are crucial for this paper. They were established by L. de Branges [B] and M. Sh. Birman and S. B. Èntina [BE].

Because of importance of these two theorems for what follows, we shall give their proofs, even though they follow verbatim those in [Y].

THEOREM 1.9.1 ([Y, Theorem 6.1.5]). *Let $\mathcal{H}$ and $\mathcal{K}$ be two Hilbert spaces. Suppose H_0 is a self-adjoint operator in $\mathcal{H}$ and $F\colon \mathcal{H} \to \mathcal{K}$ is a Hilbert–Schmidt operator. Then for a.e. $\lambda \in \mathbb{R}$ the operator-valued function $FE_\lambda^{H_0}F^* \in \mathcal{L}_1(\mathcal{K})$ is differentiable in the trace-class norm, the operator-valued function $F \operatorname{Im} R_{\lambda+iy}(H_0)F^*$ has a limit in the trace-class norm as $y \to 0$, and*

$$\frac{1}{\pi} \lim_{y\to 0} F \operatorname{Im} R_{\lambda+iy}(H_0) F^* = \frac{d}{d\lambda}(FE_\lambda F^*), \tag{1.22}$$

where the limit and the derivative are taken in the trace-class norm.

Proof. Let $T_z = FR_z(H_0)F^*$ and let $\operatorname{Im} z > 0$.

(A) Let D be a dense set of linear combinations of some basis in $\mathcal{H}$. Let $f, g \in D$. The function

$$\left\langle f, \frac{1}{\pi} \operatorname{Im} T_z g \right\rangle$$

is the Poisson integral of the measure $\Delta \mapsto \langle f, E^{H_0}_\Delta g\rangle$. By Theorem 1.3.3, there exists a set Λ_1 of full measure such that for any $f, g \in D$ and for any $\lambda \in \Lambda_1$ the limit of $\langle f, \frac{1}{\pi} \operatorname{Im} T_{\lambda+iy} g\rangle$ as $y \to 0^+$ exists.

(B) Note that the function $\operatorname{Tr}(\frac{1}{\pi} \operatorname{Im} T_{\lambda+iy})$ is the Poisson integral of the measure $\Delta \mapsto \operatorname{Tr}(F E^{H_0}_\Delta F^*)$. By Theorem 1.3.3, there exists a set Λ_2 of full measure such that for all $\lambda \in \Lambda_2$ there exists a limit of $\operatorname{Tr}(\frac{1}{\pi} \operatorname{Im} T_{\lambda+iy})$ as $y \to 0^+$. Since the operator $\operatorname{Im} T_{\lambda+iy}$ is non-negative, it follows that for any $\lambda \in \Lambda_2$ there exist numbers $C(\lambda), y_0(\lambda) > 0$ such that

$$\|\operatorname{Im} T_{\lambda+iy}\|_1 \le C(\lambda) \quad \text{for all } y < y_0(\lambda).$$

(C) It follows from (A) and (B) that for all λ from the full set $\Lambda = \Lambda_1 \cap \Lambda_2$, the operator $\operatorname{Im} T_{\lambda+iy}$ has a weak limit as $y \to 0^+$.

(D) By Lemma 1.6.1, the operator F can be written in the form $F = TG$, where T is a compact operator and $G \in \mathcal{L}_2(\mathcal{H})$. By (B), for a.e. $\lambda \in \mathbb{R}$ we have $\|G \operatorname{Im} R_{\lambda+iy}(H_0) G^*\|_1 \le C(\lambda)$ as $y \to 0^+$, and by (C) for a.e. $\lambda \in \mathbb{R}$ the operator $G \operatorname{Im} R_{\lambda+iy} G^*$ weakly converges as $y \to 0^+$. Combining this with Lemma 1.6.3, it follows that $F \operatorname{Im} R_{\lambda+iy} F^* = T(G R_{\lambda+iy} G^*) T^*$ converges in $\mathcal{L}_2(\mathcal{H})$ for a.e. $\lambda \in \mathbb{R}$.

(E) The proof of $\mathcal{L}_1$-differentiability of $\lambda \mapsto F E_\lambda F^*$ and of (1.22) is similar and we omit the details which can be found in [Y, §6.1]. ∎

Another reason for omitting the second part of the proof of this theorem is that, while for this paper it is crucial that the $\mathcal{L}_1$-limit of $F \operatorname{Im} R_{\lambda+iy}(H_0) F^*$ exists for a.e. λ, differentiability of the function $\lambda \mapsto F E_\lambda F^*$ and the equality (1.22) are not so important. In fact, as Fatou's Theorem 1.3.3 shows, the derivative of a function and the limit value of its Poisson integral are in some sense identical notions, that is, the limit of the Poisson integral can be considered as a modified definition of the derivative, and one can choose to work with either of them. In the framework of scattering theory, the limit of Poisson integral is much more convenient. On the other hand, theorems of analysis are proved for the usual derivative, and Fatou's theorem allows one to exploit the properties of the usual derivative.

Theorem 1.9.2 ([Y, Theorem 6.1.9]). *Suppose that H_0 is a self-adjoint operator in a Hilbert space $\mathcal{H}$ and $F \in \mathcal{L}_2(\mathcal{H}, \mathcal{K})$. Then for a.e. $\lambda \in \mathbb{R}$ the operator-valued function $F R_{\lambda \pm iy}(H_0) F^*$ has a limit in $\mathcal{L}_2(\mathcal{K})$ as $y \to 0$.*

Proof. Let $T_z = F R_z(H_0) F^*$ and let $\operatorname{Im} z > 0$.

(A) Claim. $|\det(1 - iT_z)| \ge 1$.

Proof. We have, using (1.16) and (1.14),

$$\begin{aligned} |\det(1 - iT_z)|^2 &= \det((1 - iT_z)^*) \det(1 - iT_z) = \det(1 + iT_{\bar z}) \det(1 - iT_z) \\ &= \det\left[(1 + iT_{\bar z})(1 - iT_z)\right] = \det(1 + iT_{\bar z} - iT_z + T_{\bar z} T_z). \end{aligned}$$

Since $iT_{\bar z} - iT_z = 2 \operatorname{Im} T_z \ge 0$ and $T_{\bar z} T_z \ge 0$, it follows from the last equality and (1.15) that

$$\det(1 + iT_{\bar z} - iT_z + T_{\bar z} T_z) \ge 1.$$

Hence, $|\det(1 - iT_z)| \ge 1$.

(B) Claim. *For a.e.* $\lambda \in \mathbb{R}$ *the limit* $\lim_{y\to 0^+} \det(1 - iT_{\lambda+iy})$ *exists.*

Proof. Let $f(z) = \det(1 - iT_z)$. The function $g(z) = 1/f(z)$ is holomorphic in the upper-half plane $\mathbb{C}_+$, and by (A) it is bounded. It follows from Theorem 1.2.1(a) that $g(\lambda + i0)$ exists for a.e. λ, and by Theorem 1.2.1(b) this limit is non-zero for a.e. λ. It follows that $f(\lambda + i0)$ exists and is finite for a.e. λ.

(C) Claim. *For a.e.* $\lambda \in \mathbb{R}$, $\|T_{\lambda+iy}\|_2 \le C(\lambda)$ *as* $y \to 0^+$.

Proof. Using (1.17), we have

$$\|T_z\|_2^2 = \operatorname{Tr}(T_{\bar z} T_z) \le \det(1 + T_{\bar z} T_z).$$

Since $iT_{\bar z} - iT_z = 2 \operatorname{Im} T_z \ge 0$, it follows from (1.15) that

$$\|T_z\|_2^2 \le \det(1 + T_{\bar z} T_z) \le \det(1 + iT_{\bar z} - iT_z + T_{\bar z} T_z) = |\det(1 - iT_z)|^2.$$

Now (B) completes the proof.

(D) Claim. *For a.e.* λ *the operator* $T_{\lambda+iy}$ *weakly converges as* $y \to 0^+$.

Proof. Let D be a dense set in $\mathcal{H}$ of linear combinations of some basis. By Theorem 1.3.4, there exists a set Λ of full measure such that for any $f, g \in D$ and for any $\lambda \in \Lambda$ the limit of $\langle f, T_{\lambda+iy} g\rangle$ as $y \to 0^+$ exists. It follows from this and (C) that $T_{\lambda+iy}$ weakly converges as $y \to 0^+$ for a.e. λ.

(E) By Lemma 1.6.1, the operator F can be written in the form $F = TG$, where T is a compact operator and $G \in \mathcal{L}_2(\mathcal{H})$. By (C), for a.e. $\lambda \in \mathbb{R}$ we have $\|GR_{\lambda+iy}G^*\|_2 \le C(\lambda)$ as $y \to 0^+$ and by (D) for a.e. $\lambda \in \mathbb{R}$ the operator $GR_{\lambda+iy}G^*$ weakly converges as $y \to 0^+$. Combining this with Lemma 1.6.3, it follows that

$$FR_{\lambda+iy}F^* = T(GR_{\lambda+iy}G^*)T^*$$

converges in $\mathcal{L}_2(\mathcal{H})$ for a.e. $\lambda \in \mathbb{R}$. ■

S. N. Naboko has shown that in this theorem convergence in $\mathcal{L}_2(\mathcal{K})$ can be replaced by convergence in $\mathcal{L}_p(\mathcal{K})$ with any $p > 1$. In general, convergence in $\mathcal{L}_1(\mathcal{K})$ does not hold (cf. [N, N_2, N_3]).

Theorem 1.9.1 plays a more important role in this paper compared to Theorem 1.9.2. Moreover, existence of the limit of $FR_{\lambda\pm iy}(H_0)F^*$ in the Hilbert–Schmidt norm is not necessary at all for what follows: existence of the limit in the usual norm will suffice. For the purposes of this paper, in the second condition of Definition 0.2.2 of the full set $\Lambda(H_0; F)$ one can replace norm convergence by $\mathcal{L}_p$-convergence with any $p \in (1, \infty]$—the set $\Lambda(H_0; F)$ will still have full Lebesgue measure. Since the norm topology is weaker than the Hilbert–Schmidt topology, the set $\Lambda(H_0; F)$ becomes larger if we use norm convergence in Definition 0.2.2(ii), but this is not a point. It turns out that to generalize the results of this paper to the case of non-compact perturbations, norm convergence is preferable; this allows us to enlarge the set of non-compact perturbations covered by the theory.

2. Framed Hilbert space

2.1. Definition. In this section we introduce the so called framed Hilbert space and study several objects associated with it. Before giving a formal definition, I would like to explain the idea which led to this notion.

Let H_0 be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and let H_1 be its trace-class perturbation. Our ultimate purpose is to explicitly define the wave matrix $w_\pm(\lambda; H_1, H_0)$ at a fixed point λ of the spectral line. The wave matrix $w_\pm(\lambda; H_1, H_0)$ acts between fiber Hilbert spaces $\mathfrak{h}_\lambda(H_0)$ and $\mathfrak{h}_\lambda(H_1)$ from the direct integrals of Hilbert spaces

$$\int_{\hat\sigma(H_0)}^{\oplus} \mathfrak{h}_\lambda(H_0)\,d\lambda \quad \text{and} \quad \int_{\hat\sigma(H_1)}^{\oplus} \mathfrak{h}_\lambda(H_1)\,d\lambda,$$

diagonalizing the absolutely continuous parts of the operators H_0 and H_1, where $\hat\sigma(H_j)$ is a core of the spectrum of H_j. Before defining $w_\pm(\lambda; H_1, H_0)$, one should first define explicitly the fiber Hilbert spaces $\mathfrak{h}_\lambda(H_0)$ and $\mathfrak{h}_\lambda(H_1)$. Moreover, given a vector $f \in \mathcal{H}$, it is necessary to be able to assign an explicit value $f(\lambda) \in \mathfrak{h}_\lambda$ of the vector f at a single point $\lambda \in \mathbb{R}$. Obviously, the vectors $f(\lambda)$ generate the fiber Hilbert space $\mathfrak{h}_\lambda$. So, one of the first important questions to ask is:

$$\text{What is } f(\lambda)? \tag{2.1}$$

Actually, since the measure $d\lambda$ in the direct integral decomposition of the Hilbert space can be replaced by any other measure $\rho(d\lambda)$ with the same spectral type, it is not difficult to see that $f(\lambda)$ does not make sense as it stands. Indeed, let us consider an operator of multiplication by a continuous function $f(x)$ on the Hilbert space $L_2([-\pi,\pi])$. The Hilbert space $L_2([-\pi,\pi])$ can be represented as a direct integral of one-dimensional Hilbert spaces $\mathfrak{h}_\lambda \simeq \mathbb{C}$:

$$L_2([-\pi,\pi]) = \int_{[-\pi,\pi]}^{\oplus} \mathbb{C}\,dx.$$

(As a measurability base one can take here the system which consists of only one function, say, e^{inx}, where n is any integer; in particular, a non-zero constant function will do.) Since $f(x)$ is continuous we can certainly say what is, say, $f(0)$. But the measure dx can be replaced by any other measure of the same spectral type; for example, by

$$d\rho(x) = \left(2 + \sin\frac{1}{x}\right) dx.$$

The spectral theorem says that the operator of multiplication M_f by $f(x)$ does not notice this change of measure; that is, the operator M_f will stay in the same unitary equivalence class. At the same time, now it is difficult to say what $f(0)$ is. That is, the value $f(\lambda) \in \mathfrak{h}_\lambda$ of a vector f at a point λ of the spectral line is affected by the choice of a measure in its spectral type. As a consequence, the expression $f(\lambda)$ does not make sense. The measure ρ defined by the above formula is far from being the worst scenario: instead of $\sin\frac{1}{x}$ one can take, say, any L_∞-function bounded below by -1. In this case, we have difficulty in defining the value of f at any point.

In order to give a meaning to $f(\lambda)$, one needs to introduce some additional structure. (One can see that fixing a measure $d\rho$ in the spectral type does not help.) There are different approaches to this problem. Firstly, if we try to single out what enables us to give a meaning to $f(x)$ for all x in the case of the measure dx, we see that this additional structure is of geometric character: it is the (Riemannian) metric. The problem is that in the setting of arbitrary self-adjoint operators we do not have a metric. But the metric is fully encoded in the Dirac operator $\frac{1}{i}\frac{d}{d\theta}$ (see [C$_1$, Chapter VI]). The operator $\frac{1}{i}\frac{d}{d\theta}$ on $L_2(\mathbb{T})$ has discrete spectrum and so it is identified by a sequence of its eigenvalues and by the orthonormal basis of its eigenvectors. This type of data consisting of numbers and vectors of the Hilbert space can be easily dealt with in the abstract situation.

So, to see in another way what kind of additional structure can allow one to define $f(\lambda)$, let us assume, to begin with, that there is a fixed unit vector $\phi_1 \in \mathcal{H}$. In this case, it is possible to define the number

$$\langle f(\lambda), \phi_1(\lambda)\rangle$$

for a.e. λ, by formula (1.4), since the above scalar product is a summable function of λ. Note that neither $f(\lambda)$ nor $\phi_1(\lambda)$ are defined yet, but their scalar product is defined.

If there are sufficiently many (unit) vectors $\phi_1, \phi_2, \ldots$, then one can hope that the knowledge of all the scalar products $\langle f(\lambda), \phi_j(\lambda)\rangle$ will allow us to recover the vector $f(\lambda) \in \mathfrak{h}_\lambda$. (Note that we do not know yet what exactly $\mathfrak{h}_\lambda$ is.) But this is still not the case. Note that the scalar product $\langle \phi_j(\lambda), \phi_k(\lambda)\rangle$ should satisfy the formal equality

$$\langle \phi_j(\lambda), \phi_k(\lambda)\rangle = \langle \phi_j|\delta(H_0 - \lambda)|\phi_k\rangle = \frac{1}{\pi}\langle \phi_j|\operatorname{Im}(H_0 - \lambda - i0)^{-1}|\phi_k\rangle, \tag{2.2}$$

where $\langle \phi|A|\psi\rangle$ is physicists' (Dirac's) notation for $\langle \phi, A\psi\rangle$. That this equality must hold for the absolutely continuous part $H_0^{(a)}$ can be seen from

$$\langle \phi_j, j_\varepsilon(H_0^{(a)} - \lambda)\phi_k\rangle = \int_{\mathbb{R}} j_\varepsilon(\mu - \lambda)\langle \phi_j(\mu), \phi_k(\mu)\rangle\, d\mu,$$

where j_ε is an approximate unit for the Dirac δ-function. In order to satisfy this key equality, we use an artificial trick. We assign to each vector ϕ_j a weight $\kappa_j > 0$ such that $(\kappa_j) = (\kappa_1, \kappa_2, \ldots) \in \ell_2$. Now, we form the matrix

$$\phi(\lambda) := \left(\kappa_j\kappa_k\frac{1}{\pi}\langle \phi_j|\operatorname{Im}(H_0 - \lambda - i0)^{-1}|\phi_k\rangle\right).$$

Using the limiting absorption principle (Theorem 1.9.1), it can be easily shown that this matrix is a non-negative trace-class matrix. Now, if we define $\phi_j(\lambda)$ as the jth column of the square root of the matrix $\phi(\lambda)$ over κ_j, then $\phi_j(\lambda)$ will become an element of ℓ_2 and the equality (2.2) will be satisfied. For all λ from some explicit set of full Lebesgue measure, which depends only on H_0 and the data (ϕ_j, κ_j), this allows us to define the value $f(\lambda)$ at λ for each $f = \phi_j$, $j = 1, 2, \ldots$, and consequently for any vector from the dense manifold of finite linear combinations of ϕ_j. Finally, the fiber Hilbert space $\mathfrak{h}_\lambda$ can be defined as the linear subspace of ℓ_2 generated by $\phi_j(\lambda)$'s.

Evidently, the data (ϕ_j, κ_j) can be encoded in a single Hilbert–Schmidt operator $F = \sum_{j=1}^\infty \kappa_j\langle \phi_j, \cdot\rangle\psi_j$, where (ψ_j) is an arbitrary orthonormal system in a possibly different Hilbert space. Actually, in the case of $\mathcal{H} = L_2(M)$ discussed above, where M is a Riemannian manifold, F can be chosen to be the appropriate negative power of the Laplace–Beltrami operator Δ.

This justifies introduction of the following

DEFINITION 2.1.1. A *frame* in a Hilbert space $\mathcal{H}$ is a Hilbert–Schmidt operator $F\colon \mathcal{H}\to\mathcal{K}$, with trivial kernel and cokernel, of the form

$$F = \sum_{j=1}^{\infty} \kappa_j \langle \phi_j, \cdot \rangle \psi_j, \tag{2.3}$$

where $\mathcal{K}$ is another Hilbert space, and where $(\kappa_j) \in \ell_2$ is a fixed decreasing sequence of s-numbers of F, all of which are non-zero, (ϕ_j) is a fixed orthonormal basis in $\mathcal{H}$, and (ψ_j) is an orthonormal basis in $\mathcal{K}$.

A *framed Hilbert space* is a pair $(\mathcal{H}, F)$ consisting of a Hilbert space $\mathcal{H}$ and a frame F in $\mathcal{H}$.

Throughout this paper we shall work with only one frame F, with some restrictions imposed later on it, and κ_j, ϕ_j and ψ_j will be as in (2.3).

What is important in the definition of a frame is the orthonormal basis (ϕ_j) and the ℓ_2-sequence of weights (κ_j) of the basis vectors. The Hilbert space $\mathcal{K}$ is of little importance, if any. For the most part of this paper, one can take $\mathcal{K} = \mathcal{H}$ and F to be self-adjoint, but later we shall see that the more general definition given above is more useful.

A frame introduces rigidity into the Hilbert space. In particular, a frame fixes a measure on the spectrum of a self-adjoint operator by the formula $\mu(\Delta) = \operatorname{Tr}(F E^H_\Delta F^*)$. In other words, a frame fixes a measure in its spectral type.

For further use, we note the trivial relations

$$F\phi_j = \kappa_j \psi_j, \qquad F^* \psi_j = \kappa_j \phi_j. \tag{2.4}$$

2.2. Spectral triple associated with an operator on a framed Hilbert space. To the pair (H_0, F) consisting of a self-adjoint operator H_0 and a frame operator F one can assign a spectral triple [C$_1$]. The involutive algebra $\mathcal{A}$ of a spectral triple $(\mathcal{A}, \mathcal{H}, |F|^{-1})$ is given by

$$\mathcal{A} = \{\phi(H) : \phi \in C_b(\mathbb{R}),\ [|F|^{-1}, \phi(H)] \in \mathcal{B}(\mathcal{H})\}.$$

Here the class C_b of all continuous bounded functions on $\mathbb{R}$ can be replaced by L_∞. Let us check that $\mathcal{A}$ is an algebra. If $\phi_1(H), \phi_2(H) \in \mathcal{A}$ and $\alpha_1, \alpha_2 \in \mathbb{C}$, then obviously $\phi_1(H)^* = \bar{\phi}(H) \in \mathcal{A}$ and $\alpha_1\phi_1(H) + \alpha_2\phi_2(H) \in \mathcal{A}$. Now, if $\phi_1(H), \phi_2(H) \in \mathcal{A}$, then the operator

$$[|F|^{-1}, \phi_1(H)\phi_2(H)] = [|F|^{-1}, \phi_1(H)]\phi_2(H) + \phi_1(H)[|F|^{-1}, \phi_2(H)]$$

is also bounded, so that $\phi_1(H)\phi_2(H) \in \mathcal{A}$. Consequently, $\mathcal{A}$ is an involutive algebra. The second axiom of the spectral triple is satisfied obviously, that is, the resolvent $(|F|^{-1}-z)^{-1}$ of the operator $|F|^{-1}$ is compact for non-real z.

2.3. Non-compact frames. In the pair (H_0, F), consisting of a self-adjoint operator H_0 and a frame operator F, H_0 and F are independent of each other. One can consider more general pairs (H_0, F) which, I believe, may be useful in generalizing the present work to the case of non-trace-class (non-compact) perturbations V.

A *generalized frame operator* F for a self-adjoint operator H_0 is an operator $F\colon \mathcal{H} \to \mathcal{K}$ such that (1) the domain of F contains all subspaces $E^{H_0}_\Delta \mathcal{H}$ with bounded Borel Δ, (2) for any bounded Borel Δ the operator $FE_{\Delta}^{H_0}$ is Hilbert–Schmidt, and (3) the kernel of $FE_{\Delta}^{H_0}$ as an operator on $E_{\Delta}^{H_0}\mathcal{H}$ is trivial.

For such pairs one can construct a sheaf of Hilbert spaces over $\mathbb{R}$ which diagonalizes H_0. Details of this construction and its applications to scattering theory for non-compact perturbations will appear in [Az_6].

2.4. The set $\Lambda(H_0; F)$ and the matrix $\phi(\lambda)$. Let H_0 be a self-adjoint operator in a framed Hilbert space $(\mathcal{H}, F)$.

By $E_\lambda = E_\lambda^{H_0}$, $\lambda \in \mathbb{R}$, we denote the family of spectral projections of H_0. For any (ordered) pair of indices (i, j) one can consider a finite (signed) measure

$$m_{ij}(\Delta) := \langle \phi_i, E_\Delta^{H_0} \phi_j \rangle. \tag{2.5}$$

We denote by

$$\Lambda_0(H_0, F) \tag{2.6}$$

the intersection of all the sets $\Lambda(m_{ij})$, $i, j \in \mathbb{N}$ (see Subsection 1.3.7), even though it depends only on H_0 and the vectors $\phi_1, \phi_2, \ldots$. So, for any $\lambda \in \Lambda_0(H_0, F)$ the limit

$$\phi_{ij}(\lambda) := \frac{1}{\pi} \kappa_i \kappa_j \langle \phi_i, \operatorname{Im} R_{\lambda+i0}(H_0) \phi_j \rangle$$

exists. It follows that, for any $\lambda \in \Lambda_0(H_0, F)$, one can form an infinite matrix

$$\phi(\lambda) = (\phi_{ij}(\lambda))_{i,j=1}^{\infty}.$$

Our aim is to consider $\phi(\lambda)$ as an operator on ℓ_2. Evidently, the matrix $\phi(\lambda)$ is symmetric in the sense that for any $i, j = 1, 2, \ldots,$

$$\overline{\phi_{ij}(\lambda)} = \phi_{ji}(\lambda).$$

But it may turn out that $\phi(\lambda)$ is not a matrix of a bounded, or even of an unbounded, operator on ℓ_2. So, we have to investigate the set of points where $\phi(\lambda)$ determines a bounded self-adjoint operator on ℓ_2. As is shown below, it turns out that $\phi(\lambda)$ is a trace-class operator on a set of full measure.

In the following definition one of the central notions of this paper is introduced.

Definition 2.4.1. The standard set $\Lambda(H_0; F)$ of full Lebesgue measure, associated with a self-adjoint operator H_0 acting on a framed Hilbert space $(\mathcal{H}, F)$, consists of those points $\lambda \in \mathbb{R}$ at which the limit of $FR_{\lambda+iy}(H_0)F^*$ (as $y \to 0^+$) exists in the uniform norm and the limit of $F \operatorname{Im} R_{\lambda+iy}(H_0) F^*$ exists in the $\mathcal{L}_1$-norm.

In other words, a number λ belongs to $\Lambda(H_0; F)$ if and only if it belongs to both sets of full measure from Theorems 1.9.1 and 1.9.2.

Proposition 2.4.2. *For any self-adjoint operator H_0 on a framed Hilbert space $(\mathcal{H}, F)$ the set $\Lambda(H_0; F)$ has full Lebesgue measure.*

Proof. This follows from Theorems 1.9.1 and 1.9.2. ■

The following proposition gives one of the two main properties of the set $\Lambda(H_0; F)$.

Proposition 2.4.3. *Let H_0 be a self-adjoint operator acting on a framed Hilbert space $(\mathcal{H}, F)$. If $\lambda \in \Lambda(H_0; F)$, then the matrix $\phi(\lambda)$ exists, is non-negative and trace-class.*

Proof. Let $\lambda \in \Lambda(H_0; F)$. Since for $\lambda \in \Lambda(H_0; F)$ the limit

$$FR_{\lambda \pm i0}(H_0)F^* = \lim_{y \to 0^+} FR_{\lambda \pm iy}(H_0)F^*$$

exists in the Hilbert–Schmidt norm, it follows that for any pair (i, j) the limit

$$P_i^* FR_{\lambda \pm i0}(H_0)F^* P_j = \lim_{y \to 0^+} P_i^* FR_{\lambda \pm iy}(H_0)F^* P_j$$

also exists in the Hilbert–Schmidt norm, where $P_j = \langle \phi_j, \cdot \rangle \psi_j$. This is equivalent to the existence of the limit

$$\langle \phi_i, R_{\lambda \pm i0}(H_0)\phi_j \rangle = \lim_{y \to 0^+} \langle \phi_i, R_{\lambda \pm iy}(H_0)\phi_j \rangle.$$

Hence, $\Lambda(H_0; F) \subset \Lambda_0(H_0, F)$; so $\phi(\lambda)$ exists for any $\lambda \in \Lambda(H_0; F)$.

The matrix $\phi(\lambda)$ is unitarily equivalent to the non-negative trace-class operator $F \frac{1}{\pi} \operatorname{Im} R_{\lambda + iy}(H_0)F^*$. Hence, $\phi(\lambda)$ is also non-negative and trace-class. ∎

LEMMA 2.4.4. *The operator function $\Lambda(H_0; F) \ni \lambda \mapsto \phi(\lambda) \in \mathcal{L}_1(\ell_2)$ is measurable.*

Indeed, $\phi(\lambda)$ is an a.e. pointwise limit of matrices $\phi(\lambda + iy)$ with continuous matrix elements.

2.5. A core of the singular spectrum $\mathbb{R} \setminus \Lambda(H_0; F)$. We call a null set $X \subset \mathbb{R}$ a *core* of the singular spectrum of H_0, if the operator $E^{H_0}_{\mathbb{R} \setminus X} H_0$ is absolutely continuous. Evidently, any core of the singular spectrum contains the pure point spectrum. Apart from it, a core of the singular spectrum contains a null Borel support of the singular continuous spectrum.

LEMMA 2.5.1. *Let H_0 be a self-adjoint operator on $\mathcal{H}$ and let Λ be a full set. If $\mathbb{R} \setminus \Lambda$ is not a core of the singular spectrum of H_0, then there exists a null set $X \subset \Lambda$ such that $E_X \neq 0$.*

Proof. Let Z_a be a full set such that E_{Z_a} is the projection onto the absolutely continuous subspace of $H_0 E_\Lambda$. Such a set exists by [Y, Lemma 1.3.6]. If $\mathbb{R} \setminus \Lambda$ is not a core of the singular spectrum, then the operator $H_0 E_\Lambda$ is not absolutely continuous. So, the set $X := \Lambda \setminus Z_a$ is a null set and $E_X \neq 0$. ∎

PROPOSITION 2.5.2. *For any self-adjoint operator H_0 on a framed Hilbert space $(\mathcal{H}, F)$, the set $\mathbb{R} \setminus \Lambda_0(H_0, F)$ is a core of the singular spectrum of H_0.*

Proof. Assume the contrary. Then by Lemma 2.5.1 there exists a null subset X of $\Lambda_0(H_0, F)$ such that $E_X \neq 0$. Since (ϕ_j) is a basis, there exists ϕ_j such that $E_X \phi_j \neq 0$. Hence, $\langle E_X \phi_j, \phi_j \rangle \neq 0$, that is,

$$m_{jj}^{(s)}(X) = m_{jj}(X) \neq 0,$$

where m_{jj} is the spectral measure of ϕ_j (see (2.5)). Since $X \subset \Lambda(m_{jj})$, this contradicts the fact that the complement of $\Lambda(m_{jj})$ is a Borel support of $m_{jj}^{(s)}$ (see Theorem 1.3.6). ∎

Since $\Lambda(H_0; F) \subset \Lambda_0(H_0, F)$, we obtain

COROLLARY 2.5.3. *For any self-adjoint operator H_0 on a framed Hilbert space $(\mathcal{H}, F)$, the set $\mathbb{R} \setminus \Lambda(H_0; F)$ is a core of the singular spectrum of H_0.*

Since $\Lambda(H_0;F)$ has full measure, this corollary means that the set $\Lambda(H_0;F)$ cuts out the singular spectrum of H_0 from $\mathbb{R}$. Given a frame operator $F \in \mathcal{L}_2(\mathcal{H},\mathcal{K})$, we consider the set $\mathbb{R} \setminus \Lambda(H_0;F)$ as a standard core of the singular spectrum of H_0, associated with the given frame F.

2.6. The Hilbert spaces $\mathcal{H}_\alpha(F)$. Let $\alpha \in \mathbb{R}$. In analogy with Sobolev spaces W^2_α (see e.g. [RS$_2$, §IX.6], [C$_2$]), given a framed Hilbert space $(\mathcal{H},F)$, we introduce the Hilbert spaces $\mathcal{H}_\alpha(F)$. By definition, $\mathcal{H}_\alpha(F)$ is the completion of the linear manifold

$$\mathcal{D} = \mathcal{D}(F) := \Big\{ f \in \mathcal{H} : f = \sum_{j=1}^{N} \beta_j \phi_j,\ N < \infty \Big\} \tag{2.7}$$

in the norm

$$\|f\|_{\mathcal{H}_\alpha(F)} = \big\| |F|^{-\alpha} f \big\|,$$

with the scalar product

$$\langle f, g\rangle_{\mathcal{H}_\alpha(F)} = \langle |F|^{-\alpha} f, |F|^{-\alpha} g\rangle.$$

That is, if $f = \sum_{j=1}^N \beta_j\phi_j$, then

$$\|f\|_{\mathcal{H}_\alpha(F)} = \Big(\sum_{j=1}^{N} |\beta_j|^2 \kappa_j^{-2\alpha} \Big)^{1/2}. \tag{2.8}$$

Since F has trivial kernel, $\|\cdot\|_{\mathcal{H}_\alpha(F)}$ is indeed a norm. The scalar product of vectors $f = \sum_{j=1}^N \alpha_j\phi_j$ and $g = \sum_{j=1}^N \beta_j\phi_j$ in $\mathcal{H}_\alpha(F)$ is given by the formula

$$\langle f, g\rangle_{\mathcal{H}_\alpha(F)} = \sum_{j=1}^{N} \bar{\alpha}_j \beta_j \kappa_j^{-2\alpha}.$$

The Hilbert space $\mathcal{H}_\alpha(F)$ has a natural orthonormal basis $(\kappa_j^\alpha \phi_j)$. Since

$$|F|^\gamma (\kappa_j^\alpha \phi_j) = \kappa_j^{\alpha+\gamma}\phi_j,$$

we obtain

Lemma 2.6.1. *For any $\alpha, \gamma \in \mathbb{R}$ the operator $|F|^\gamma \colon \mathcal{D} \to \mathcal{D}$ is unitary as an operator from $\mathcal{H}_\alpha(F)$ to $\mathcal{H}_{\alpha+\gamma}(F)$.*

It follows that all Hilbert spaces $\mathcal{H}_\alpha(F)$ are naturally isomorphic, the natural isomorphism being an appropriate power of $|F|$.

Plainly, $\mathcal{H}_0(F) = \mathcal{H}$. Let $\alpha, \beta \in \mathbb{R}$. If $\alpha < \beta$, then $\mathcal{H}_\beta(F) \subset \mathcal{H}_\alpha(F)$. The inclusion operator

$$i_{\alpha,\beta} \colon \mathcal{H}_\beta(F) \hookrightarrow \mathcal{H}_\alpha(F)$$

is compact with Schmidt representation

$$i_{\alpha,\beta} = \sum_{j=1}^{\infty} \kappa_j^{\beta-\alpha} \langle \kappa_j^\beta \phi_j, \cdot\rangle_{\mathcal{H}_\beta} \kappa_j^\alpha \phi_j.$$

It follows that the s-numbers of the inclusion operator i are $s_j(i) = \kappa_j^{\beta-\alpha}$. In particular, the inclusion operator

$$i_{\alpha,\alpha+1} \colon \mathcal{H}_{\alpha+1}(F) \hookrightarrow \mathcal{H}_\alpha(F)$$

is Hilbert–Schmidt with s-numbers $s_j = \kappa_j$.

Since we shall work in a fixed framed Hilbert space $(\mathcal{H}, F)$, the argument F of the Hilbert spaces $\mathcal{H}_\alpha(F)$ will often be omitted.

Proposition 2.6.2. *Let $\{A_\iota \in \mathcal{B}(\mathcal{H}) : \iota \in I\}$ be a net of bounded operators on a Hilbert space with frame F. The net of operators*

$$|F|A_\iota|F| \colon \mathcal{H} \to \mathcal{H}$$

converges in $\mathcal{B}(\mathcal{H})$ (respectively, in $\mathcal{L}_p(\mathcal{H})$) if and only if the net of operators

$$A_\iota \colon \mathcal{H}_1 \to \mathcal{H}_{-1}$$

converges in $\mathcal{B}(\mathcal{H}_1(F), \mathcal{H}_{-1}(F))$ (respectively, in $\mathcal{L}_p(\mathcal{H}_1, \mathcal{H}_{-1})$).

Elements of $\mathcal{H}_1$ are regular (smooth), while elements of $\mathcal{H}_{-1}$ are non-regular. In this sense, the frame operator F increases smoothness of vectors.

Remark. If $\alpha > 0$, then the triple $(\mathcal{H}_\alpha, \mathcal{H}, \mathcal{H}_{-\alpha})$ forms a rigged Hilbert space. So, a frame in a Hilbert space generates a natural rigging. At the same time, a frame evidently contains essentially more information than a rigging.

2.6.1. Diamond conjugate. Let $\alpha \in \mathbb{R}$. On the product $\mathcal{H}_\alpha \times \mathcal{H}_{-\alpha}$ there exists a unique bounded form $\langle \cdot, \cdot \rangle_{\alpha,-\alpha}$ such that for any $f, g \in \mathcal{H}_{|\alpha|}$,

$$\langle f, g \rangle_{\alpha,-\alpha} = \langle f, g \rangle.$$

Let $\mathcal{K}$ be a Hilbert space. For any bounded operator $A \colon \mathcal{H}_\alpha \to \mathcal{K}$, there exists a unique bounded operator $A^\diamondsuit \colon \mathcal{K} \to \mathcal{H}_{-\alpha}$ such that for any $f \in \mathcal{K}$ and $g \in \mathcal{H}_\alpha$,

$$\langle A^\diamondsuit f, g \rangle_{-\alpha,\alpha} = \langle f, Ag \rangle_{\mathcal{K}}.$$

In particular, if $A \colon \mathcal{H}_1 \to \mathcal{K}$ and $f, g \in \mathcal{H}_1$, then

$$\langle f, A^\diamondsuit Ag \rangle_{1,-1} = \langle Af, Ag \rangle_{\mathcal{K}}. \tag{2.9}$$

There is a connection between the diamond conjugate and the usual conjugate:

$$A^\diamondsuit = |F|^{-2\alpha} A^*$$

where $A^* \colon \mathcal{K} \to \mathcal{H}_\alpha$ and $|F|^{-2\alpha} \colon \mathcal{H}_\alpha \to \mathcal{H}_{-\alpha}$. It follows from Lemma 2.6.1 that if A belongs to $\mathcal{L}_p(\mathcal{H}_\alpha, \mathcal{K})$, then $A^\diamondsuit$ belongs to $\mathcal{L}_p(\mathcal{K}, \mathcal{H}_{-\alpha})$.

2.7. The trace-class matrix $\phi(\lambda + iy)$. In this and further sections we collect some objects associated with a frame in a Hilbert space and list their properties for future use.

Let H_0 be a self-adjoint operator on a framed Hilbert space $(\mathcal{H}, F)$. Let λ be a fixed point of $\Lambda(H_0; F)$. For any $y \geq 0$, we introduce the matrix

$$\phi(\lambda + iy) = \frac{1}{\pi}(\kappa_i \kappa_j \langle \phi_i, \operatorname{Im} R_{\lambda+iy}(H_0)\phi_j \rangle) \tag{2.10}$$

and consider it as an operator on ℓ_2.

We note several elementary properties of $\phi(\lambda + iy)$.

(i) For all $y \geq 0$, $\phi(\lambda + iy)$ is a non-negative trace-class operator on ℓ_2 and its trace is equal to the trace of $\frac{1}{\pi} F \operatorname{Im} R_{\lambda+iy}(H_0) F^*$. This follows from Theorem 1.9.1 and the fact that $\phi(\lambda + iy)$ is unitarily equivalent to $\frac{1}{\pi} F \operatorname{Im} R_{\lambda+iy}(H_0) F^*$.

(ii) For all $y > 0$, the kernel of $\phi(\lambda + iy)$ is trivial. This follows from the fact that the kernel of $F \operatorname{Im} R_{\lambda+iy}(H_0)F^*$ is trivial. Indeed, otherwise for some non-zero $f \in \mathcal{K}$, $F \operatorname{Im} R_{\lambda+iy}(H_0)F^* f = 0$, hence $\ker R_{\lambda+iy}(H_0) \ni F^* f \neq 0$, which is impossible.
(iii) The matrix $\phi(\lambda + iy)$ is a real-analytic function of the parameter $y > 0$ with values in $\mathcal{L}_1(\ell_2)$, and it is continuous in $\mathcal{L}_1(\ell_2)$ up to $y = 0$, as follows from Theorem 1.9.1.
(iv) We have $s_n(\phi(\lambda + iy)) \le y^{-1}\kappa_n^2$. This follows from the equality $s_n(A^*A) = s_n(AA^*)$ and the estimate (1.8).

2.8. The Hilbert–Schmidt matrix $\eta(\lambda + iy)$. Let $\lambda \in \Lambda(H_0; F)$. For any $y \ge 0$, we also introduce the matrix

$$\eta(\lambda + iy) = \sqrt{\phi(\lambda + iy)}. \tag{2.11}$$

We list elementary properties of $\eta(\lambda + iy)$.

(i) For all $y \ge 0$, $\eta(\lambda + iy)$ is a non-negative Hilbert–Schmidt operator on ℓ_2.
(ii) If $y > 0$, then the kernel of $\eta(\lambda + iy)$ is trivial.
(iii) The matrix $\eta(\lambda + iy)$ is a real-analytic function of the parameter $y > 0$ with values in $\mathcal{L}_2(\mathcal{H})$.
(iv) The matrix $\eta(\lambda + iy)$ is continuous in $\mathcal{L}_2(\mathcal{H})$ up to $y = 0$.
(v) We have the estimate $s_n(\eta(\lambda + iy)) \le y^{-1/2}\kappa_n$.

2.9. Eigenvalues $\alpha_j(\lambda + iy)$ of $\eta(\lambda + iy)$. Let $\lambda \in \Lambda(H_0; F)$. We denote by $\alpha_j(\lambda + iy)$ the jth eigenvalue of $\eta(\lambda + iy)$ (counting multiplicities).

We list elementary properties of $\alpha_j(\lambda + iy)$.

(i) For $y > 0$, all eigenvalues $\alpha_j(\lambda + iy)$ are strictly positive.
(ii) For $y \ge 0$, the sequence $(\alpha_j(\lambda + iy))$ belongs to ℓ_2.
(iii) The functions $(0, \infty) \ni y \mapsto \alpha_j(\lambda + iy)$ can be chosen to be real-analytic (after proper renumbering). This follows from Theorem 1.8.2 and item 2.8(iii).
(iv) All $\alpha_j(\lambda + iy)$ converge as $y \to 0$. This follows from Theorem 1.8.2 and 2.8(iv).

2.10. Zero and non-zero type indices. Let $\lambda \in \Lambda(H_0; F)$. While the eigenvalues $\alpha_j(\lambda + iy)$ of the matrix $\eta(\lambda + iy)$ are strictly positive for $y > 0$, the limit values $\alpha_j(\lambda)$ of some of them can be zero. We say that the eigenvalue function $\alpha_j(\lambda + iy)$ is of *non-zero type* if its limit is not zero. Otherwise we say that it is of *zero type*. We denote the set of non-zero type indices by $\mathcal{Z}_\lambda$.

Though it is not necessary, we agree to enumerate the functions $\alpha_j(\lambda + iy)$ in such a way that the sequence $\{\alpha_j(\lambda + i0)\}$ is decreasing.

2.11. Vectors $e_j(\lambda + iy)$. For any $\lambda \in \Lambda(H_0; F)$ we consider the sequence of normalized eigenvectors

$$e_j(\lambda + iy) \in \ell_2, \quad j = 1, 2, \ldots,$$

of the non-negative Hilbert–Schmidt matrix $\eta(\lambda + iy)$. These vectors are also eigenvectors of $\phi(\lambda + iy)$. We enumerate the functions $e_j(\lambda + iy)$ in such a way that

$$\eta(\lambda + iy)e_j(\lambda + iy) = \alpha_j(\lambda + iy)e_j(\lambda + iy), \quad y > 0, \tag{2.12}$$

where the enumeration of $\alpha_j(\lambda + iy)$ is as in Subsection 2.10.

We list elementary properties of $e_j(\lambda+iy)$'s.

(i) If $y>0$, then the sequence $e_j(\lambda+iy)\in\ell_2$, $j=1,2,\dots$, is an orthonormal basis of ℓ_2.

(ii) The functions $(0,\infty)\ni y\mapsto e_j(\lambda+iy)\in\ell_2$ can be chosen to be real-analytic. This follows from Theorem 1.8.2 and item 2.8(iii).

(iii) For indices j of non-zero type, the functions $[0,\infty)\ni y\mapsto e_j(\lambda+iy)\in\ell_2$ are continuous up to $y=0$. This follows from Theorem 1.8.2 and 2.8(iv).

(iv) We say that $e_j(\lambda+iy)$ is of (non-)zero type if the corresponding eigenvalue function $\alpha_j(\lambda+iy)$ is of (non-)zero type. Non-zero type vectors $e_j(\lambda+iy)$ have limit values $e_j(\lambda+i0)$, which form an orthonormal system in ℓ_2, in view of Theorem 1.8.2. Note that zero-type vectors $e_j(\lambda+iy)$ may not converge as $y\to 0$.

(v) For non-zero type indices j the vectors $e_j(\lambda+i0)$ are measurable.

2.12. Vectors $\eta_j(\lambda+iy)$. Let $\lambda\in\Lambda(H_0;F)$. We introduce the vector $\eta_j(\lambda+iy)$ as the jth column of the Hilbert–Schmidt matrix $\eta(\lambda+iy)$ (see (2.11)). This definition implies that

$$\langle\eta_j(\lambda+iy),\eta_k(\lambda+iy)\rangle=\phi_{jk}(\lambda+iy). \tag{2.13}$$

We list elementary properties of $\eta_j(\lambda+iy)$'s.

(i) For all $y\ge 0$, all vectors $\eta_j(\lambda+iy)$ belong to ℓ_2.

(ii) For all $y\ge 0$, the norms of the vectors $\eta_j(\lambda+iy)$ constitute a sequence which belongs to ℓ_2. This follows from the fact that $\eta(\lambda+iy)$ is a Hilbert–Schmidt operator for all $y\ge 0$.

(iii) If $y>0$, then the set of vectors $\{\eta_j(\lambda+iy)\}$ is complete in ℓ_2. Indeed, we have

$$e_j(\lambda+iy)=\alpha_j^{-1}(\lambda+iy)\sum_{k=1}^{\infty}e_{kj}(\lambda+iy)\eta_k(\lambda+iy),\qquad y\ge 0, \tag{2.14}$$

because (2.12) implies that

$$\begin{aligned}
e_j(\lambda+iy)&=\alpha_j^{-1}(\lambda+iy)\eta(\lambda+iy)e_j(\lambda+iy)\\
&=\alpha_j^{-1}\begin{pmatrix}\eta_{11}&\eta_{12}&\dots\\ \eta_{21}&\eta_{22}&\dots\\ \dots&\dots&\dots\end{pmatrix}\begin{pmatrix}e_{1j}\\ e_{2j}\\ \dots\end{pmatrix}=\alpha_j^{-1}\begin{pmatrix}\eta_{11}e_{1j}+\eta_{12}e_{2j}+\dots\\ \eta_{21}e_{1j}+\eta_{22}e_{2j}+\dots\\ \dots\end{pmatrix}\\
&=\alpha_j^{-1}(\lambda+iy)\sum_{k=1}^{\infty}e_{kj}(\lambda+iy)\eta_k(\lambda+iy),\qquad y\ge 0,
\end{aligned}$$

where, in the case of $y=0$, the equalities hold for indices j of non-zero type. Hence, the set of vectors $\{\eta_1(\lambda+iy),\eta_2(\lambda+iy),\dots\}$ is complete. Note also that the linear combination above is absolutely convergent, according to (ii).

(iv) Let $y>0$. If for some $\beta=(\beta_j)\in\ell_2$ the equality

$$\sum_{j=1}^{\infty}\beta_j\eta_j(\lambda+iy)=0$$

holds, then $(\beta_j) = 0$. Indeed, assume the contrary. We have

$$\eta(\lambda+iy)\beta = \begin{bmatrix} \beta_1\eta_{11}(\lambda+iy) + \beta_2\eta_{12}(\lambda+iy) + \cdots \\ \cdots \\ \beta_1\eta_{i1}(\lambda+iy) + \beta_2\eta_{i2}(\lambda+iy) + \cdots \\ \cdots \end{bmatrix}$$
$$= \beta_1\eta_1(\lambda+iy) + \beta_2\eta_2(\lambda+iy) + \cdots$$
$$= 0,$$

where the second equality makes sense, since the series $\sum_{j=1}^{\infty} \beta_j\eta_j(\lambda+iy)$ is absolutely convergent by 2.12(ii). It follows that β is an eigenvector of $\eta(\lambda+iy)$ corresponding to a zero eigenvalue. Since, by 2.8(ii), for $y > 0$ the matrix $\eta(\lambda+iy)$ does not have zero eigenvalues, we get a contradiction.

(v) The vectors $\eta_j(\lambda+iy)$ converge to $\eta_j(\lambda)$ in ℓ_2 as $y \to 0$. This follows from property 2.8(iv) of $\eta(\lambda+iy)$.

2.13. Unitary matrix $e(\lambda+iy)$. Let $\lambda \in \Lambda(H_0; F)$. We can form a matrix

$$e(\lambda+iy) = (e_{jk}(\lambda+iy)),$$

whose columns are $e_j(\lambda+iy)$, $j = 1, 2, \ldots$. Since the vectors $e_j(\lambda+iy)$, $j = 1, 2, \ldots$, form an orthonormal basis of ℓ_2, this matrix is unitary and it diagonalizes the matrix $\eta(\lambda+iy)$:

$$e(\lambda+iy)^*\eta(\lambda+iy)e(\lambda+iy) = \operatorname{diag}(\alpha_1(\lambda+iy), \alpha_2(\lambda+iy), \ldots),$$

where $(\alpha_j(\lambda+iy)) \in \ell_2$ are the eigenvalues of $\eta(\lambda+iy)$ (see Subsection 2.9).

2.14. Vectors $\phi_j(\lambda+iy)$. Let $\lambda \in \Lambda(H_0; F)$. Now we introduce vectors

$$\phi_j(\lambda+iy) = \kappa_j^{-1}\eta_j(\lambda+iy) \in \ell_2. \tag{2.15}$$

It may seem to be more consistent to denote by $\phi_j(\lambda+iy)$ the jth column of the matrix $\phi(\lambda+iy)$. But, firstly, we do not need columns of $\phi(\lambda+iy)$, secondly, there is an advantage of this notation. Namely, $\phi_j(\lambda)$ can be considered as the value of the vector $\phi_j \in \mathcal{H}$ at $\lambda \in \Lambda(H_0; F)$, as we shall see later (see Section 3).

Some properties of $\phi_j(\lambda+iy)$:

(i) All vectors $\phi_j(\lambda+iy)$ belong to ℓ_2. This follows from $\eta_j(\lambda+iy) \in \ell_2$ (see 2.12(i)).

(ii) If $y > 0$, then the set of vectors $\{\phi_j(\lambda+iy)\}$ is complete in ℓ_2. This follows from the similar property of $\{\eta_j(\lambda+iy)\}$ (see 2.12(iii)).

(iii) Let $y > 0$. If $(\kappa_j^{-1}\beta_j) \in \ell_2$ and

$$\sum_{j=1}^{\infty} \beta_j\phi_j(\lambda+iy) = 0,$$

then $(\beta_j) = 0$.

(iv) The following equality holds:

$$\langle \phi_j(\lambda+iy), \phi_k(\lambda+iy)\rangle = \frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+iy}(H_0)\phi_k\rangle. \tag{2.16}$$

This follows immediately from the definition of $\phi_j(\lambda+iy)$'s. Indeed, using (2.15), (2.13) and (2.10),

$$\langle \phi_j(\lambda+iy), \phi_k(\lambda+iy)\rangle = \kappa_j^{-1}\kappa_k^{-1}\langle \eta_j(\lambda+iy), \eta_k(\lambda+iy)\rangle$$
$$= \kappa_j^{-1}\kappa_k^{-1}\phi_{jk}(\lambda+iy) = \frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+iy}(H_0)\phi_k\rangle.$$

(v) It follows from (2.14) and (2.15) that each $e_j(\lambda+iy)$ can be written as a linear combination of $\phi_j(\lambda+iy)$'s with coefficients of the form $\kappa_j\beta_j$, where $(\beta_j)\in \ell_2$:

$$e_j(\lambda+iy) = \alpha_j^{-1}(\lambda+iy)\sum_{k=1}^{\infty}\kappa_k e_{kj}(\lambda+iy)\phi_k(\lambda+iy). \tag{2.17}$$

Moreover, this representation is unique, according to (iii).

(vi) For all $j=1,2,\ldots$, $\|\phi_j(\lambda+iy)\|_{\ell_2} \le (y\pi)^{-1/2}$.

(vii) $\phi_j(\lambda+iy)$ converges to $\phi_j(\lambda)$ in ℓ_2 as $y\to 0$ (recall that $\lambda\in\Lambda(H_0;F)$). This follows from 2.12(v).

(viii) We have

$$\langle \phi_j(\lambda), \phi_k(\lambda)\rangle_{\ell_2} = \frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\phi_k\rangle_{\mathcal{H}}.$$

Indeed, since for $\lambda\in\Lambda(H_0;F)$ the limit on the right hand side exists by 2.7(iii), this follows from (vii) and (iv).

2.15. The operator $\mathcal{E}_{\lambda+iy}$. Let $\lambda\in\Lambda(H_0;F)$. Let

$$\mathcal{E}_{\lambda+iy}\colon \mathcal{H}_1 \to \ell_2$$

be the linear operator defined on the frame vectors by the formula

$$\mathcal{E}_{\lambda+iy}\phi_j = \phi_j(\lambda+iy). \tag{2.18}$$

We list some properties of $\mathcal{E}_{\lambda+iy}$, which more or less immediately follow from the definition.

(i) For $y>0$,

$$\langle \mathcal{E}_{\lambda+iy}\phi_j, \mathcal{E}_{\lambda+iy}\phi_k\rangle_{\ell_2} = \frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+iy}(H_0)\phi_k\rangle_{\mathcal{H}}.$$

It follows that

$$\mathcal{E}^*_{\lambda+iy}\mathcal{E}_{\lambda+iy} = \frac{1}{\pi}\operatorname{Im} R_{\lambda+iy}(H_0). \tag{2.19}$$

(ii) Let $y>0$. The operator $\mathcal{E}_{\lambda+iy}$ is a Hilbert–Schmidt operator as an operator from $\mathcal{H}_1$ to ℓ_2. Moreover,

$$\|\mathcal{E}_{\lambda+iy}\|^2_{\mathcal{L}_2(\mathcal{H}_1,\ell_2)} = \frac{1}{\pi}\operatorname{Tr}_{\mathcal{K}}(F\operatorname{Im} R_{\lambda+iy}(H_0)F^*).$$

Indeed, evaluating the trace of $\mathcal{E}^*_{\lambda+iy}\mathcal{E}_{\lambda+iy}$ in the orthonormal basis $\{\kappa_j\phi_j\}$ of $\mathcal{H}_1$, we get, using (i) and (2.4),

$$\begin{aligned}\sum_{j=1}^{\infty}\langle \mathcal{E}_{\lambda+iy}^{*}\mathcal{E}_{\lambda+iy}\kappa_j\phi_j,\kappa_j\phi_j\rangle_{\mathcal{H}_1} &= \sum_{j=1}^{\infty}\kappa_j^2\langle \mathcal{E}_{\lambda+iy}\phi_j,\mathcal{E}_{\lambda+iy}\phi_j\rangle_{\ell_2} \\ &= \frac{1}{\pi}\sum_{j=1}^{\infty}\kappa_j^2\langle \phi_j,\operatorname{Im} R_{\lambda+iy}(H_0)\phi_j\rangle_{\mathcal{H}} && \text{by (i)} \\ &= \frac{1}{\pi}\sum_{j=1}^{\infty}\langle F^*\psi_j,\operatorname{Im} R_{\lambda+iy}(H_0)F^*\psi_j\rangle_{\mathcal{H}} && \text{by (2.4)} \\ &= \frac{1}{\pi}\operatorname{Tr}_{\mathcal{K}}(F\operatorname{Im} R_{\lambda+iy}(H_0)F^*). && \text{by (1.9).}\end{aligned}$$

(iii) The norm of $\mathcal{E}_{\lambda+iy}\colon \mathcal{H}_1 \to \ell_2$ is $\le \|\eta(\lambda+iy)\|_2$. Indeed, if $\beta = (\beta_j) \in \ell_2$, then $f := \sum_{j=1}^{\infty}\kappa_j\beta_j\phi_j \in \mathcal{H}_1$ with $\|f\|_{\mathcal{H}_1} = \|\beta\|$, and, using (2.18), (2.15) and the Schwarz inequality, one gets

$$\begin{aligned}\|\mathcal{E}_{\lambda+iy}f\| &= \Big\|\sum_{j=1}^{\infty}\kappa_j\beta_j\phi_j(\lambda+iy)\Big\| = \Big\|\sum_{j=1}^{\infty}\beta_j\eta_j(\lambda+iy)\Big\| \\ &\le \|\beta\|\cdot\Big(\sum_{j=1}^{\infty}\|\eta_j(\lambda+iy)\|^2\Big)^{1/2} = \|f\|_{\mathcal{H}_1}\cdot\|\eta(\lambda+iy)\|_2.\end{aligned}$$

(iv) For all $y > 0$, the operator $\mathcal{E}_{\lambda+iy}\colon \mathcal{H}_1 \to \ell_2$ has trivial kernel. Indeed, otherwise for some non-zero vector $f \in \mathcal{H}_1$,

$$0 = \langle \mathcal{E}_{\lambda+iy}f,\mathcal{E}_{\lambda+iy}f\rangle = \frac{1}{\pi}\langle f,\operatorname{Im} R_{\lambda+iy}(H_0)f\rangle.$$

Combining this equality with the formula

$$\operatorname{Im} R_{\lambda+iy}(H_0) = yR_{\lambda-iy}(H_0)R_{\lambda+iy}(H_0),$$

one infers that $R_{\lambda+iy}(H_0)$ has non-trivial kernel. But this is impossible.

(v) The operator $\mathcal{E}_{\lambda+iy}\colon \mathcal{H}_1 \to \ell_2$ as a function of $y > 0$ is real-analytic in $\mathcal{L}_2(\mathcal{H}_1,\ell_2)$.

(vi) The operator $\mathcal{E}_{\lambda+iy}\colon \mathcal{H}_1 \to \ell_2$ converges in the Hilbert–Schmidt norm to $\mathcal{E}_\lambda$ as $y \to 0$. Indeed, in the orthonormal basis $\{\kappa_j\phi_j\}$ of $\mathcal{H}_1$,

$$\begin{aligned}\|\mathcal{E}_{\lambda+iy}-\mathcal{E}_\lambda\|_{\mathcal{L}_2(\mathcal{H}_1)}^2 &= \sum_{j=1}^{\infty}\|(\mathcal{E}_{\lambda+iy}-\mathcal{E}_\lambda)(\kappa_j\phi_j)\|^2 && \text{by (1.11)} \\ &= \sum_{j=1}^{\infty}\|\kappa_j\phi_j(\lambda+iy)-\kappa_j\phi_j(\lambda)\|^2 && \text{by (2.18)} \\ &= \sum_{j=1}^{\infty}\|\eta_j(\lambda+iy)-\eta_j(\lambda)\|^2 && \text{by (2.15)} \\ &= \|\eta(\lambda+iy)-\eta(\lambda)\|_2^2 \to 0 && \text{by (1.11),}\end{aligned}$$

where the convergence holds by 2.8(iv).

(vii) It follows that the equality in (i) holds for $y = 0$ as well,

$$\langle \mathcal{E}_\lambda\phi_j,\mathcal{E}_\lambda\phi_k\rangle_{\ell_2} = \frac{1}{\pi}\langle \phi_j,\operatorname{Im} R_{\lambda+i0}(H_0)\phi_k\rangle_{\mathcal{H}}.$$

Moreover, the operator $\mathcal{E}_\lambda\colon \mathcal{H}_1 \to \ell_2$ is also Hilbert–Schmidt and

$$\|\mathcal{E}_\lambda\|^2_{\mathcal{L}_2(\mathcal{H}_1,\ell_2)} = \frac{1}{\pi}\operatorname{Tr}_{\mathcal{K}}(F \operatorname{Im} R_{\lambda+i0}(H_0)F^*).$$

2.16. Vectors $b_j(\lambda+iy) \in \mathcal{H}_1$. Let $y>0$ and $\lambda \in \Lambda(H_0;F)$. For each $j=1,2,\dots$ we introduce the vector $b_j(\lambda+iy) \in \mathcal{H}_1$ as a unique vector from the Hilbert space $\mathcal{H}_1$ with

$$\mathcal{E}_{\lambda+iy} b_j(\lambda+iy) = e_j(\lambda+iy). \tag{2.20}$$

Property 2.14(v) of $\phi_j(\lambda+iy) = \mathcal{E}_{\lambda+iy}\phi_j$ implies that the vector

$$b_j(\lambda+iy) = \alpha_j^{-1}(\lambda+iy)\sum_{k=1}^\infty \kappa_k e_{kj}(\lambda+iy)\phi_k \tag{2.21}$$

satisfies the above equation, where $e_{kj}(\lambda+iy)$ is the kth coordinate of $e_j(\lambda+iy)$. Property 2.14(iii) of $\phi_j(\lambda+iy)$ implies that the representation is unique.

The representation (2.21) shows that the functions $(0,\infty) \ni y \mapsto b_j(\lambda+iy) \in \mathcal{H}_1$ are continuous, since, by the Schwarz inequality and $\|e_j(\lambda+iy)\| = 1$, the series on the right hand side of (2.21) absolutely converges locally uniformly with respect to $y>0$.

We list some properties of the vectors $b_j(\lambda+iy)$.

(i) We have

$$\|b_j(\lambda+iy)\|_{\mathcal{H}} \le \alpha_j^{-1}(\lambda+iy)\|F\|_2, \qquad \|b_j(\lambda+iy)\|_{\mathcal{H}_1} = \alpha_j^{-1}(\lambda+iy).$$

(ii) The vectors $b_j(\lambda+iy)$, $j=1,2,\dots$, are linearly independent.

(iii) The system of vectors $\{b_j(\lambda+iy)\}$ is complete in $\mathcal{H}_1$ (and consequently in $\mathcal{H}$ as well). This follows from the equality

$$\phi_l = \kappa_l^{-1}\sum_{j=1}^\infty \bar e_{lj}(\lambda+iy)\alpha_j(\lambda+iy)b_j(\lambda+iy), \qquad l=1,2,\dots, \tag{2.22}$$

which follows from (2.21) and the unitarity of the matrix $(e_{jk}(\lambda+iy))$.

(iv) We have

$$\langle \mathcal{E}_{\lambda+iy} b_j(\lambda+iy), \mathcal{E}_{\lambda+iy} b_k(\lambda+iy)\rangle = \delta_{jk}. \tag{2.23}$$

(v) We have

$$\frac{y}{\pi}\langle R_{\lambda\pm iy}(H_0)b_j(\lambda+iy), R_{\lambda\pm iy}(H_0)b_k(\lambda+iy)\rangle = \delta_{jk}.$$

Indeed,

$$\begin{aligned}
&\frac{y}{\pi}\langle R_{\lambda+iy}(H_0)b_j(\lambda+iy), R_{\lambda+iy}(H_0)b_k(\lambda+iy)\rangle \\
&\qquad = \frac{y}{\pi}\langle b_j(\lambda+iy), R_{\lambda-iy}(H_0)R_{\lambda+iy}(H_0)b_k(\lambda+iy)\rangle \\
&\qquad = \langle b_j(\lambda+iy), \frac{1}{\pi}\operatorname{Im} R_{\lambda+iy}(H_0)b_k(\lambda+iy)\rangle \\
&\qquad = \langle b_j(\lambda+iy), \mathcal{E}^*_{\lambda+iy}\mathcal{E}_{\lambda+iy}b_k(\lambda+iy)\rangle \quad \text{by (2.19)} \\
&\qquad = \langle \mathcal{E}_{\lambda+iy}b_j(\lambda+iy), \mathcal{E}_{\lambda+iy}b_k(\lambda+iy)\rangle \\
&\qquad = \delta_{jk} \quad \text{by (2.23).}
\end{aligned}$$

(vi) The set of vectors $\sqrt{y/\pi}\{R_{\lambda+iy}(H_0)b_j(\lambda+iy)\}$ is an orthonormal basis in $\mathcal{H}$. By (v), it is enough to show that this set is complete. If for a non-zero vector g,

$$\langle R_{\lambda+iy}(H_0)b_j(\lambda+iy), g\rangle = 0 \quad \text{for all } j,$$

then

$$\langle b_j(\lambda+iy), R_{\lambda-iy}(H_0)g\rangle = 0 \quad \text{for all } j.$$

By (iii), one infers that $R_{\lambda-iy}(H_0)g = 0$. This is impossible, since $R_{\lambda-iy}(H_0)$ has trivial kernel.

(vii) The set $\sqrt{y/\pi}\{R_{\lambda\pm iy}(H_0)b_j(\lambda+iy)\}$ is an orthonormal basis of $\mathcal{H}$ for each choice of the sign $\pm$. This follows from the previous items.

(viii) If j is of non-zero type, then $b_j(\lambda+iy) \in \mathcal{H}_1$ converges in $\mathcal{H}_1$ to $b_j(\lambda+i0) \in \mathcal{H}_1$. This follows from the convergence of $e_j(\lambda+iy)$ in ℓ_2 (see 2.11(iii)) and (2.21).

3. The evaluation operator $\mathcal{E}_\lambda$

As mentioned before, a frame in a Hilbert space $\mathcal{H}$ on which a self-adjoint operator H_0 acts, allows one to define explicitly the fiber Hilbert space $\mathfrak{h}_\lambda$ of the direct integral of Hilbert spaces diagonalizing H_0, with the purpose of defining $f(\lambda)$ as an element of $\mathfrak{h}_\lambda$ for a dense set $\mathcal{H}_1$ of vectors and any λ from a fixed set $\Lambda(H_0;F)$ of full Lebesgue measure. In this section we give this construction.

3.1. Definition of $\mathcal{E}_\lambda$. Let H_0 be a self-adjoint operator on a fixed framed Hilbert space $(\mathcal{H}, F)$, where the frame F is given by (2.3). For $\lambda \in \Lambda(H_0;F)$ (see Definition 2.4.1), we have the Hilbert–Schmidt operator (see item 2.15(vi))

$$\mathcal{E}_\lambda \colon \mathcal{H}_1 \to \ell_2,$$

defined by the formula

$$\mathcal{E}_\lambda f = \sum_{j=1}^{\infty} \beta_j \eta_j(\lambda), \tag{3.1}$$

where $f = \sum_{j=1}^{\infty} \beta_j \kappa_j \phi_j \in \mathcal{H}_1$, $(\beta_j) \in \ell_2$ (see 2.12(v) for the definition of $\eta_j(\lambda)$). (Remark: the formula (3.1) is one of the most important definitions in this paper.) Since, by 2.12(ii), $(\|\eta_j(\lambda)\|) \in \ell_2$, the series above converges absolutely: by the Schwarz inequality

$$\sum_{j=1}^{\infty} \|\beta_j \eta_j(\lambda)\|_{\ell_2} \le \|\beta\|_{\ell_2} \Big(\sum_{j=1}^{\infty} \|\eta_j(\lambda)\|_{\ell_2}^2\Big)^{1/2} = \|\beta\|_{\ell_2} \|\eta(\lambda)\|_2.$$

The set $\mathcal{E}_\lambda \mathcal{H}_1$ is a pre-Hilbert space. We denote the closure of this set in ℓ_2 by $\mathfrak{h}_\lambda$:

$$\mathfrak{h}_\lambda := \overline{\mathcal{E}_\lambda \mathcal{H}_1}. \tag{3.2}$$

It is clear that the dimension function $\Lambda(H_0;F) \ni \lambda \mapsto \dim \mathfrak{h}_\lambda$ is Borel measurable, since, by definition,

$$\dim \mathfrak{h}_\lambda = \operatorname{rank}(\eta(\lambda)) \in \{0, 1, 2, \ldots, \infty\},$$

and it is clear that the matrix $\eta(\lambda)$ is Borel measurable. Since the matrix $\phi(\lambda)$ is self-adjoint, it is also clear that

$$\dim \mathfrak{h}_\lambda = \operatorname{rank}(\phi(\lambda)).$$

One can give one more formula for $\dim \mathfrak{h}_\lambda$:

$$\operatorname{Card}\{j : j \text{ is of non-zero type}\} = \dim \mathfrak{h}_\lambda.$$

LEMMA 3.1.1. *The system of vector-functions* $\{\phi_j(\lambda) : j = 1, 2, \ldots\}$ *satisfies the axioms of measurability base* (*Definition* 1.7.1) *for the family of Hilbert spaces* $\{\mathfrak{h}_\lambda\}_{\lambda \in \Lambda(H_0;F)}$, *given by* (3.2).

Proof. For any fixed $\lambda \in \Lambda(H_0; F)$, the vectors $\phi_1(\lambda), \phi_2(\lambda), \ldots$ generate $\mathfrak{h}_\lambda$ by definition. Measurability of the functions $\Lambda(H_0; F) \ni \lambda \mapsto \langle \phi_j(\lambda), \phi_k(\lambda)\rangle$ follows from 2.14(viii). So, both axioms of measurability base hold. ■

The field of Hilbert spaces

$$\{\mathfrak{h}_\lambda : \lambda \in \Lambda(H_0; F)\}$$

with measurability base

$$\lambda \mapsto \mathcal{E}_\lambda \phi_j = \phi_j(\lambda), \quad j = 1, 2, \ldots, \tag{3.3}$$

determines a direct integral of Hilbert spaces (see Subsection 1.7)

$$\mathcal{H} := \int^{\oplus}_{\Lambda(H_0;F)} \mathfrak{h}_\lambda \, d\lambda. \tag{3.4}$$

The vector $\phi_j(\lambda)$ is to be interpreted as the value of the vector ϕ_j at λ, as we shall see later. Note that though the vectors $\phi_j(\lambda) \in \mathfrak{h}_\lambda$, $j = 1, 2, \ldots$, depend on the sequence (κ_j) of weights of the frame F, their norms and scalar products

$$\|\phi_j(\lambda)\|_{\mathfrak{h}_\lambda}, \quad \langle \phi_j(\lambda), \phi_k(\lambda)\rangle$$

are independent of the weights, as follows directly from 2.14(viii). This also means that if two frames F_1 and F_2 have different weights, but the same frame vectors, and if λ belongs to both full sets $\Lambda(H_0; F_1)$ and $\Lambda(H_0; F_2)$, then the Hilbert spaces $\mathfrak{h}_\lambda(H_0, F_1)$ and $\mathfrak{h}_\lambda(H_0, F_2)$ are naturally isomorphic. The isomorphism is given by the correspondence

$$\phi_j^{(1)}(\lambda) \leftrightarrow \phi_j^{(2)}(\lambda), \quad j = 1, 2, \ldots,$$

where $\phi_j^{(k)}(\lambda)$, $k = 1, 2$, is the vector constructed using the frame F_k.

EXAMPLE 3.1.2. Let $\lambda \in [0, 2\pi)$. Let $\mathcal{H} = L_2(\mathbb{T}) \ominus \{\text{constants}\}$ and let

$$F = \sum_{j \in \mathbb{Z}^*} |j|^{-1} \langle \phi_j, \cdot \rangle \phi_j,$$

where $\phi_j = e^{-ij\lambda}$ and $\mathbb{Z}^* = \{\pm 1, \pm 2, \ldots\}$. Let H_0 be multiplication by λ on $[0, 2\pi) \equiv \mathbb{T}$. In this case

$$\phi(\lambda) = (|jk|^{-1} e^{i(j-k)\lambda})_{j,k \in \mathbb{Z}^*}$$

and $\Lambda(H_0; F) = \mathbb{R}$. For all $\lambda \in [0, 2\pi)$, this matrix has rank one, so that there is only one index of non-zero type and $\dim \mathfrak{h}_\lambda = 1$. This corresponds to the fact that H_0 has simple spectrum. Vectors f from $\mathcal{H}_1$ are absolutely continuous functions with L_2 derivative. The value of ϕ_j at λ should be interpreted as the jth column of $\eta(\lambda) = \sqrt{\phi(\lambda)}$ over $|j|$. For the only non-zero type index 1 we have

$$\alpha_1(0)^2 = 2\sum_{n=1}^{\infty} n^{-2}.$$

The matrix $\eta(\lambda)$ is usually difficult to calculate, but in this case it can be easily calculated. Since $\phi(\lambda)$ is one-dimensional, it follows that

$$\eta(\lambda) = \alpha_1^{-1}(0)\phi(\lambda).$$

So, in this case it is possible to write down an explicit formula for the evaluation operator $\mathcal{E}_\lambda$. If $f \in \mathcal{H}_1$, then the Fourier series of f is

$$f = \sum_{j\in\mathbb{Z}^*} |j|^{-1}\beta_j e^{-ij\lambda},$$

where $(\beta_j) \in \ell_2(\mathbb{Z}^*)$ and by (3.1),

$$\mathcal{E}_\lambda f = \eta(\lambda)\beta = \alpha_1(0)^{-1} \sum_{k\in\mathbb{Z}^*} |k|^{-1}\beta_k e^{-ik\lambda}(|j|^{-1}e^{ij\lambda})_{j\in\mathbb{Z}^*} = f(\lambda)\psi(\lambda),$$

where $\psi(\lambda) = \alpha_1(0)^{-1}(|j|^{-1}e^{ij\lambda})_{j\in\mathbb{Z}^*}$ is a normalized vector from $\ell_2(\mathbb{Z}^*)$. The one-dimensional Hilbert space $\mathfrak{h}_\lambda$ is spanned by $\psi(\lambda)$.

Lemma 3.1.3. *For any $j = 1, 2, \ldots$, the function $\mathcal{E}\phi_j$ belongs to $\mathcal{H}$ and $\|\mathcal{E}\phi_j\|_{\mathcal{H}} \le 1$.*

Proof. We only need to show that $\phi_j(\lambda) = \mathcal{E}_\lambda\phi_j$ is square summable and that the estimate holds. It follows from 2.14(viii) that

$$\langle \mathcal{E}\phi_j, \mathcal{E}\phi_j\rangle_{\mathcal{H}} = \int_{\Lambda(H_0;F)} \langle \phi_j(\lambda), \phi_j(\lambda)\rangle\, d\lambda = \frac{1}{\pi}\int_{\Lambda(H_0;F)} \langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\phi_j\rangle\, d\lambda =: (E).$$

Since $\frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+iy}(H_0)\phi_j\rangle$ is the Poisson integral of the function $\langle \phi_j, E_\lambda^{H_0}\phi_j\rangle$, it follows from Theorem 1.3.3 that

$$\frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\phi_j\rangle = \frac{d}{d\lambda}\langle \phi_j, E_\lambda^{H_0}\phi_j\rangle$$

for a.e. λ. Consequently,

$$(E) = \int_{\Lambda(H_0;F)} \frac{d}{d\lambda}\langle \phi_j, E_\lambda^{H_0}\phi_j\rangle\, d\lambda \le 1. \ \blacksquare$$

Corollary 3.1.4. *For any pair of indices j and k the function*

$$\Lambda(H_0;F) \ni \lambda \mapsto \langle \phi_j(\lambda), \phi_k(\lambda)\rangle_{\mathfrak{h}_\lambda}$$

is summable and its L_1-norm is ≤ 1.

Proof. This follows from the Schwarz inequality and Lemma 3.1.3. $\blacksquare$

A function $\Lambda(H_0;F) \ni \lambda \mapsto f(\lambda) \in \ell_2$ will be called $\mathcal{H}$-*measurable* if $f(\lambda) \in \mathfrak{h}_\lambda$ for a.e. $\lambda \in \Lambda(H_0;F)$, $f(\cdot)$ is measurable with respect to the measurability base (3.3) and $f \in \mathcal{H}$ (i.e. if f is square summable).

We can define a linear operator $\mathcal{E}\colon \mathcal{H}_1 \to \mathcal{H}$ with dense domain $\mathcal{D}$ by the formula

$$(\mathcal{E}\phi_j)(\lambda) = \phi_j(\lambda), \tag{3.5}$$

where $\mathcal{D}$ is defined by (2.7).

One can define a standard minimal core $\mathcal{A}(H_0, F)$ of the absolutely continuous spectrum of H_0, acting on a framed Hilbert space, by the formula

$$\mathcal{A}(H_0, F) = \bigcup_{i,j=1}^{\infty} \mathcal{A}(m_{ij}),$$

where $m_{ij}(\Delta) = \langle E_\Delta \phi_i, \phi_j \rangle$ is a (signed) spectral measure, and $\mathcal{A}(m)$ is a minimal support of the absolutely continuous part of m, defined by (1.5).

PROPOSITION 3.1.5. *The dimension of the fiber Hilbert space $\mathfrak{h}_\lambda$ is not zero if and only if $\lambda \in \mathcal{A}(H_0, F)$.*

Proof. ($\Leftarrow$). If $\lambda \in \mathcal{A}(H_0, F)$, then $\lambda \in \mathcal{A}(m_{ij})$ for some pair (i, j). This means that the limit $\operatorname{Im} \mathcal{C}_{m_{ij}}(\lambda + i0)$ exists and is not zero. This implies that $\phi(\lambda) = (\phi_{ij}(\lambda)) \neq 0$, as well as $\eta(\lambda) \neq 0$. So, the Hilbert space $\mathfrak{h}_\lambda$ is generated by at least one non-zero vector $\phi_j(\lambda)$.

($\Rightarrow$). If $\dim \mathfrak{h}_\lambda \neq 0$, then by definition (3.2) of $\mathfrak{h}_\lambda$ for some index j the vector $\phi_j(\lambda) = \kappa_j^{-1} \eta_j(\lambda)$ is non-zero. Hence, the matrix $\eta(\lambda)$ is non-zero. It follows that $\phi(\lambda)$ is non-zero. If $\phi_{ij}(\lambda) \neq 0$, then $\lambda \in \mathcal{A}(m_{ij})$. So, $\lambda \in \mathcal{A}(H_0, F)$. ∎

It follows from this proposition that the direct integral (3.4) can be rewritten as

$$\mathcal{H} = \int_{\mathcal{A}(H_0,F)}^{\oplus} \mathfrak{h}_\lambda \, d\lambda. \tag{3.6}$$

Hence, instead of the full set $\Lambda(H_0; F)$ one can use $\mathcal{A}(H_0, F)$. However, since $\Lambda(H_0; F)$ has full Lebesgue measure, it is more convenient to work with.

Recall that the vectors $e_j(\lambda), j = 1, 2, \ldots$, corresponding to non-zero type indices j are the limit values of the non-zero type eigenvectors $e_j(\lambda + iy), j = 1, 2, \ldots$, of $\eta(\lambda + iy) = \sqrt{\phi(\lambda + iy)}$.

LEMMA 3.1.6. *The system of ℓ_2-vectors $\{e_j(\lambda) : j$ is of non-zero type$\}$ is an orthonormal basis of $\mathfrak{h}_\lambda$.*

Proof. Firstly, by 2.11(iv), the system of vectors $\{e_j(\lambda) : j$ is of non-zero type$\}$ is orthonormal. In part (A) below it is shown that this system is a subset of $\mathfrak{h}_\lambda$; in part (B) it is shown that the system is complete in $\mathfrak{h}_\lambda$.

(A) By definition (3.2) of $\mathfrak{h}_\lambda$, it is generated by $\{\phi_1(\lambda), \phi_2(\lambda), \ldots\}$, or, which is the same, by $\{\eta_1(\lambda), \eta_2(\lambda), \ldots\}$. For a non-zero type index j, one can take the limit $y \to 0^+$ in (2.14) to get

$$e_j(\lambda) = \alpha_j(\lambda)^{-1} \sum_{k=0}^{\infty} e_{kj}(\lambda) \eta_k(\lambda).$$

It follows that $\{e_j(\lambda) : j$ is of non-zero type$\} \subset \mathfrak{h}_\lambda$.

(B) For any index i,

$$\eta_i(\lambda + iy) = \sum_{k=1}^{\infty} \alpha_k(\lambda + iy) e_{ik}(\lambda + iy) e_k(\lambda + iy). \tag{3.7}$$

Indeed, this equality is equivalent to

$$\langle \eta_i(\lambda + iy), e_j(\lambda + iy) \rangle = \alpha_j(\lambda + iy) e_{ij}(\lambda + iy).$$

This last equality follows from (2.12). Passing to the limit in (3.7), one gets

$$\eta_i(\lambda) = \sum_{k=1, k\in\mathcal{Z}_\lambda}^{\infty} \alpha_k(\lambda) e_{ik}(\lambda) e_k(\lambda).$$

It follows that the system $\{e_j(\lambda) : j \text{ is of non-zero type}\}$ is complete in $\mathfrak{h}_\lambda$. ∎

This lemma implies that $\{e_j(\lambda)\}$ is an orthonormal measurability base for the direct integral $\mathcal{H}$.

Let $P_\lambda \in \mathcal{B}(\ell_2)$ be the projection onto $\mathfrak{h}_\lambda$.

Lemma 3.1.7. *There exists a measurable operator-valued function* $\Lambda(H_0; F) \ni \lambda \mapsto \psi(\lambda) \in \mathcal{C}(\ell_2)$ *such that* $\psi(\lambda)$ *is a self-adjoint operator and*

$$\psi(\lambda)\phi(\lambda) = P_\lambda.$$

Proof. Since $\phi(\lambda)$ is a non-negative compact operator, this follows from the spectral theorem. We just set $\psi(\lambda) = 0$ on $\ker \phi(\lambda)$ and $\psi(\lambda) = \phi(\lambda)^{-1}$ on $\ker \phi(\lambda)^\perp$. ∎

Corollary 3.1.8. *The family of orthogonal projections* $P_\lambda \colon \ell_2 \to \mathfrak{h}_\lambda$ *is weakly measurable.*

Proof. This follows from Lemmas 2.4.4 and 3.1.7. ∎

Lemma 3.1.9. *A function* $f\colon \Lambda(H_0; F) \ni \lambda \mapsto f(\lambda) \in \mathfrak{h}_\lambda$ *is* $\mathcal{H}$*-measurable if and only if it is measurable as a function* $\Lambda(H_0; F) \to \ell_2$ *and is square summable.*

Proof. (If) Since the functions $\phi_j(\lambda)$ are measurable, if a function $f\colon \Lambda(H_0; F) \to \ell_2$ is measurable and $f(\lambda) \in \mathfrak{h}_\lambda$, then all the functions $\langle f(\lambda), \phi_j(\lambda)\rangle_{\mathfrak{h}_\lambda} = \langle f(\lambda), \phi_j(\lambda)\rangle_{\ell_2}$ are measurable. Hence, f is $\mathcal{H}$-measurable.

(Only if) Let $f(\lambda) \in \mathfrak{h}_\lambda$ be $\mathcal{H}$-measurable, i.e. for any j,

$$\langle \phi_j(\lambda), f(\lambda)\rangle$$

is measurable and $\|f(\lambda)\|_{\mathfrak{h}_\lambda} \in L_2(\Lambda, d\lambda)$. This implies that the vector

$$(\kappa_j \langle \phi_j(\lambda), f(\lambda)\rangle) = (\langle \eta_j(\lambda), f(\lambda)\rangle) = \eta(\lambda) f(\lambda)$$

is measurable. So, the function $\eta^2(\lambda) f(\lambda) = \phi(\lambda) f(\lambda)$ is also measurable. Since by Lemma 3.1.7 there exists a measurable function $\psi(\lambda)$ such that $\psi(\lambda)\phi(\lambda) = P_\lambda$, the function $f(\lambda)$ is also measurable. ∎

Proposition 3.1.10. *Let* $\chi_\Delta(\cdot)$ *be the characteristic function of* Δ. *The set of finite linear combinations of functions*

$$\Lambda(H_0; F) \ni \lambda \mapsto \chi_\Delta(\lambda)\phi_j(\lambda) \in \ell_2,$$

where Δ *is an arbitrary Borel subset of* Λ *and* $j = 1, 2, \ldots,$ *is dense in* $\mathcal{H}$.

Proof. This follows from Lemma 1.7.4. ∎

3.2. $\mathcal{E}$ is an isometry. Note that the system $\{\phi_j^{(a)}\}$ is complete in $\mathcal{H}^{(a)}$, though it is not, in general, linearly independent.

Proposition 3.2.1. *Let H_0 be a self-adjoint operator on a framed Hilbert space $(\mathcal{H}, F)$. The operator $\mathcal{E}\colon \mathcal{H}_1 \to \mathfrak{H}$, defined by (3.5), is bounded as an operator from $\mathcal{H}$ to $\mathfrak{H}$, so that one can define $\mathcal{E}$ on the whole $\mathcal{H}$ by continuity. The operator $\mathcal{E}\colon \mathcal{H} \to \mathfrak{H}$ thus defined vanishes on $\mathcal{H}^{(s)}$ and is isometric on $\mathcal{H}^{(a)}$.*

Proof. Firstly, we show that $\mathcal{E}$ is bounded. It follows from item 2.14(viii) that

$$\begin{aligned}\langle \mathcal{E}\phi_j, \mathcal{E}\phi_k\rangle_{\mathfrak{H}} &= \int_\Lambda \langle \mathcal{E}_\lambda\phi_j, \mathcal{E}_\lambda\phi_k\rangle_{\mathfrak{h}_\lambda}\, d\lambda = \int_\Lambda \langle \phi_j(\lambda), \phi_k(\lambda)\rangle_{\mathfrak{h}_\lambda}\, d\lambda \\ &= \frac{1}{\pi}\int_\Lambda \langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\, \phi_k\rangle\, d\lambda.\end{aligned}$$

Since by Theorem 1.3.3,

$$\frac{1}{\pi}\langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\phi_k\rangle = \frac{d}{d\lambda}\langle \phi_j, E_\lambda\phi_k\rangle \quad \text{for a.e. } \lambda \in \Lambda, \tag{3.8}$$

it follows that

$$\langle \mathcal{E}\phi_j, \mathcal{E}\phi_k\rangle_{\mathfrak{H}} = \int_\Lambda \frac{d\langle \phi_j, E_\lambda\phi_k\rangle}{d\lambda}\, d\lambda.$$

This implies that

$$\langle \mathcal{E}\phi_j, \mathcal{E}\phi_k\rangle_{\mathfrak{H}} = \int_\Lambda \frac{d\langle \phi_j, E_\lambda^{(a)}\phi_k\rangle}{d\lambda}\, d\lambda = \langle \phi_j, E_\Lambda^{(a)}\phi_k\rangle = \langle \phi_j^{(a)}, \phi_k^{(a)}\rangle. \tag{3.9}$$

This equality implies that for any $f \in \mathcal{D}$ (see (2.7) for the definition of $\mathcal{D}$) $\|\mathcal{E}f\| = \|f^{(a)}\| \le \|f\|$, and so $\mathcal{E}$ is bounded. Since also $\|\mathcal{E}f\| = \|P^{(a)}f\|$ for all f from the dense set $\mathcal{D}$, it follows that $\|\mathcal{E}f\| = \|P^{(a)}f\|$ for any $f \in \mathcal{H}$. This implies that $\mathcal{E}$ vanishes on $\mathcal{H}^{(s)}$ and it is an isometry on $\mathcal{H}^{(a)}$. ■

This proposition implies that for any $f \in \mathcal{H}$ we have a vector-function $f(\lambda) = \mathcal{E}_\lambda(f)$ as an element of the direct integral (3.4). The function $f(\lambda)$ is defined for a.e. $\lambda \in \Lambda$, while for regular vectors $f \in \mathcal{H}_1$, $f(\lambda)$ is defined for all $\lambda \in \Lambda(H_0; F)$.

Lemma 3.2.2. *For any $f, g \in \mathcal{H}^{(a)}$,*

$$\langle f, g\rangle = \int_\Lambda \langle f(\lambda), g(\lambda)\rangle\, d\lambda.$$

Proof. Indeed, the right hand side of this equality is, by definition, $\langle \mathcal{E}f, \mathcal{E}g\rangle_{\mathfrak{H}}$, which by (3.9) is equal to $\langle f, g\rangle_{\mathcal{H}}$. ■

3.3. $\mathcal{E}$ is unitary. The aim of this subsection is to show that the restriction of the operator $\mathcal{E}\colon \mathcal{H} \to \mathfrak{H}$ to $\mathcal{H}^{(a)}$ is unitary.

Lemma 3.3.1. *Let Δ be a Borel subset of $\Lambda = \Lambda(H_0; F)$. If $f \in E_{\Lambda\setminus\Delta}\mathcal{H}$, then $f(\lambda)$ is zero on Δ for a.e. $\lambda \in \Delta$.*

Proof. (A) If $g = \sum_{j=1}^N \alpha_j\phi_j \in \mathcal{D}$ (see (2.7)), then

$$\|E_\Delta g\|^2 = \int_\Delta \langle g(\lambda), g(\lambda)\rangle\, d\lambda.$$

Indeed,

$$\begin{aligned}\int_\Delta \langle g(\lambda), g(\lambda)\rangle\, d\lambda &= \sum_{j=1}^N \sum_{k=1}^N \bar{\alpha}_j \alpha_k \int_\Delta \langle \phi_j(\lambda), \phi_k(\lambda)\rangle\, d\lambda \\ &= \sum_{j=1}^N \sum_{k=1}^N \bar{\alpha}_j \alpha_k \int_\Delta \frac{d}{d\lambda} \langle \phi_j, E_\lambda \phi_k\rangle\, d\lambda \\ &= \sum_{j=1}^N \sum_{k=1}^N \bar{\alpha}_j \alpha_k \int_\Delta \frac{d}{d\lambda} \langle \phi_j, E_\lambda^{(a)} \phi_k\rangle\, d\lambda \\ &= \sum_{j=1}^N \sum_{k=1}^N \bar{\alpha}_j \alpha_k \langle \phi_j, E_\Delta^{(a)} \phi_k\rangle = \|E_\Delta^{(a)} g\|^2,\end{aligned}$$

where the second equality follows from Theorem 1.3.4 and the third follows from Corollary 1.3.7.

Since $\Delta \subset \Lambda(H_0; F)$, Corollary 2.5.3 implies that $E_\Delta^{(a)} = E_\Delta$ so $\|E_\Delta^{(a)} g\|^2 = \|E_\Delta g\|^2$.

(B) To prove the lemma, note that $f \in E_{\Lambda\setminus\Delta}\mathcal{H}$ implies that f is an absolutely continuous vector for H_0. Consequently, there exists a sequence $f_1, f_2, \dots$ of vectors from $P^{(a)}\mathcal{D}$ converging to f (in $\mathcal{H}$). Then by Lemma 3.2.2,

$$\int_{\Lambda(H_0;F)} \langle f(\lambda) - f_n(\lambda), f(\lambda) - f_n(\lambda)\rangle\, d\lambda = \|f - f_n\|^2 \to 0.$$

Since by (A),

$$\int_\Delta \langle f_n(\lambda), f_n(\lambda)\rangle\, d\lambda = \|E_\Delta f_n\|^2 = \|E_\Delta (f - f_n)\|^2 \le \|f - f_n\|^2 \to 0,$$

it follows that $\int_\Delta \langle f(\lambda), f(\lambda)\rangle\, d\lambda = 0$. So, $f(\lambda) = 0$ for a.e. $\lambda \in \Delta$. ■

COROLLARY 3.3.2. *Let Δ be a Borel subset of $\Lambda(H_0; F)$ and let $f, g \in \mathcal{H}$. If $E_\Delta f = E_\Delta g$, then $f(\lambda) = g(\lambda)$ for a.e. $\lambda \in \Delta$.*

COROLLARY 3.3.3. *For any Borel subset Δ of $\Lambda(H_0; F)$ and any $f \in \mathcal{H}$,*

$$\mathcal{E}(E_\Delta f)(\lambda) = \chi_\Delta(\lambda) f(\lambda), \qquad \text{a.e. } \lambda \in \mathbb{R}.$$

COROLLARY 3.3.4. *Let Δ be a Borel subset of $\Lambda(H_0; F)$. For any $f, g \in \mathcal{H}$,*

$$\langle E_\Delta f, E_\Delta g\rangle = \int_\Delta \langle f(\lambda), g(\lambda)\rangle\, d\lambda.$$

PROPOSITION 3.3.5. *The map $\mathcal{E}\colon \mathcal{H}^{(a)} \to \mathcal{H}$ is unitary.*

Proof. It has already been proven (Proposition 3.2.1) that $\mathcal{E}$ is an isometry with initial space $\mathcal{H}^{(a)}$. So, it is enough to show that the range of $\mathcal{E}$ coincides with $\mathcal{H}$. Corollary 3.3.3 implies that the range of $\mathcal{E}$ contains all functions of the form $\chi_\Delta(\cdot)\phi_j(\cdot)$, where Δ is an arbitrary Borel subset of $\Lambda(H_0; F)$ and $j = 1, 2, \dots$. Consequently, Proposition 3.1.10 completes the proof. ■

3.4. Diagonality of H_0 in $\mathcal{H}$. The aim of this subsection is to prove Theorem 3.4.2, which asserts that the direct integral $\mathfrak{H}$ is a spectral representation of $\mathcal{H}$ for the operator $H_0^{(a)}$.

Using the standard step-function approximation argument, Corollary 3.3.3 implies

THEOREM 3.4.1. *For any bounded Borel function h on $\Lambda(H_0; F)$ and any $f \in \mathcal{H}$,*

$$\mathcal{E}_\lambda(h(H_0)f) = h(\lambda)\mathcal{E}_\lambda f \quad \textit{for a.e. } \lambda \in \Lambda.$$

This theorem implies the following result.

THEOREM 3.4.2. *$H_0^{(a)}$ is naturally isomorphic to the operator of multiplication by λ on $\mathfrak{H}$ via the unitary mapping $\mathcal{E} \colon \mathcal{H}^{(a)} \to \mathfrak{H}$:*

$$\mathcal{E}_\lambda(H_0 f) = \lambda \mathcal{E}_\lambda f \quad \textit{for a.e. } \lambda \in \mathbb{R}.$$

Nonetheless, we give another proof of this theorem.

LEMMA 3.4.3 ([Y, (1.3.12)]). *Let H be a self-adjoint operator on Hilbert space $\mathcal{H}$, and let $f, g \in \mathcal{H}$. Then for a.e. $\lambda \in \mathbb{R}$,*

$$\lambda \frac{d}{d\lambda}\langle f, E_\lambda g\rangle = \frac{d}{d\lambda}\langle H_0 f, E_\lambda g\rangle.$$

Proof of Theorem 3.4.2. It is enough to show that for any $f \in E_\Delta \mathcal{H}$, and for a.e. $\lambda \in \Delta$ the equality $\mathcal{E}_\lambda(H_0 f) = \lambda f(\lambda)$ holds, where Δ is any bounded Borel subset of Λ.

This is equivalent to the statement: for any $g \in E_\Delta \mathcal{H}$,

$$\int_\Delta \langle \mathcal{E}_\lambda(H_0 f), g(\lambda)\rangle \, d\lambda = \int_\Delta \lambda \langle f(\lambda), g(\lambda)\rangle \, d\lambda.$$

By continuity of $H_0 E_\Delta^{H_0}$ and of the multiplicator $\lambda \chi_\Delta(\lambda)$, it is enough to consider the case of $f = E_\Delta \phi_j \in \mathcal{H}^{(a)}$ and $g = E_\Delta \phi_k \in \mathcal{H}^{(a)}$. Then, by (3.8) and Corollary 3.3.2, the right hand side of the previous formula is

$$\int_\Delta \lambda \frac{d}{d\lambda}\langle \phi_j, E_\lambda \phi_k\rangle \, d\lambda = \int_\Delta \frac{d}{d\lambda}\langle H_0\phi_j, E_\lambda \phi_k\rangle \, d\lambda = \langle H_0 \phi_j, E_\Delta \phi_k\rangle,$$

where Lemma 3.4.3 has been used. Now, Corollary 3.3.4 completes the proof. ∎

A complete set of unitary invariants of the absolutely continuous part $H_0^{(a)}$ of the operator H_0 is given by the sequence $(\Lambda_0, \Lambda_1, \Lambda_2, \ldots)$, where

$$\Lambda_n = \{\lambda \in \Lambda(H_0; F) : \dim \mathfrak{h}_\lambda = n\}.$$

One of the versions of the spectral theorem says that there exists a direct integral representation

$$\mathcal{H}^{(a)} \cong \int_{\hat\sigma}^{\oplus} \mathfrak{h}_\lambda \, \rho(d\lambda)$$

of the Hilbert space $\mathcal{H}^{(a)}$, which diagonalizes $H_0^{(a)}$, where $\hat\sigma$ is a core of the spectrum of H_0, and ρ is a measure from the spectral type of H_0. Actually, instead of changing the measure ρ in its spectral type, it is possible to change (renormalize) the scalar product of the fiber Hilbert spaces $\mathfrak{h}_\lambda$. In the construction of the direct integral, given in this section, a frame in $\mathcal{H}$ in particular fixes a renormalization of scalar products in fiber Hilbert spaces.

The operator $\mathcal{E}_\lambda$ is the evaluation operator which answers the question (2.1). As we have seen, for any vector $f \in \mathcal{H}_1$ and any point λ of the set $\Lambda(H_0; F)$ of full Lebesgue measure, one can define the value of the vector f at λ by the formula

$$f(\lambda) = \mathcal{E}_\lambda f.$$

Vectors f which belong to $\mathcal{H}_1$ can be defined at every point of the set $\Lambda(H_0; F)$, since they are regular; or, rather, vectors of $\mathcal{H}_1$ should be considered regular, since they can be defined at every point of $\Lambda(H_0; F)$. If a vector f is not regular, that is, if $f \notin \mathcal{H}_1$, then one can define its value only at almost every point of $\Lambda(H_0; F)$. Results of this section fully justify this interpretation of the operator $\mathcal{E}_\lambda$.

Remark. Recall that a vector f is called cyclic for a self-adjoint operator H_0 if the vectors $H_0^k f$, $k = 0, 1, 2, \ldots$, generate the whole Hilbert space $\mathcal{H}$. The construction of the direct integral obviously implies that if H_0 has a cyclic vector then $\dim \mathfrak{h}_\lambda \le 1$ for all $\lambda \in \Lambda(H_0; F)$.

Remark. Clearly, the family $\Omega_1 := \{e_j(\lambda)\}$ is a measurability base and it generates the same set of measurable vector-functions as the measurability base $\Omega_0 := \{\phi_j(\lambda)\}$; that is, $\hat{\Omega}_0 = \hat{\Omega}_1$. The family Ω_1 is an orthonormal measurability base.

4. The resonance set $R(\lambda; \{H_r\}, F)$

In the previous section we have defined the evaluation operator $\mathcal{E}_\lambda$. The evaluation operator is defined on the set $\Lambda(H_0; F)$. Clearly, the complement of $\Lambda(H_0; F)$ consists of points where the operator H_0 behaves in some sense badly. Indeed, by Corollary 2.5.3 the set $\mathbb{R} \setminus \Lambda(H_0; F)$ is a core of the singular spectrum of H_0. So, one of the reasons why a vector $f \in \mathcal{H}$ cannot be defined at some point $\lambda \in \mathbb{R}$ is that λ can be an eigenvalue of H_0. Since eventually the operator H_0 is going to be perturbed, one needs to investigate what happens to the set $\Lambda(H_0; F)$ when H_0 is perturbed. In this section we consider this set of questions.

Many results of this section are generally well-known (for rank-one perturbations); cf. e.g. [Ar, Ag, SW, S$_3$]. I do not claim any originality as regards them.

4.1. Resonance points of a path of operators. So far we have considered a single fixed self-adjoint operator H_0 on a Hilbert space $\mathcal{H}$ with a frame F. Now we are going to perturb H_0 by self-adjoint trace-class operators.

We say that an operator-function $\mathbb{R} \ni r \mapsto A(r)$ is piecewise analytic in an appropriate norm if there is a finite or infinite increasing sequence of numbers r_j, $j \in \mathbb{Z}$, with no finite accumulation points, such that the restriction of $A(r)$ to any interval (r_{j-1}, r_j) has analytic continuation in the norm to a neighbourhood of the closure of that interval. We do not assume continuity of a piecewise analytic path, unless otherwise specified.

Given a frame $F \in \mathcal{L}_2(\mathcal{H}, \mathcal{K})$ in a Hilbert space $\mathcal{H}$, we introduce a vector space $\mathcal{A}(F)$ of trace-class operators by

$$\mathcal{A}(F) = \{FJF^* : J \in \mathcal{B}(\mathcal{K})\}. \tag{4.1}$$

For an operator $FJF^* \in \mathcal{A}(F)$ we define its norm by

$$\|FJF^*\|_{\mathcal{A}(F)} = \|J\|.$$

Obviously, the vector space $\mathcal{A}(F)$ with such a norm is a Banach space.

ASSUMPTION 4.1.1. *Let $F\colon \mathcal{H} \to \mathcal{K}$ be a frame operator in a Hilbert space $\mathcal{H}$. We assume that the path*

$$\mathbb{R} \ni r \mapsto H_r$$

of self-adjoint operators in $\mathcal{H}$ satisfies the following conditions:

(i) $H_r = H_0 + V_r$,
(ii) $V_r = F^* J_r F$, *where J_r is a bounded self-adjoint operator on the Hilbert space $\mathcal{K}$,*
(iii) *the path $\mathbb{R} \ni r \mapsto J_r \in \mathcal{B}(\mathcal{K})$ is continuous and piecewise real-analytic.*

In other words, $H_r \in H_0 + \mathcal{A}(F)$ and the path $\{H_r\}$ is $\mathcal{A}(F)$-analytic.

Clearly, $V_0 = 0$. Obviously, the path $\{V_r\}$ is continuous and piecewise real-analytic with values in $\mathcal{L}_1(\mathcal{K})$, so that the trace-class derivative

$$\dot{V}_r = F^* \dot{J}_r F$$

exists and is trace-class. Since the derivative $\dot{V}_r$ belongs to $\mathcal{A}(F)$, it can be considered as an operator $\mathcal{H}_{-1} \to \mathcal{H}_1$. Clearly,

$$\dot{V}_r\colon \mathcal{H}_{-1} \to \mathcal{H}_1 \text{ is a bounded operator.} \tag{4.2}$$

Assumption 4.1.1 is not too restrictive, as the following lemma shows.

LEMMA 4.1.2. *Let H be a self-adjoint operator in $\mathcal{H}$ and let V be a self-adjoint trace-class operator in $\mathcal{H}$. There exists a frame $F \in \mathcal{L}_2(\mathcal{H}, \mathcal{K})$ and a path $\{H_r\}$ which satisfies Assumption 4.1.1 such that $H_0 = H$ and $H_1 = H + V$.*

Proof. Let $H_r = H + rV$ and $\mathcal{K} = \mathcal{H}$. If V has trivial kernel, then one can take $F = \sqrt{|V|}$, so that $V = F^* \operatorname{sign}(V) F$. If V has non-trivial kernel, then one can take $F = \sqrt{|V|} + I \cdot \tilde{F}$, where I is the projection onto $\ker(V)$ and $\tilde{F}$ is a self-adjoint Hilbert–Schmidt operator on the Hilbert space $I\mathcal{H}$. ∎

Let

$$T_z(H_r) = F R_z(H_r) F^*.$$

LEMMA 4.1.3. *If operators $A_\alpha, A \in \mathcal{B}(\mathcal{H})$ are invertible and $A_\alpha \to A$ uniformly, then $A_\alpha^{-1} \to A^{-1}$ uniformly.*

The following lemma and its proof are well-known (cf. e.g. [Ag, Theorem 4.2], [Y, Lemma 4.7.8]). They are given for completeness.

LEMMA 4.1.4. *The operator $1 + J_r T_z(H_0)$ is invertible for all $r \in \mathbb{R}$ and all $z \in \mathbb{C} \setminus \mathbb{R}$.*

Proof. The second resolvent identity implies that (Aronszajn's equation [Ar], cf. also [SW, S_3])

$$T_z(H_r)(1 + J_r T_z(H_0)) = T_z(H_0). \tag{4.3}$$

Since $T_z(H_0)$ is compact, if $1+J_rT_z(H_0)$ is not invertible, then there exists a non-zero $\psi \in \mathcal{K}$ such that

$$(1 + J_rT_z(H_0))\psi = 0. \tag{4.4}$$

Combining this equality with (4.3) gives $T_z(H_0)\psi = 0$, so (4.4) gives $\psi = 0$. This contradiction shows that $1 + J_rT_z(H_0)$ is invertible. ■

While the operator $1+J_rT_z(H_0)$ is invertible for all non-real values of z, the operator $1 + J_rT_{\lambda+i0}(H_0)$ may not be invertible at some points. The set of points where $1 + J_rT_{\lambda+i0}(H_0)$ is not invertible is of special importance.

Proposition 4.1.5. *Let $\{H_r : r \in [a,b]\}$ be a path of self-adjoint operators on $\mathcal{H}$ with frame F, which satisfies Assumption* 4.1.1. *Let $\lambda \in \Lambda(H_0; F)$. For any $s \in [a,b]$ the following assertions are equivalent:*

($1_\pm$) *the operator $1 + J_sT_{\lambda\pm i0}(H_0)$ is not invertible;*
($2_\pm$) *the operator $1 + T_{\lambda\pm i0}(H_0)J_s$ is not invertible;*
($3_\pm$) *the operator $1 + V_sR_{\lambda\pm i0}(H_0)$ is not invertible in $\mathcal{H}_1$;*
($4_\pm$) *the operator $1 + R_{\lambda\pm i0}(H_0)V_s$ is not invertible in $\mathcal{H}_{-1}$.*

Proof. The condition ($1_\pm$) is equivalent to ($2_\pm$) by (1.6). The condition ($1_\pm$) is equivalent to ($2_\mp$) since a bounded operator T is invertible if and only if T^* is invertible. Equivalence of ($1_\pm$) and ($3_\pm$) and equivalence of ($2_\pm$) and ($4_\pm$) follow from the fact that F^* is an isomorphism of $\mathcal{K}$ and $\mathcal{H}_1$ and F is an isomorphism of $\mathcal{H}_{-1}$ and $\mathcal{K}$. ■

Definition 4.1.6. We denote by

$$R(\lambda; \{H_r\}, F) \tag{4.5}$$

the set of all those real numbers s for which any (and hence all) of the conditions of Proposition 4.1.5 holds. We call this set the *resonance set* at λ.

Lemma 4.1.7. *The set $R(\lambda; \{H_r\}, F)$ is discrete, i.e. it has no finite accumulation points.*

Proof. Since V_r is a piecewise analytic function, this follows directly from the analytic Fredholm alternative (Theorem 1.8.3). ■

Lemma 4.1.8. *Let $\lambda \in \mathbb{R}$ be such that the limit $T_{\lambda+i0}(H_0)$ exists in the norm topology. Then the limit $T_{\lambda+i0}(H_r)$ exists in the norm topology if and only if $r \notin R(\lambda; \{H_r\}, F)$.*

Proof. (Only if) Assume that $T_{\lambda+i0}(H_r)$ exists. Taking the norm limit $y = \operatorname{Im} z \to 0$ in (4.3), one gets

$$T_{\lambda+i0}(H_r)(1 + J_rT_{\lambda+i0}(H_0)) = T_{\lambda+i0}(H_0). \tag{4.6}$$

Since $T_{\lambda+i0}(H_0)$ is compact, $1 + J_rT_{\lambda+i0}(H_0)$ is not invertible if and only if there exists a non-zero $\psi \in \mathcal{H}$ such that $(1 + J_rT_{\lambda+i0}(H_0))\psi = 0$. This and (4.6) imply that $T_{\lambda+i0}(H_0)\psi = 0$. Hence $\psi = 0$. This contradiction shows that $1 + J_rT_{\lambda+i0}(H_0)$ is invertible.

(If) By (4.3) and Lemma 4.1.4,

$$T_{\lambda+iy}(H_r) = T_{\lambda+iy}(H_0)[1 + J_rT_{\lambda+iy}(H_0)]^{-1}. \tag{4.7}$$

If $1 + J_r T_{\lambda+i0}(H_0)$ is invertible, then by Lemma 4.1.3 the limit of the right hand side as $y \to 0^+$ exists in the norm topology. ∎

THEOREM 4.1.9. *Let $\{H_r\}$ be a path of self-adjoint operators on $\mathcal{H}$ with frame F, which satisfies Assumption* 4.1.1. *Let $\lambda \in \Lambda(H_0; F)$. For all $r \notin R(\lambda; \{H_r\}, F)$ we have $\lambda \in \Lambda(H_r; F)$, where $R(\lambda; \{H_r\}, F)$ is the discrete subset of $\mathbb{R}$ defined in* (4.5).

Proof. (A) Since $\lambda \in \Lambda(H_0; F)$, the limit $T_{\lambda+i0}(H_0)$ exists in the norm topology. It follows from Lemma 4.1.8 that the norm limit of

$$T_{\lambda+iy}(H_r) = F R_{\lambda+iy}(H_r) F^*$$

also exists.

Now, in order to prove that $\lambda \in \Lambda(H_r; F)$, we need to show that the limit of $F \operatorname{Im} R_{\lambda+iy}(H_r) F^*$ exists in $\mathcal{L}_1$-norm.

(B) We have

$$\operatorname{Im} T_z(H_r) = (1 + T_{\bar{z}}(H_0) J_r)^{-1} \operatorname{Im} T_z(H_0)(1 + J_r T_z(H_0))^{-1} \tag{4.8}$$

by (4.7).

(C) Since $r \notin R(\lambda; \{H_r\}, F)$, it follows from Lemmas 4.1.3 and 4.1.4 that

$$(1 + T_{\bar{z}}(H_0) J_r)^{-1} \quad \text{and} \quad (1 + J_r T_z(H_0))^{-1}$$

converge in $\|\cdot\|$ as $y = \operatorname{Im} z \to 0^+$. Since, by the definition of $\Lambda(H_0; F)$, $\operatorname{Im} T_z(H_0)$ converges to $\operatorname{Im} T_{\lambda+i0}(H_0)$ in $\mathcal{L}_1(\mathcal{K})$, it follows from (4.8) that $\operatorname{Im} T_z(H_r)$ also converges in $\mathcal{L}_1(\mathcal{K})$ as $\operatorname{Im} z \to 0^+$. Hence, $\lambda \in \Lambda(H_r; F)$.

That $R(\lambda; \{H_r\}, F)$ is a discrete subset of $\mathbb{R}$ follows from Lemma 4.1.7. ∎

Theorem 4.1.9 shows that the resonance subset of the plane (λ, r) behaves differently with respect to the spectral parameter λ and with respect to the coupling constant r. While for a fixed r the resonance set is a more or less arbitrary null set, and, consequently, can be very bad, for a fixed λ the resonance set is a discrete subset of $\mathbb{R}$.

The discreteness of $R(\lambda; \{H_r\}, F)$ for a.e. λ is used in an essential way in Subsection 7.3.

PROPOSITION 4.1.10. *If $\lambda \in \Lambda(H_0; F)$ is an eigenvalue of H_r, then $r \in R(\lambda; \{H_r\}, F)$.*

Proof. Since, by Corollary 2.5.3, the complement of $\Lambda(H_r; F)$ is a support of the singular spectrum of H_r, which includes all eigenvalues of H_r, it follows that if $\lambda \in \Lambda(H_0; F)$ is an eigenvalue of H_r, then $\lambda \notin \Lambda(H_r; F)$, so that by Theorem 4.1.9, $r \in R(\lambda; \{H_r\}, F)$. ∎

This proposition partly explains why elements of $R(\lambda; \{H_r\}, F)$ are called resonance points. Note that the inclusion $r \in R(\lambda; \{H_r\}, F)$ does not necessarily imply that λ is an eigenvalue of H_r.

THEOREM 4.1.11. *Let $\lambda \in \Lambda(H_0; F)$. Then $\lambda \notin \Lambda(H_r; F)$ if and only if $r \in R(\lambda; \{H_r\}, F)$.*

Proof. The "only if" part has been established in Theorem 4.1.9. The "if" part says that $\lambda \in \Lambda(H_r; F)$ implies $r \notin R(\lambda; \{H_r\}, F)$. This follows from Lemma 4.1.8. ∎

REMARK. As can be seen from the proofs, existence of $T_{\lambda+i0}(H_0)$ in $\mathcal{L}_\infty(\mathcal{K})$ or existence of $\operatorname{Im} T_{\lambda+i0}(H_0)$ in $\mathcal{L}_1(\mathcal{K})$ is not essential for the above theorem. In the definition of

$\Lambda(H_0; F)$ the ideals $\mathcal{L}_1(\mathcal{K})$ and $\mathcal{L}_\infty(\mathcal{K})$ can be replaced by any $\mathcal{L}_p(\mathcal{K})$, $p \in [1, \infty]$, or even by any pair of invariant operator ideals $\mathfrak{S}_1$ and $\mathfrak{S}_2$. That is, one can consider the sets

$$\Lambda(H_0, F; \mathfrak{S}_1, \mathfrak{S}_2) = \{\lambda \in \mathbb{R} : F \operatorname{Im} R_{\lambda+i0}(H_0)F^* \text{ exists in } \mathfrak{S}_1 \text{ and } F R_{\lambda+i0}(H_0)F^* \text{ exists in } \mathfrak{S}_2\},$$

so that, in particular, $\Lambda(H_0; F) = \Lambda(H_0, F; \mathcal{L}_1, \mathcal{L}_\infty)$. What the last theorem is saying is that, as long as r_0 is not a resonance point, the regularity of λ is the same for $r = 0$ and $r = r_0$.

4.2. Essentially regular points. Let $\mathcal{A} = H_0 + \mathcal{A}(F)$ be the affine space of self-adjoint operators associated with a pair (H_0, F). Theorem 4.1.11 shows that regularity of a point $\lambda \in \mathbb{R}$ with respect to an operator $H \in \mathcal{A}$ does not depend on the path $\{H_r\}$. This observation suggests the following definition.

Let us fix a frame operator F on a Hilbert space $\mathcal{H}$ and an affine space $\mathcal{A} = H_0 + \mathcal{A}(F)$ of self-adjoint operators.

DEFINITION 4.2.1. We say that a real number λ is *essentially regular* if there exists an operator $H \in \mathcal{A}$ such that $\lambda \in \Lambda(H; F)$.

The set of essentially regular numbers will be denoted by $\Lambda(\mathcal{A}; F)$. So, by definition,

$$\Lambda(\mathcal{A}; F) = \bigcup_{H \in \mathcal{A}} \Lambda(H; F).$$

We say that a real number λ is *essentially singular* if it is not essentially regular. Obviously, the set $\Lambda(\mathcal{A}; F)$ of essentially regular points has full Lebesgue measure. By definition, the *essentially singular spectrum* of a pair $(\mathcal{A}, F)$ is the set of all essentially singular points. The essentially singular spectrum is a null set.

DEFINITION 4.2.2. If a real number λ is essentially regular, then an operator $H \in \mathcal{A}$ will be called *resonant* at λ if $\lambda \notin \Lambda(H; F)$. Otherwise, we say that H is *regular* or *non-resonant* at λ.

We denote the set of operators regular at λ by

$$\Gamma(\lambda; \mathcal{A}, F) = \Gamma(\lambda).$$

The complement of $\Gamma(\lambda; \mathcal{A}, F)$ in $\mathcal{A}$ will be called the *resonance set* and will be denoted by $R(\lambda; \mathcal{A}, F)$.

Note that if λ is essentially singular, then every operator $H \in \mathcal{A}$ is resonant at λ, though formally in this case the notion of an operator resonant at λ does not make sense.

The following reformulation of Theorem 4.1.11 will be useful.

THEOREM 4.2.3. *Let λ be an essentially regular point, and let H_0 be an operator regular at λ. Let $V = F^*JF$ and let $H = H_0 + V$. The operator H is regular at λ if and only if the operator*

$$1 + JT_{\lambda+i0}(H_0)$$

is invertible.

Definition 4.2.4. Let λ be an essentially regular point, and let H_0 be an operator resonant at λ. An operator $V \in \mathcal{A}(F)$ is *regularizing* if the operator $H_0 + V$ is regular at λ. An operator V is a *regularizing direction* if the operator $H_0 + rV$ is regular at λ for some $r \in \mathbb{R}$.

Theorem 4.2.5. *For every essentially regular point $\lambda \in \mathbb{R}$, the resonance set $R(\lambda; \mathcal{A}, F)$ is a closed nowhere dense subset of $\mathcal{A}$. Moreover, the intersection of any real-analytic path (in particular, a straight line) in $\mathcal{A}$ with $R(\lambda; \mathcal{A}, F)$ is either a discrete set or coincides with the path itself.*

Proof. Since λ is an essentially regular point, there exists an operator $H_0 \in \mathcal{A}$ regular at λ. If H is another operator regular at λ and if $F^*JF = H - H_0$, then it follows from Theorem 4.1.11 that the operator

$$1 + JT_{\lambda+i0}(H_0)$$

is invertible. Since for small norm-perturbations of J the latter operator remains invertible, it follows from Theorem 4.1.11 that some neighborhood of H in $\mathcal{A}$ also lies in $\Gamma(\lambda; \mathcal{A}, F)$. It follows that $\Gamma(\lambda; \mathcal{A}, F)$ is an open set, that is, $R(\lambda; \mathcal{A}, F)$ is closed.

Now, assume that $R(\lambda; \mathcal{A}, F)$ contains an open ball U. Since λ is essentially regular, there exists $H_0 \in \Gamma(\lambda; \mathcal{A}, F)$. Let l be the straight line which passes through H_0 and the center of the ball U. By Theorem 4.1.11, the intersection $U \cap l$ must be a discrete set, which is clearly impossible. This proves that $R(\lambda; \mathcal{A}, F)$ has empty interior and hence it is nowhere dense (since it is closed).

Let l be a real-analytic path in $\mathcal{A}$. That $R(\lambda; \mathcal{A}, F)$ either contains l or intersects l in a discrete set follows from Theorem 4.1.11 and Lemma 4.1.7. ∎

5. Wave matrix $w_\pm(\lambda; H_r, H_0)$

In the main setting of the abstract scattering theory, which considers trace-class perturbations V of arbitrary self-adjoint operators H_0, one first shows existence of the wave operators (Kato–Rosenblum theorem, [Ka$_1$, R], cf. also [Y, §6.2])

$$W_\pm(H_1, H_0) \colon \mathcal{H}^{(a)}(H_0) \to \mathcal{H}^{(a)}(H_1),$$

where $H_1 = H_0 + V$, and next one shows existence of the wave matrices

$$w_\pm(\lambda; H_1, H_0) \colon \mathfrak{h}_\lambda(H_0) \to \mathfrak{h}_\lambda(H_1) \tag{5.1}$$

for almost every $\lambda \in \mathbb{R}$, where $\mathfrak{h}_\lambda(H_j)$ is a fiber Hilbert space from a direct integral diagonalizing the absolutely continuous parts $H_j^{(a)}$, $j = 1, 2$, of the operators H_j. A drawback of this definition is that, for a given point $\lambda \in \mathbb{R}$, it is not possible to say whether $w_\pm(\lambda; H_1, H_0)$ is defined or not. This is because the fiber Hilbert spaces $\mathfrak{h}_\lambda(H_j)$ are not explicitly defined: they exist for almost every λ, but for a fixed λ the space $\mathfrak{h}_\lambda(H_j)$ is not defined.

However, if we fix a frame F in the Hilbert space $\mathcal{H}$, then for $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_1; F)$ it becomes possible to define the wave matrices $w_\pm(\lambda; H_1, H_0)$ as operators

(5.1), where $\mathfrak{h}_\lambda(H_j)$, $j = 1, 2$, are the fiber Hilbert spaces associated with the fixed frame by (3.2).

While the original proof of Kato and Rosenblum used time-dependent methods, the method of this paper is based on the stationary approach to abstract scattering theory from [BE, Y]. Combination of ideas from [BE, Y] with the construction of the direct integral, given in Section 3, allows us to define wave matrices $w_\pm(\lambda; H_r, H_0)$ for all λ from the set $\Lambda(H_0; F) \cap \Lambda(H_r; F)$ of full Lebesgue measure and prove all their main properties, including the multiplicative property.

In this section H_0 is a self-adjoint operator on $\mathcal{H}$ with frame F, and V is a trace-class self-adjoint operator for which the path $V_r = rV$ satisfies the condition (4.2). We note again that for any trace-class self-adjoint operator V there exists a frame F such that (4.2) holds for $V_r = rV$. Consequently, the condition (4.2) does not impose any additional restrictions on the perturbation V, except the trace-class condition.

5.1. Operators $\mathfrak{a}_\pm(\lambda; H_r, H_0)$. In [Ag], instead of sandwiching the resolvent, it is considered as acting on appropriately defined Hilbert spaces. Following this idea, we consider the limit value $R_{\lambda+i0}(H_0)$ of the resolvent as an operator

$$R_{\lambda+i0}(H_0) \colon \mathcal{H}_1 \to \mathcal{H}_{-1}.$$

Recall that all Hilbert spaces $\mathcal{H}_\alpha$, $\alpha \in \mathbb{R}$, are naturally isomorphic with the isomorphism being

$$|F|^{\beta-\alpha} \colon \mathcal{H}_\alpha \to \mathcal{H}_\beta.$$

So, if we have an operator-function $A(y), y > 0$, with values in some subclass of $\mathcal{B}(\mathcal{H})$, such that the limit

$$\lim_{y \to 0} |F|^\alpha A(y) |F|^\beta$$

exists in the topology of that class, then the limit

$$\lim_{y \to 0} A(y)$$

exists in the topology of the corresponding subclass of $\mathcal{B}(\mathcal{H}_\beta, \mathcal{H}_{-\alpha})$. In this way we write $A(0)$, meaning by this an operator from $\mathcal{H}_\beta$ to $\mathcal{H}_{-\alpha}$. It is not necessary to use this convention, but otherwise we would need to write a lot of F's in the subsequent formulas, thus making them cumbersome.

Thus, in an expression like

$$R_{\lambda \mp iy}(H_0) V_r$$

with $y > 0$, both $R_{\lambda \mp iy}(H_0)$ and V_r can be understood as operators from $\mathcal{H}$ to $\mathcal{H}$, *or* the operator V_r can be understood as an operator from $\mathcal{H}_{-1}$ to $\mathcal{H}_1$ while $R_{\lambda \mp iy}(H_0)$ can be understood as an operator from $\mathcal{H}_1$ to $\mathcal{H}_{-1}$. But when we take the limit $y \to 0$ and write

$$R_{\lambda \mp i0}(H_0) V_r$$

both operators should be understood in the second sense, so that the product above is an operator from $\mathcal{H}_{-1}$ to $\mathcal{H}_{-1}$. That is, in the product the operator $V_r \colon \mathcal{H}_{-1} \to \mathcal{H}_1$ means actually the operator $|F| V_r |F|$, acting in the following way:

$$\mathcal{H}_1 \xleftarrow{|F|} \mathcal{H} \xleftarrow{V_r} \mathcal{H} \xleftarrow{|F|} \mathcal{H}_{-1}.$$

In the Hilbert space $\mathcal{H}$ the operator $R_{\lambda\mp i0}(H_0)V_r$ (if one wishes) should be written as $|F|R_{\lambda\mp i0}(H_0)|F|V_r$, where V_r is understood as acting from $\mathcal{H}$ to $\mathcal{H}$.

In what follows, we constantly use this convention without further reference.

Lemma 5.1.1. *If $\lambda \in \Lambda(H_r;F)$, then*

$$R_{\lambda\pm iy}(H_r) \to R_{\lambda\pm i0}(H_r) \quad \text{in } \mathcal{L}_\infty(\mathcal{H}_1,\mathcal{H}_{-1}) \text{ as } y \to 0^+.$$

Proof. This follows from Proposition 2.6.2 and the definition of $\Lambda(H_0;F)$. ∎

Lemma 5.1.2. *If $\lambda \in \Lambda(H_r;F)$, then*

$$\operatorname{Im} R_{\lambda+iy}(H_r) \to \operatorname{Im} R_{\lambda+i0}(H_r) \quad \text{in } \mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1}) \text{ as } y \to 0^+.$$

Proof. This follows from Theorem 1.9.1 and Proposition 2.6.2. ∎

We now investigate the forms (cf. [Y, Definition 2.7.2])

$$\mathfrak{a}_\pm(H_r,H_0;f,g;\lambda) := \lim_{y\to 0^+} \frac{y}{\pi}\langle R_{\lambda\pm iy}(H_r)f, R_{\lambda\pm iy}(H_0)g\rangle.$$

Unlike [Y, Definition 2.7.2], we treat $\mathfrak{a}_\pm(H_r,H_0;\lambda)$ not as a form, but as an operator from $\mathcal{H}_1$ to $\mathcal{H}_{-1}$. In [Y, §5.2] it is proved that this form is well-defined for a.e. $\lambda \in \mathbb{R}$. In the next proposition we give an explicit set of full measure on which $\mathfrak{a}_\pm(H_r,H_0;\lambda)$ exists.

Proposition 5.1.3. *If $\lambda \in \Lambda(H_r;F)\cap\Lambda(H_0;F)$, then the limit*

$$\lim_{y\to 0^+} \frac{y}{\pi} R_{\lambda\mp iy}(H_r)R_{\lambda\pm iy}(H_0) \tag{5.2}$$

exists in $\mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1})$.

Proof. We have (cf. e.g. [Y, (2.7.10)])

$$\begin{aligned}\frac{y}{\pi} R_{\lambda\mp iy}(H_r)R_{\lambda\pm iy}(H_0) &= \frac{1}{\pi}\operatorname{Im} R_{\lambda+iy}(H_r)[1+V_rR_{\lambda\pm iy}(H_0)] \\ &= [1-R_{\lambda\mp iy}(H_r)V_r]\cdot\frac{1}{\pi}\operatorname{Im} R_{\lambda+iy}(H_0).\end{aligned} \tag{5.3}$$

Since $\lambda \in \Lambda(H_0;F)\cap\Lambda(H_r;F)$, Lemma 5.1.2 implies that the limits of $\operatorname{Im} R_{\lambda+iy}(H_0)$ and $\operatorname{Im} R_{\lambda+iy}(H_r)$ exist in $\mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1})$. Also, by Lemma 5.1.1, the limits of $R_{\lambda\pm iy}(H_0)$ and $R_{\lambda\pm iy}(H_r)$ exist in $\mathcal{L}_\infty(\mathcal{H}_1,\mathcal{H}_{-1})$, while $V_r\colon \mathcal{H}_{-1}\to\mathcal{H}_1$ is a bounded operator (see (4.2)). It follows that the limit (5.2) exists in $\mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1})$. ∎

Definition 5.1.4. Let $\lambda \in \Lambda(H_r;F)\cap\Lambda(H_0;F)$. The operators

$$\mathfrak{a}_\pm(\lambda;H_r,H_0)\colon \mathcal{H}_1 \to \mathcal{H}_{-1}$$

are the limits (5.2) taken in the $\mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1})$ topology.

Proposition 5.1.5. *If $\lambda \in \Lambda(H_r;F)\cap\Lambda(H_0;F)$, then, in $\mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1})$,*

$$\mathfrak{a}_\pm(\lambda;H_r,H_0) = [1-R_{\lambda\mp i0}(H_r)V_r]\cdot\frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_0) = \frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_r)[1+V_rR_{\lambda\pm i0}(H_0)]. \tag{5.4}$$

Proof. This follows from (5.3), Lemmas 5.1.1, 5.1.2, Proposition 5.1.3 and (4.2). ∎

Note that products such as $R_{\lambda\mp i0}(H_r)V_r \cdot \frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_0)$ should be and are understood as acting in the following way:

$$\mathcal{H}_{-1} \xleftarrow{R_{\lambda\mp i0}(H_r)} \mathcal{H}_1 \xleftarrow{V_r} \mathcal{H}_{-1} \xleftarrow{\frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_0)} \mathcal{H}_1.$$

LEMMA 5.1.6. *Let* $\lambda \in \Lambda(H_r;F)\cap\Lambda(H_0;F)$ *and let* $f \in \mathcal{H}_1$*. If* $\mathcal{E}_\lambda(H_0)f = 0$*, then* $\mathfrak{a}_\pm(\lambda; H_r, H_0)f = 0$.

Proof. This follows from (see 2.15(vii) and (2.9))

$$\mathcal{E}_\lambda^\diamondsuit(H_0)\mathcal{E}_\lambda(H_0) = \frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_0) \tag{5.5}$$

(an equality in $\mathcal{L}_1(\mathcal{H}_1,\mathcal{H}_{-1})$) and Proposition 5.1.5. ■

5.2. Definition of the wave matrix $w_\pm(\lambda; H_r, H_0)$. Since from now on we need direct integral representations (3.4) for different operators $H_r = H_0 + V_r$, we denote the fiber Hilbert space corresponding to H_r by $\mathfrak{h}_\lambda^{(r)}$ or by $\mathfrak{h}_\lambda(H_r)$.

In this section we define the wave matrix $w_\pm(\lambda; H_r, H_0)$ as a form and prove that it is well-defined and bounded, so that it defines an operator.

DEFINITION 5.2.1. Let $\lambda \in \Lambda(H_r;F)\cap\Lambda(H_0;F)$. The *wave matrix* $w_\pm(\lambda; H_r, H_0)$ is a densely defined form $w_\pm(\lambda; H_r, H_0)\colon \mathfrak{h}_\lambda^{(r)} \times \mathfrak{h}_\lambda^{(0)} \to \mathbb{C}$, defined by the formula

$$w_\pm(\lambda; H_r, H_0)(\mathcal{E}_\lambda(H_r)f, \mathcal{E}_\lambda(H_0)g) = \langle f, \mathfrak{a}_\pm(\lambda; H_r, H_0)g\rangle_{1,-1}, \tag{5.6}$$

where $f, g \in \mathcal{H}_1$.

It is worth noting that this definition depends on endpoint operators H_0 and H_r, but it does not depend on the path $\{H_s\}_{s\in[0,r]}$ connecting the endpoints.

One needs to show that the wave matrix is well-defined.

PROPOSITION 5.2.2. *For any* $\lambda \in \Lambda(H_r;F)\cap\Lambda(H_0;F)$ *the form* $w_\pm(\lambda; H_r, H_0)$ *is well-defined, and it is bounded with norm* ≤ 1.

Proof. That $w_\pm(\lambda; H_r, H_0)$ is well-defined follows from Lemma 5.1.6.

Further, by the Schwarz inequality, for any $f, g \in \mathcal{H}_1$,

$$\begin{aligned}\frac{y}{\pi}|\langle f, R_{\lambda-iy}(H_r)R_{\lambda+iy}(H_0)g\rangle| &= \frac{y}{\pi}|\langle R_{\lambda+iy}(H_r)f, R_{\lambda+iy}(H_0)g\rangle| \\ &\le \frac{y}{\pi}|\langle R_{\lambda+iy}(H_r)f, R_{\lambda+iy}(H_r)f\rangle|^{1/2}|\langle R_{\lambda+iy}(H_0)g, R_{\lambda+iy}(H_0)g\rangle|^{1/2} \\ &= \frac{1}{\pi}|\langle f, \operatorname{Im} R_{\lambda+iy}(H_r)f\rangle|^{1/2}\cdot|\langle g, \operatorname{Im} R_{\lambda+iy}(H_0)g\rangle|^{1/2}.\end{aligned} \tag{5.7}$$

Taking the limit $y \to 0^+$, one gets, using Lemma 5.1.2, Proposition 5.1.3 and (5.5),

$$|\langle f, \mathfrak{a}_\pm(\lambda; H_r, H_0)g\rangle_{1,-1}| \le \|\mathcal{E}_\lambda(H_r)f\|_{\mathfrak{h}_\lambda^{(r)}} \cdot \|\mathcal{E}_\lambda(H_0)g\|_{\mathfrak{h}_\lambda^{(0)}}.$$

It follows that the wave matrix is bounded with bound ≤ 1. ■

So, the form $w_\pm(\lambda; H_r, H_0)$ is defined on $\mathfrak{h}_\lambda^{(r)} \times \mathfrak{h}_\lambda^{(0)}$. We will identify the form $w_\pm(\lambda)$ with the corresponding operator from $\mathfrak{h}_\lambda^{(0)}$ to $\mathfrak{h}_\lambda^{(r)}$, so that

$$w_\pm(\lambda; H_r, H_0)(\mathcal{E}_\lambda(H_r)f, \mathcal{E}_\lambda(H_0)g) = \langle \mathcal{E}_\lambda(H_r)f, w_\pm(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0)g\rangle,$$

where $f, g \in \mathcal{H}_1$. Note that it follows from the definition of $w_\pm(\lambda; H_r, H_0)$ that

$$\mathcal{E}^\diamondsuit_\lambda(H_r) w_\pm(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) = \mathfrak{a}_\pm(\lambda; H_r, H_0). \tag{5.8}$$

The following proposition follows immediately from the definition of $w_\pm(\lambda; H_r, H_0)$.

PROPOSITION 5.2.3.

1. *Let* $\lambda \in \Lambda(H_0; F)$. *Then*

$$w_\pm(\lambda; H_0, H_0) = \mathrm{Id}.$$

2. *Let* $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$. *Then*

$$w^*_\pm(\lambda; H_r, H_0) = w_\pm(\lambda; H_0, H_r). \tag{5.9}$$

Proof. 1. Using (5.6), (5.4), (5.5) and (2.9), for any $f, g \in \mathcal{H}_1$ we have

$$\begin{aligned}
&\langle \mathcal{E}_\lambda(H_0) f, w_\pm(\lambda; H_0, H_0) \mathcal{E}_\lambda(H_0) g \rangle\rangle_{\mathfrak{h}^{(0)}_\lambda} \\
&\qquad = \langle f, \mathfrak{a}_\pm(\lambda; H_0, H_0) g \rangle_{1,-1} = \frac{1}{\pi} \langle f, \operatorname{Im} R_{\lambda+i0}(H_0) g \rangle_{1,-1} \\
&\qquad = \langle f, \mathcal{E}^\diamondsuit_\lambda(H_0) \mathcal{E}_\lambda(H_0) g \rangle_{1,-1} = \langle \mathcal{E}_\lambda(H_0) f, \mathcal{E}_\lambda(H_0) g \rangle_{\mathfrak{h}^{(0)}_\lambda}.
\end{aligned}$$

Since $\mathcal{E}_\lambda \mathcal{H}_1$ is, by definition, dense in $\mathfrak{h}_\lambda$ (see (3.2)) and since, by Proposition 5.2.2, the wave matrix $w_\pm(\lambda; H_r, H_0)$ is bounded, the last equality implies that $w_\pm(\lambda; H_0, H_0) = 1$.

2. This follows directly from the definition of $w_\pm(\lambda; H_r, H_0)$. The details are omitted since later we derive this property of the wave matrix from the multiplicative property. ■

5.3. Multiplicative property of the wave matrix. We have shown that the wave matrix is a bounded operator from $\mathfrak{h}^{(0)}_\lambda$ to $\mathfrak{h}^{(r)}_\lambda$. The next thing to do is to show that it is a unitary operator. Unitarity of the wave matrix is a consequence of the multiplicative property and the norm bound $\|w_\pm\| \le 1$.

In this subsection we establish the multiplicative property of the wave matrix. We shall extensively use objects such as $\phi_j(\lambda + iy)$, $b_j(\lambda + iy)$ and so on, associated to a self-adjoint operator H_r on a fixed framed Hilbert space $(\mathcal{H}, F)$. Which self-adjoint operator these objects are associated with will be clear from the context. For example, if one meets an expression $R_{\lambda+iy}(H_r) b_j(\lambda + iy)$, then this means that $b_j(\lambda + iy)$ is associated with H_r.

LEMMA 5.3.1. *Let* $\lambda \in \Lambda(H_0; F)$. *If* $f = \sum_{k=1}^\infty \beta_k \kappa_k \phi_k \in \mathcal{H}_1$ *(so that* $(\beta_j) \in \ell_2$*), then*

$$\langle \mathcal{E}_{\lambda+iy}(H_0) f, e_j(\lambda + iy) \rangle_{\ell_2} = \alpha_j(\lambda + iy) \langle \beta, e_j(\lambda + iy) \rangle_{\ell_2}.$$

Proof. One has

$$\begin{aligned}
\langle \mathcal{E}_{\lambda+iy}(H_0) f, e_j(\lambda + iy) \rangle &= \Big\langle \mathcal{E}_{\lambda+iy}(H_0) \sum_{k=1}^\infty \beta_k \kappa_k \phi_k, e_j(\lambda + iy) \Big\rangle \\
&= \Big\langle \sum_{k=1}^\infty \beta_k \kappa_k \mathcal{E}_{\lambda+iy}(H_0) \phi_k, e_j(\lambda + iy) \Big\rangle \\
&= \Big\langle \sum_{k=1}^\infty \beta_k \eta_k(\lambda + iy), e_j(\lambda + iy) \Big\rangle \quad \text{by (2.15)}
\end{aligned}$$

$$= \sum_{k=1}^{\infty} \bar{\beta}_k \langle \eta_k(\lambda+iy), e_j(\lambda+iy)\rangle$$
$$= \sum_{k=1}^{\infty} \bar{\beta}_k \alpha_j(\lambda+iy) e_{kj}(\lambda+iy) = \alpha_j(\lambda+iy)\langle \beta, e_j(\lambda+iy)\rangle_{\ell_2}.$$

The second equality holds since $\mathcal{E}_{\lambda+iy}$ is a bounded operator from $\mathcal{H}_1$ to ℓ_2. The fourth equality holds since the series $\sum_{k=1}^{\infty} \beta_k \eta_k$ is absolutely convergent. The fifth equality holds since $e_j(\lambda+iy)$ is an eigenvector of the matrix $\eta(\lambda+iy)$ with the eigenvalue $\alpha_j(\lambda+iy)$. ∎

For the definition of an index of zero type see Subsection 2.10.

LEMMA 5.3.2. *Let $\lambda \in \Lambda(H_0;F)$ and $f \in \mathcal{H}_1$. If j is an index of zero type, then*

$$\langle \mathcal{E}_{\lambda+iy}(H_0)f, e_j(\lambda+iy)\rangle \to 0 \quad \text{as } y \to 0.$$

Proof. By Lemma 5.3.1 (and its representation for f) and the definition of $e_j(\lambda+iy)$,

$$|\langle \mathcal{E}_{\lambda+iy}(H_0)f, e_j(\lambda+iy)\rangle| = \alpha_j(\lambda+iy)|\langle \beta, e_j(\lambda+iy)\rangle_{\ell_2}|$$
$$\le \alpha_j(\lambda+iy)\|\beta\|\|e_j(\lambda+iy)\| = \alpha_j(\lambda+iy)\|\beta\|.$$

If j is an index of zero type, then, by definition, $\alpha_j(\lambda+iy) \to 0$ as $y \to 0$. ∎

LEMMA 5.3.3. *Let $\lambda \in \Lambda(H_r;F) \cap \Lambda(H_0;F)$. If j is of zero type, then for any $f \in \mathcal{H}_1$,*

$$\frac{y}{\pi}\langle R_{\lambda\pm iy}(H_r)f, R_{\lambda\pm iy}(H_0)b_j(\lambda+iy)\rangle \to 0 \quad \text{as } y \to 0. \tag{5.10}$$

Proof. The first equality in (5.3) and 2.15(i) imply that

$$\frac{y}{\pi}\langle R_{\lambda\pm iy}(H_r)f, R_{\lambda\pm iy}(H_0)b_j(\lambda+iy)\rangle$$
$$= \langle \mathcal{E}_{\lambda+iy}(H_0)[1+V_r R_{\lambda\pm iy}(H_r)]f, \mathcal{E}_{\lambda+iy}(H_0)b_j(\lambda+iy)\rangle$$
$$= \langle \mathcal{E}_{\lambda+iy}(H_0)[1+V_r R_{\lambda\pm iy}(H_r)]f, e_j(\lambda+iy)\rangle, \tag{5.11}$$

where the second equality follows from the definition (2.20) of $b_j(\lambda+iy)$. Since by Lemma 5.1.1 the resolvent $R_{\lambda\pm iy}(H_r)$ converges as an operator from $\mathcal{H}_1$ to $\mathcal{H}_{-1}$, and since V maps $\mathcal{H}_{-1}$ to $\mathcal{H}_1$ (see (4.2)), it follows that $VR_{\lambda\pm iy}(H_r)f$ converges in $\mathcal{H}_1$ as $y \to 0$. Now, applying Lemma 5.3.1 and using the fact that for indices j of zero type the eigenvalues $\alpha_j(\lambda+iy)$ converge to 0, we deduce (5.10). ∎

The following lemma is well-known and therefore its proof is omitted.

LEMMA 5.3.4. *If a non-increasing sequence $f_1, f_2, \ldots$ of continuous functions on $[0,1]$ converges pointwise to 0, then it also converges to 0 uniformly.*

LEMMA 5.3.5. *Let $\lambda \in \Lambda(H_0;F)$. The sum*

$$\sum_{j=N}^{\infty} \alpha_j(\lambda+iy)^2$$

converges to 0 as $N \to \infty$ uniformly with respect to $y \in [0,1]$.

Proof. Let $f_N(y)$ be this sum. Since $f_1(y) = \|\eta(\lambda+iy)\|_2^2$, it follows from 2.8(iii) and (iv) that $f_1(y)$, and, consequently, all $f_N(y)$ are continuous functions of y in $[0,1]$. So, we have a non-increasing sequence $f_N(y)$ of continuous non-negative functions, converging pointwise to 0 as $N \to \infty$. It follows from Lemma 5.3.4 that the sequence $f_N(y)$ converges to 0 as $N \to \infty$ uniformly with respect to $y \in [0,1]$. ■

LEMMA 5.3.6. *Let $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$. If $f \in \mathcal{H}_1$, then the sequence*

$$\left(\frac{y}{\pi}\right)^2 \sum_{j=N}^{\infty} |\langle R_{\lambda \pm iy}(H_r) f, R_{\lambda \pm iy}(H_0) b_j(\lambda + iy)\rangle|^2, \qquad N = 1, 2, \ldots,$$

converges to 0 as $N \to \infty$, uniformly with respect to $y > 0$.

Proof. We prove the lemma for the plus sign. The formula (5.11) and Lemma 5.3.1 imply that

$$\begin{aligned} (E) := \left(\frac{y}{\pi}\right)^2 & \sum_{j=N}^{\infty} |\langle R_{\lambda+iy}(H_r) f, R_{\lambda+iy}(H_0) b_j(\lambda + iy)\rangle|^2 \\ &= \sum_{j=N}^{\infty} |\langle \mathcal{E}_{\lambda+iy}(H_0)[1 + V_r R_{\lambda+iy}(H_r)] f, e_j(\lambda + iy)\rangle|^2 \\ &= \sum_{j=N}^{\infty} |\alpha_j(\lambda + iy)\langle \beta(\lambda + iy), e_j(\lambda + iy)\rangle|^2, \end{aligned}$$

where $\beta(\lambda + iy) = (\beta_k(\lambda + iy)) \in \ell_2$, and

$$[1 + V_r R_{\lambda+iy}(H_r)] f = \sum_{k=1}^{\infty} \beta_k(\lambda + iy) \kappa_k \phi_k \in \mathcal{H}_1.$$

Since $[1 + V_r R_{\lambda+iy}(H_r)] f$ converges in $\mathcal{H}_1$ as $y \to 0$, the sequence $(\beta_k(\lambda + iy))$ converges in ℓ_2 as $y \to 0$. It follows that $\|\beta(\lambda + iy)\|_{\ell_2} \le C$ for all $y \in [0,1]$. Hence,

$$(E) \le C^2 \sum_{j=N}^{\infty} \alpha_j(\lambda + iy)^2.$$

By Lemma 5.3.5, the last expression converges to 0 uniformly. ■

In the following theorem we prove the multiplicative property of the wave matrix. This is well-known [Y], but the novelty is that we give an explicit set of full measure such that for all λ from that set the wave matrices are explicitly defined and the multiplicative property holds.

THEOREM 5.3.7. *Let $\{H_r\}$ be a path satisfying Assumption 4.1.1. If $\lambda \in \Lambda(H_0; F)$ and if r_0, r_1, r_2 are not resonance points of the path $\{H_r\}$ for this λ (that is, if $r_0, r_1, r_2 \notin R(\lambda; \{H_r\}, F)$), then*

$$w_\pm(\lambda; H_{r_2}, H_{r_0}) = w_\pm(\lambda; H_{r_2}, H_{r_1}) w_\pm(\lambda; H_{r_1}, H_{r_0}).$$

Proof. We prove this equality for the + sign. Let $f, g \in \mathcal{H}_1$. It follows from 2.16(vi) that

$$\begin{aligned} \frac{y}{\pi} & \langle R_{\lambda+iy}(H_{r_2}) f, R_{\lambda+iy}(H_{r_0}) g\rangle \\ &= \left(\frac{y}{\pi}\right)^2 \sum_{j=1}^{\infty} \langle R_{\lambda+iy}(H_{r_2}) f, R_{\lambda+iy}(H_{r_1}) b_j(\lambda + iy)\rangle \\ & \qquad \cdot \langle R_{\lambda+iy}(H_{r_1}) b_j(\lambda + iy), R_{\lambda+iy}(H_{r_0}) g\rangle, \qquad (5.12) \end{aligned}$$

where the series converges absolutely, since the set of vectors $\{\sqrt{y/\pi}R_{\lambda+iy}(H_{r_1})b_j(\lambda+iy)\}$ is orthonormal and complete (see 2.16(vi)). Applying the Schwarz inequality to (5.12) and using Lemma 5.3.6, one can take the limit $y \to 0$ in this formula. By Lemma 5.3.3, the summands with zero-type j disappear after letting $y \to 0$.

It now follows from Definition 5.1.4 of $\mathfrak{a}_\pm$ and 2.16(viii) that

$$\langle f, \mathfrak{a}_+(\lambda; H_{r_2}, H_{r_0})g\rangle_{1,-1} = \sum_{j=1}^{\infty}\langle f, \mathfrak{a}_+(\lambda; H_{r_2}, H_{r_1})b_j(\lambda+i0)\rangle_{1,-1}\langle b_j(\lambda+i0), \mathfrak{a}_+(\lambda; H_{r_1}, H_{r_0})g\rangle_{1,-1}, \qquad (5.13)$$

where the summation is over indices of non-zero type. By definition (5.6) of $w_\pm$, it follows from (5.13) that

$$\begin{aligned}
&\langle \mathcal{E}_\lambda^{(r_2)} f, w_\pm(\lambda; H_{r_2}, H_{r_0})\mathcal{E}_\lambda^{(r_0)} g\rangle \\
&= \sum_{j=1}^{\infty}\langle \mathcal{E}_\lambda^{(r_2)} f, w_\pm(\lambda; H_{r_2}, H_{r_1})\mathcal{E}_\lambda^{(r_1)} b_j(\lambda+i0)\rangle\langle \mathcal{E}_\lambda^{(r_1)} b_j(\lambda+i0), w_\pm(\lambda; H_{r_1}, H_{r_0})\mathcal{E}_\lambda^{(r_0)} g\rangle \\
&= \sum_{j=1}^{\infty}\langle \mathcal{E}_\lambda^{(r_2)} f, w_\pm(\lambda; H_{r_2}, H_{r_1})e_j(\lambda+i0)\rangle\langle e_j(\lambda+i0), w_\pm(\lambda; H_{r_1}, H_{r_0})\mathcal{E}_\lambda^{(r_0)} g\rangle \\
&= \langle \mathcal{E}_\lambda^{(r_2)} f, w_\pm(\lambda; H_{r_2}, H_{r_1})w_\pm(\lambda; H_{r_1}, H_{r_0})\mathcal{E}_\lambda^{(r_0)} g\rangle, \qquad (5.14)
\end{aligned}$$

where in the last equality Lemma 3.1.6 was used. The second equality above follows from (2.20), 2.15(vi) and 2.11(iv). Since the set $\mathcal{E}_\lambda\mathcal{H}_1$ is dense in $\mathfrak{h}_\lambda$, the proof is complete. ∎

Corollary 5.3.8. *Let $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$. Then $w_\pm(\lambda; H_r, H_0)$ is a unitary operator from $\mathfrak{h}_\lambda^{(0)}$ to $\mathfrak{h}_\lambda^{(r)}$ and* (5.9) *holds.*

Proof. Indeed, using the first part of Proposition 5.2.3 and the multiplicative property of the wave matrix (Theorem 5.3.7), one infers that

$$w_\pm(\lambda; H_0, H_r)w_\pm(\lambda; H_r, H_0) = w_\pm(\lambda; H_0, H_0) = 1,$$
$$w_\pm(\lambda; H_r, H_0)w_\pm(\lambda; H_0, H_r) = w_\pm(\lambda; H_r, H_r) = 1.$$

Since $\|w_\pm(\lambda; H_r, H_0)\| \le 1$ by Proposition 5.2.2, it follows that $w_\pm(\lambda; H_r, H_0)$ is a unitary operator and

$$w_\pm^*(\lambda; H_r, H_0) = w_\pm(\lambda; H_0, H_r). \ ∎$$

Remark 5.3.9. There is an essential difference between the operators $\sqrt{y/\pi}R_{\lambda+iy}(H_0)$ (or $\sqrt{y/\pi}R_{\lambda-iy}(H_0)$) and $\mathcal{E}_{\lambda+iy}(H_0)$. While they have some common features (see formulae 2.16(iv) and 2.16(v)), the second operator is better than the first one. Actually, as can be seen from the definitions of $\sqrt{\frac{y}{\pi}}R_{\lambda+iy}(H_0)$ and $\mathcal{E}_{\lambda+iy}(H_0)$, these operators "differ" by the phase part. This statement is enforced by the fact that the $\mathcal{L}_2(\mathcal{H}_1, \mathcal{H})$ norm of the difference

$$\sqrt{y/\pi}\, R_{\lambda+iy}(H_0) - \sqrt{y_1/\pi}\, R_{\lambda+iy_1}(H_0)$$

remains bounded as $y, y_1 \to 0$, even though it does not converge to 0. Convergence is hindered by the non-convergent phase part, which is absent in $\mathcal{E}_{\lambda+iy}(H_0)$.

5.4. The wave operator. Recall that a family of operators $A_\lambda \colon \mathfrak{h}_\lambda(H_0) \to \mathfrak{h}_\lambda(H_1)$ is measurable if it maps measurable vector-functions to measurable vector-functions. Recall that if

$$A = \int_\Lambda^\oplus A(\lambda)\, d\lambda \quad \text{and} \quad B = \int_\Lambda^\oplus B(\lambda)\, d\lambda,$$

then

$$AB = \int_\Lambda^\oplus A(\lambda)B(\lambda)\, d\lambda.$$

We define the wave operator $W_\pm$ as the direct integral of wave matrices:

$$W_\pm(H_r, H_0) := \int_{\Lambda(H_r;F)\cap\Lambda(H_0;F)}^\oplus w_\pm(\lambda; H_r, H_0)\, d\lambda. \tag{5.15}$$

It is clear from (5.6) that the operator-function

$$\Lambda(H_r;F)\cap\Lambda(H_0;F) \ni \lambda \mapsto w_\pm(\lambda; H_r, H_0)$$

is measurable, so that the integral above makes sense.

The following well-known theorem (cf. [Y, Chapter 2]) is a direct consequence of the definition (5.15) of the wave operator $W_\pm$, Theorem 5.3.7 and Corollary 5.3.8.

THEOREM 5.4.1. *Let $\{H_r\}$ be a path of self-adjoint operators which satisfies Assumption* 4.1.1. *The wave operator $W_\pm(H_r, H_0) \colon \mathcal{H}^{(a)}(H_0) \to \mathcal{H}^{(a)}(H_r)$ possesses the following properties.*

(i) *$W_\pm(H_r, H_0)$ is a unitary operator.*
(ii) *$W_\pm(H_r, H_0) = W_\pm(H_r, H_s)W_\pm(H_s, H_0)$.*
(iii) *$W_\pm^*(H_r, H_0) = W_\pm(H_0, H_r)$.*
(iv) *$W_\pm(H_0, H_0) = 1$.*

If we define $W_\pm(H_r, H_0)$ to be zero on $\mathcal{H}^{(s)}(H_0)$, then (iv) becomes

$$W_\pm(H_0, H_0) = P^{(a)}(H_0).$$

That is, $W_\pm(H_r, H_0)$ becomes a partial isometry with initial space $\mathcal{H}^{(a)}(H_0)$ and final space $\mathcal{H}^{(a)}(H_r)$. So,

$$W_\pm(H_r, H_0) = W_\pm(H_r, H_0)P^{(a)}(H_0) = P^{(a)}(H_r)W_\pm(H_r, H_0).$$

THEOREM 5.4.2 (cf. [Y, Theorem 2.1.4]). *For any bounded measurable function h on $\mathbb{R}$,*

$$h(H_r)W_\pm(H_r, H_0) = W_\pm(H_r, H_0)h(H_0). \tag{5.16}$$

Also,

$$H_r W_\pm(H_r, H_0) = W_\pm(H_r, H_0)H_0. \tag{5.17}$$

Proof. This follows from the definition (5.15) of $W_\pm$ and Theorem 3.4.1. ■

As a consequence, we also get the Kato–Rosenblum theorem.

COROLLARY 5.4.3. *The operators $H_0^{(a)}$ and $H_1^{(a)}$, considered as operators on the absolutely continuous subspaces $\mathcal{H}^{(a)}(H_0)$ and $\mathcal{H}^{(a)}(H_1)$ respectively, are unitarily equivalent.*

This follows from (5.17).

6. Connection with the time-dependent definition of the wave operator

In this section we show that the wave operator defined by (5.15) coincides with the classical time-dependent definition. In this subsection I follow [Y]. Though the proofs follow almost verbatim those in [Y] (in [Y] the proofs are given in a more general setting), they are given here for the reader's convenience and completeness. On the other hand, availability of the evaluation operator $\mathcal{E}_\lambda$ allows us to simplify the proofs slightly.

6.1. Time-dependent definition of the wave operator. In abstract scattering theory the wave operator is usually defined by the formula (cf. e.g. [Y, (2.1.1)])

$$W_\pm(H_r, H_0) = \lim_{t\to\pm\infty} e^{itH_r} e^{-itH_0} P^{(a)}(H_0) =: \overset{\mathrm{s}}{W}_\pm(H_r, H_0), \tag{6.1}$$

where the limit is taken in the strong operator topology. Since we define the wave operator in a different way, this formula becomes a theorem.

We denote by $P_r^{(a)}$ the projection $P^{(a)}(H_r)$.

The weak wave operators $\overset{\mathrm{w}}{W}_\pm$ are defined, if they exist, by the formula

$$\overset{\mathrm{w}}{W}_\pm(H_r, H_0) := \lim_{t\to\pm\infty} P_r^{(a)} e^{itH_r} e^{-itH_0} P_0^{(a)}, \tag{6.2}$$

where the limit is taken in the weak operator topology.

The proof of the existence of the wave operator in the strong operator topology uses the existence of the weak wave operator and the multiplicative property of it. The proof of the latter constitutes the main difficulty of the stationary approach.

The following lemma is taken from [Y, Lemma 5.3.1].

Lemma 6.1.1. *If $g \in \mathcal{H}$ is such that $\|\mathcal{E}_\lambda g\|_{\mathfrak{h}_\lambda} \le N$ for a.e. $\lambda \in \Lambda(H_0; F)$, then*

$$\int_{-\infty}^{\infty} \|F e^{-itH_0} P_0^{(a)} g\|^2\,dt \le 2\pi N^2 \|F\|_2^2.$$

Proof. (A) For any frame vector ϕ_j the following estimate holds:

$$\int_{-\infty}^{\infty} |\langle e^{-itH_0} P_0^{(a)} g, \phi_j\rangle|^2\,dt \le 2\pi N^2.$$

To see this note that $g(\lambda)$ is defined for a.e. $\lambda \in \Lambda(H_0; F)$ as an element of the direct integral $\mathcal{H}$. It follows from Theorem 3.4.1 and Lemma 3.2.2 that

$$\langle e^{-itH_0} P_0^{(a)} g, \phi_j\rangle = \int_{\Lambda(H_0;F)} e^{-i\lambda t} \langle g(\lambda), \phi_j(\lambda)\rangle\,d\lambda = \sqrt{2\pi}\hat{f}_j(t),$$

where $f_j(\lambda) = \langle g(\lambda), \phi_j(\lambda)\rangle$ and $\hat{f}_j$ is the Fourier transform of f_j. It follows that

$$\int_{-\infty}^{\infty} |\langle e^{-itH_0} P_0^{(a)} g, \phi_j\rangle|^2\,dt = 2\pi \int_{-\infty}^{\infty} |\hat{f}_j(t)|^2\,dt = 2\pi \int_{\Lambda(H_0;F)} |f_j(\lambda)|^2\,d\lambda$$
$$= 2\pi \int_{\Lambda(H_0;F)} |\langle g(\lambda), \phi_j(\lambda)\rangle|^2\,d\lambda \le 2\pi N^2 \int_{\Lambda(H_0;F)} \|\phi_j(\lambda)\|^2\,d\lambda \le 2\pi N^2.$$

We write here $\Lambda(H_0; F)$ instead of $\mathbb{R}$, but since $\Lambda(H_0; F)$ has full Lebesgue measure, it makes no difference. The proof of (A) is complete.

(B) Using the Parseval equality one has (recall that (ψ_j) is the orthonormal basis from the definition (2.3) of the frame operator F)

$$(E) := \int_{-\infty}^{\infty} \|Fe^{-itH_0}P_0^{(a)}g\|^2\,dt = \int_{-\infty}^{\infty} \sum_{j=1}^{\infty} |\langle Fe^{-itH_0}P_0^{(a)}g, \psi_j\rangle|^2\,dt$$

$$= \int_{-\infty}^{\infty} \sum_{j=1}^{\infty} \kappa_j^2 |\langle e^{-itH_0}P_0^{(a)}g, \phi_j\rangle|^2\,dt = \sum_{j=1}^{\infty} \kappa_j^2 \int_{-\infty}^{\infty} |\langle e^{-itH_0}P_0^{(a)}g, \phi_j\rangle|^2\,dt.$$

Now, it follows from (A) that

$$(E) \le \sum_{j=1}^{\infty} \kappa_j^2 \cdot 2\pi N^2 = 2\pi N^2 \|F\|_2^2.$$

The proof is complete. ∎

For the following theorem, see e.g. [Y, Theorem 5.3.2].

THEOREM 6.1.2. *The weak wave operators* (6.2) *exist.*

Proof. (A) For any $f, f_0 \in \mathcal{H}$ we have

$$|\langle e^{it_2H_r}e^{-it_2H_0}f_0, f\rangle - \langle e^{it_1H_r}e^{-it_1H_0}f_0, f\rangle| \le \|J_r\| \Big(\int_{t_1}^{t_2} \|Fe^{-it_2H_0}f_0\|^2\,dt\Big)^{1/2} \Big(\int_{t_1}^{t_2} \|Fe^{-it_2H_r}f\|^2\,dt\Big)^{1/2}.$$

Indeed, for any $f, f_0 \in \mathcal{H}$,

$$\frac{d}{dt}\langle e^{-itH_0}f_0, e^{-itH_r}f\rangle = \langle(-iH_0)e^{-itH_0}f_0, e^{-itH_r}f\rangle + \langle e^{-itH_0}f_0, (-iH_r)e^{-itH_r}f\rangle$$
$$= -i\langle (H_r - H_0)e^{-itH_0}f_0, e^{-itH_r}f\rangle$$
$$= -i\langle V_r e^{-itH_0}f_0, e^{-itH_r}f\rangle = -i\langle J_rFe^{-itH_0}f_0, Fe^{-itH_r}f\rangle,$$

where in the last equality the decomposition $V_r = F^*J_rF$ was used. It follows that

$$\langle e^{it_2H_r}e^{-it_2H_0}f_0, f\rangle - \langle e^{it_1H_r}e^{-it_1H_0}f_0, f\rangle = -i\int_{t_1}^{t_2} \langle J_rFe^{-it_2H_0}f_0, Fe^{-it_2H_r}f\rangle\,dt.$$

Using the Schwarz inequality, this implies that

$$|\langle e^{it_2H_r}e^{-it_2H_0}f_0, f\rangle - \langle e^{it_1H_r}e^{-it_1H_0}f_0, f\rangle|$$
$$\le \|J_r\| \int_{t_1}^{t_2} \|Fe^{-it_2H_0}f_0\|\,\|Fe^{-it_2H_r}f\|\,dt$$
$$\le \|J_r\| \Big(\int_{t_1}^{t_2} \|Fe^{-it_2H_0}f_0\|^2\,dt\Big)^{1/2} \Big(\int_{t_1}^{t_2} \|Fe^{-it_2H_r}f\|^2\,dt\Big)^{1/2}.$$

(B) Let $N \in \mathbb{R}$. Let $g, g_0 \in \mathcal{H}$ be such that for a.e. $\lambda \in \Lambda(H_0; F)$,

$$\|\mathcal{E}_\lambda(H_0)P_0^{(a)}g_0\|_{\mathfrak{h}_\lambda^{(0)}} \le N \quad\text{and}\quad \|\mathcal{E}_\lambda(H_r)P_r^{(a)}g\|_{\mathfrak{h}_\lambda^{(r)}} \le N. \tag{6.3}$$

Applying the estimate (A) to the pair of vectors $f = P^{(a)}(H_r)g$ and $f_0 = P^{(a)}(H_0)g_0$, it now follows from the estimates (6.3) and Lemma 6.1.1, that

$$|\langle e^{-it_2H_r}e^{-it_2H_0}P^{(a)}(H_0)g_0, P^{(a)}(H_r)g\rangle - \langle e^{-it_1H_r}e^{-it_1H_0}P^{(a)}(H_0)g_0, P^{(a)}(H_r)g\rangle| \le \|J_r\| \cdot 2\pi N^2 \|F\|_2^2.$$

Consequently, the right hand side vanishes when $t_1, t_2 \to \pm\infty$. It follows that the limits

$$\lim_{t\to\pm\infty} \langle P_r^{(a)} e^{itH_r} e^{-itH_0} P_0^{(a)} g_0, g\rangle$$

exist. Since the set of vectors g_0, g which satisfy the estimate (6.3) for some N is dense in $\mathcal{H}$, it follows from the last estimate that the weak wave operators (6.2) exist. ∎

The following theorem and its proof follow verbatim [Y, Theorem 2.2.1].

THEOREM 6.1.3. *If the weak wave operators* $\overset{\mathrm{w}}{W}_\pm(H_r, H_0)$ *exist and*

$$\overset{\mathrm{w}}{W}_\pm(H_r, H_0)^* \, \overset{\mathrm{w}}{W}_\pm(H_r, H_0) = P_0^{(a)}, \tag{6.4}$$

then the strong wave operators $\overset{\mathrm{s}}{W}_\pm(H_r, H_0)$ *exist and coincide with the weak wave operators* $\overset{\mathrm{w}}{W}_\pm(H_r, H_0)$.

Proof. We have

$$\begin{aligned} E_\pm(t) &:= \|e^{itH_r} e^{-itH_0} P_0^{(a)} f - \overset{\mathrm{w}}{W}_\pm f\|^2 \\ &= \langle e^{itH_r} e^{-itH_0} P_0^{(a)} f - \overset{\mathrm{w}}{W}_\pm f, e^{itH_r} e^{-itH_0} P_0^{(a)} f - \overset{\mathrm{w}}{W}_\pm f\rangle \\ &= \langle P_0^{(a)} f, f\rangle - 2\,\mathrm{Re}\langle e^{itH_r} e^{-itH_0} P_0^{(a)} f, \overset{\mathrm{w}}{W}_\pm f\rangle + \langle \overset{\mathrm{w}}{W}_\pm f, \overset{\mathrm{w}}{W}_\pm f\rangle. \end{aligned}$$

Since $\overset{\mathrm{w}}{W}_\pm = P_r^{(a)} \, \overset{\mathrm{w}}{W}_\pm$, it follows from (6.2) that the second term on the right hand side of this equality converges to $-2\langle \overset{\mathrm{w}}{W}_\pm f, \overset{\mathrm{w}}{W}_\pm f\rangle$ as $t \to \pm\infty$. It now follows from (6.4) that

$$\lim_{t\to\pm\infty} E_\pm(t) = \langle P_0^{(a)} f, f\rangle - \langle \overset{\mathrm{w}}{W}{}_\pm^* \, \overset{\mathrm{w}}{W}_\pm f, f\rangle = 0.$$

That is, the strong wave operators $\overset{\mathrm{s}}{W}_\pm$ exist and are equal to $\overset{\mathrm{w}}{W}_\pm$. ∎

The next theorem is taken from [Y, Chapter 2].

THEOREM 6.1.4. *The strong wave operators* $\overset{\mathrm{s}}{W}_\pm$ *exist and coincide with* $W_\pm$.

Proof. (A) Let $f, g \in \mathcal{H}_1$ and let $\Lambda = \Lambda(H_r; F) \cap \Lambda(H_0; F)$. For every $\lambda \in \Lambda$ the vectors $f^{(r)}(\lambda) = \mathcal{E}_\lambda(H_r) f$ and $g^{(0)}(\lambda) = \mathcal{E}_\lambda(H_0) g$ are well-defined and the functions $f^{(r)}(\cdot)$ and $g^{(0)}(\cdot)$ are $\mathcal{H}$-measurable in the corresponding direct integrals, so that

$$\tilde f := P_r^{(a)} f = \int_\Lambda^\oplus f^{(r)}(\lambda)\, d\lambda, \qquad \tilde g := P_0^{(a)} g = \int_\Lambda^\oplus g^{(0)}(\lambda)\, d\lambda.$$

It follows from the definitions (5.15) and (5.6) of $W_\pm$ and $w_\pm(\lambda)$ that

$$\begin{aligned} \langle \tilde f, W_\pm(H_r, H_0)\tilde g\rangle &= \int_\Lambda \langle f^{(r)}(\lambda), w_\pm(\lambda; H_r, H_0) g^{(0)}(\lambda)\rangle_{\mathfrak{h}_\lambda^{(r)}}\, d\lambda \\ &= \int_\Lambda \langle \tilde f, \mathfrak{a}_\pm(\lambda; H_r, H_0)\tilde g\rangle_{1,-1}\, d\lambda. \end{aligned}$$

By the definition (5.1.4) of $\mathfrak{a}_\pm(\lambda)$, it follows from the last equality that

$$\langle \tilde f, W_\pm(H_r, H_0)\tilde g\rangle = \int_\Lambda \lim_{y\to 0} \frac{y}{\pi} \langle R_{\lambda\pm iy}(H_r)\tilde f, R_{\lambda\pm iy}(H_0)\tilde g\rangle\, d\lambda. \tag{6.5}$$

(B) We now show that the limit and the integral can be interchanged. Let Y be a Borel subset of Λ and let

$$f_y = \frac{y}{\pi} \langle R_{\lambda \pm iy}(H_r)\tilde f, R_{\lambda \pm iy}(H_0)\tilde g\rangle.$$

The Schwarz inequality implies

$$\begin{aligned}\int_Y |f_y|\,d\lambda &\leq \frac{y}{\pi}\int_Y \|R_{\lambda\pm iy}(H_r)\tilde f\|\,\|R_{\lambda\pm iy}(H_0)\tilde g\|\,d\lambda \\ &\leq \left(\frac{y}{\pi}\int_Y \|R_{\lambda\pm iy}(H_r)\tilde f\|^2\,d\lambda\right)^{1/2}\left(\frac{y}{\pi}\int_Y \|R_{\lambda\pm iy}(H_0)\tilde g\|^2\,d\lambda\right)^{1/2} \\ &\leq \left(\frac{1}{\pi}\int_Y \langle \operatorname{Im} R_{\lambda+iy}(H_r)\tilde f, \tilde f\rangle\,d\lambda\right)^{1/2}\left(\frac{1}{\pi}\int_Y \langle \operatorname{Im} R_{\lambda+iy}(H_0)\tilde g, \tilde g\rangle\,d\lambda\right)^{1/2}.\end{aligned}$$

Since $\tilde f$ is an absolutely continuous vector for H_r and since $\tilde g$ is an absolutely continuous vector for H_0, the functions $\frac{1}{\pi}\langle \operatorname{Im} R_{\lambda+iy}(H_r)\tilde f, \tilde f\rangle$ and $\frac{1}{\pi}\langle \operatorname{Im} R_{\lambda+iy}(H_0)\tilde g, \tilde g\rangle$ are Poisson integrals of the summable functions $\frac{d}{d\lambda}\langle E^{H_r}_\lambda \tilde f, \tilde f\rangle$ and $\frac{d}{d\lambda}\langle E^{H_0}_\lambda \tilde g, \tilde g\rangle$ respectively. From Lemma 1.3.2 and from the above estimate it now follows that for f_y the conditions of Vitali's Theorem 1.3.1 hold. This completes the proof of (A).

(C) We have $\overset{\mathrm{w}}{W}_\pm(H_r, H_0) = W_\pm(H_r, H_0)$. Indeed, using [Y, (2.7.2)], it follows from (6.5) and (B) that

$$\langle \tilde f, W_\pm(H_r, H_0)\tilde g\rangle = \lim_{\varepsilon\to 0} 2\varepsilon \int_0^\infty e^{-2\varepsilon t}\langle e^{\mp itH_r}\tilde f, e^{\mp itH_0}\tilde g\rangle\,dt.$$

Since, by Theorem 6.1.2, the function $t \mapsto \langle e^{\mp itH_r}\tilde f, e^{\mp itH_0}\tilde g\rangle$ has a limit, as $t\to\infty$, equal to $\langle \tilde f, \overset{\mathrm{w}}{W}_\pm(H_r, H_0)\tilde g\rangle$, it follows that the right hand side of the last equality is also equal to $\langle \tilde f, \overset{\mathrm{w}}{W}_\pm(H_r, H_0)\tilde g\rangle$. Hence,

$$\langle \tilde f, W_\pm(H_r, H_0)\tilde g\rangle = \langle \tilde f, \overset{\mathrm{w}}{W}_\pm(H_r, H_0)\tilde g\rangle.$$

Since for any self-adjoint operator H the set $P^{(a)}(H)\mathcal{H}_1$ is dense in $\mathcal{H}^{(a)}(H)$ and since both operators $\overset{\mathrm{w}}{W}_\pm(H_r, H_0)$ and $W_\pm(H_r, H_0)$ vanish on the singular subspace $\mathcal{H}^{(s)}(H_0)$ of H_0, it follows that $W_\pm(H_r, H_0) = \overset{\mathrm{w}}{W}_\pm(H_r, H_0)$.

(D) Since for $W_\pm$ the multiplicative property holds (Theorem 5.4.1(ii)), it follows from (C) that the multiplicative property holds also for the weak wave operator $\overset{\mathrm{w}}{W}_\pm$. Further, by Theorem 6.1.3 existence of the weak wave operator and the multiplicative property imply that the strong wave operator $\overset{\mathrm{s}}{W}_\pm$ exists and coincides with the wave operator as defined in (5.15). ∎

Remark 6.1.5. The operator $\overset{\mathrm{s}}{W}_\pm(H_r, H_0)$ acts on $\mathcal{H}$, while $W_\pm(H_r, H_0)$ acts on the direct integral $\mathfrak{H}$. In Theorem 6.1.4 by $W_\pm(H_r, H_0)$ one, of course, means the operator

$$\mathcal{E}^*(H_r)W_\pm(H_r, H_0)\mathcal{E}(H_0)\colon \mathcal{H}\to\mathcal{H}.$$

Theorem 6.1.4, in particular, shows that the operators $W_\pm(H_r, H_0)$ are independent of the choice of the frame F in the sense that the operators $\mathcal{E}^*(H_r)W_\pm(H_r, H_0)\mathcal{E}(H_0)$ are independent of F.

7. The scattering matrix

7.1. Definition of the scattering matrix. In [Y] the scattering matrix $S(\lambda; H_1, H_0)$ is defined via a direct integral decomposition of the scattering operator $\mathbf{S}(H_1, H_0)$. In our approach, we first define $S(\lambda; H_1, H_0)$, while the scattering operator $\mathbf{S}(H_1, H_0)$ is defined as a direct integral of $S(\lambda; H_1, H_0)$.

DEFINITION 7.1.1. For $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$ the *scattering matrix* $S(\lambda; H_r, H_0)$ is defined by the formula

$$S(\lambda; H_r, H_0) := w_+^*(\lambda; H_r, H_0) w_-(\lambda; H_r, H_0). \tag{7.1}$$

We list some properties of the scattering matrix which immediately follow from this definition (cf. [Y, Chapter 7]).

THEOREM 7.1.2. *Let* $\{H_r\}$ *be a path of operators which satisfy Assumption* 4.1.1. *Let* $\lambda \in \Lambda(H_0; F)$ *and* $r \notin R(\lambda; \{H_r\}, F)$. *Then:*

(i) $S(\lambda; H_r, H_0) \colon \mathfrak{h}_\lambda^{(0)} \to \mathfrak{h}_\lambda^{(0)}$ *is a unitary operator.*

(ii) *For any* h *such that* $r + h \notin R(\lambda; \{H_r\}, F)$,

$$S(\lambda; H_{r+h}, H_0) = w_+^*(\lambda; H_r, H_0) S(\lambda; H_{r+h}, H_r) w_-(\lambda; H_r, H_0).$$

(iii) *For any* h *such that* $r + h \notin R(\lambda; \{H_r\}, F)$,

$$S(\lambda; H_{r+h}, H_0) = w_+^*(\lambda; H_r, H_0) S(\lambda; H_{r+h}, H_r) w_+(\lambda; H_r, H_0) S(\lambda; H_r, H_0).$$

Proof. (i) By Corollary 5.3.8 the operators $w_+^*(\lambda; H_r, H_0)$ and $w_-(\lambda; H_r, H_0)$ are unitary. It follows that their product $S(\lambda; H_r, H_0) = w_+^*(\lambda; H_r, H_0) w_-(\lambda; H_r, H_0)$ is also unitary.

(ii) From the definition of the scattering matrix (7.1) and the multiplicative property of the wave matrix (Theorem 5.3.7) it follows that

$$\begin{aligned} S(\lambda; H_{r+h}, H_0) &= w_+^*(\lambda; H_{r+h}, H_0) w_-(\lambda; H_{r+h}, H_0) \\ &= (w_+(\lambda; H_{r+h}, H_r) w_+(\lambda; H_r, H_0))^* w_-(\lambda; H_{r+h}, H_r) w_-(\lambda; H_r, H_0) \\ &= w_+(\lambda; H_r, H_0)^* w_+(\lambda; H_{r+h}, H_r)^* w_-(\lambda; H_{r+h}, H_r) w_-(\lambda; H_r, H_0) \\ &= w_+(\lambda; H_r, H_0)^* S(\lambda; H_{r+h}, H_r) w_-(\lambda; H_r, H_0). \end{aligned}$$

Note that since $r, r + h \notin R(\lambda; \{H_r\}, F)$, all the operators above make sense.

(iii) It follows from (ii) and unitarity of the wave matrix (Corollary 5.3.8) that

$$\begin{aligned} S(\lambda; H_{r+h}, H_0) &= w_+(\lambda; H_r, H_0)^* S(\lambda; H_{r+h}, H_r) w_-(\lambda; H_r, H_0) \\ &= w_+(\lambda; H_r, H_0)^* S(\lambda; H_{r+h}, H_r) w_+(\lambda; H_r, H_0) \\ &\quad \cdot [w_+^*(\lambda; H_r, H_0) w_-(\lambda; H_r, H_0)] \\ &= w_+^*(\lambda; H_r, H_0) S(\lambda; H_{r+h}, H_r) w_+(\lambda; H_r, H_0) S(\lambda; H_r, H_0). \quad \blacksquare \end{aligned}$$

We define the *scattering operator* by the formula

$$\mathbf{S}(H_r, H_0) := \int_{\Lambda(H_r; F) \cap \Lambda(H_0; F)}^{\oplus} S(\lambda; H_r, H_0)\, d\lambda. \tag{7.2}$$

It follows from the definition of the wave operator (5.15) and the definition of the scattering matrix that

$$\mathbf{S}(H_r, H_0) = W_+^*(H_r, H_0) W_-(H_r, H_0),$$

which is the usual definition of the scattering operator.

By Remark 6.1.5, the definition (7.2) is independent of the choice of the frame operator F.

THEOREM 7.1.3 ([Y, Chapter 7]). *The scattering operator* (7.2) *has the following properties:*

(i) *The scattering operator* $\mathbf{S}(H_r, H_0)\colon \mathcal{H}^{(a)}(H_0) \to \mathcal{H}^{(a)}(H_0)$ *is unitary.*
(ii) $\mathbf{S}(H_{r+h}, H_0) = W_+(H_0, H_r)\mathbf{S}(H_{r+h}, H_r)W_-(H_r, H_0)$.
(iii) $\mathbf{S}(H_{r+h}, H_0) = W_+(H_0, H_r)\mathbf{S}(H_{r+h}, H_r)W_+(H_r, H_0)\mathbf{S}(H_r, H_0)$.
(iv) $\mathbf{S}(H_r, H_0)H_0 = H_0\mathbf{S}(H_r, H_0)$. *holds.*

Proof. (i) follows from Theorem 7.1.2(i); (ii) from Theorem 7.1.2(ii); (iii) from Theorem 7.1.2(iii); and (iv) from (7.1) and Theorem 7.2. ∎

7.2. Stationary formula for the scattering matrix. The aim of this subsection is to prove the stationary formula for the scattering matrix.

LEMMA 7.2.1. *If* $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$, *then*

$$\begin{aligned}(1 + R_{\lambda-i0}(H_0)V_r) \cdot \operatorname{Im} R_{\lambda+i0}(H_r) \cdot (1 + V_r R_{\lambda-i0}(H_0))\\ = \operatorname{Im} R_{\lambda+i0}(H_0)\big[(1 - 2iV_r[1 - R_{\lambda+i0}(H_r)V_r]) \operatorname{Im} R_{\lambda+i0}(H_0)\big] \quad (7.3)\end{aligned}$$

in $\mathcal{L}_1(\mathcal{H}_1, \mathcal{H}_{-1})$.

Proof. We write

$$R_0 = R_{\lambda+i0}(H_0), \quad R_0^* = R_{\lambda-i0}(H_0), \quad R_r = R_{\lambda+i0}(H_r), \quad R_r^* = R_{\lambda-i0}(H_r).$$

Then the last formula becomes

$$(1 + R_0^* V_r) \cdot \operatorname{Im} R_r \cdot (1 + V_r R_0^*) = \operatorname{Im} R_0[1 - 2iV_r(1 - R_r V_r) \operatorname{Im} R_0]. \quad (7.4)$$

Note that by the second resolvent identity

$$R_r = (1 - R_r V_r)R_0. \quad (7.5)$$

Using (5.4), one has

$$(1 + R_0^* V_r) \operatorname{Im} R_r = \operatorname{Im} R_0(1 - V_r R_r).$$

Further, using (7.5),

$$\begin{aligned}1 - 2iV_r(1 - R_r V_r) \operatorname{Im} R_0 &= 1 - V_r(1 - R_r V_r)(R_0 - R_0^*)\\ &= 1 - V_r(1 - R_r V_r)R_0 + V_r(1 - R_r V_r)R_0^*\\ &= 1 - V_r R_r + V_r(1 - R_r V_r)R_0^* = (1 - V_r R_r)(1 + V_r R_0^*).\end{aligned}$$

Combining the last two formulae completes the proof. ∎

In the following theorem, we establish for trace-class perturbations the well-known stationary formula for the scattering matrix (cf. [Y, Theorems 5.5.3, 5.5.4, 5.7.1]).

THEOREM 7.2.2. *For any $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$ we have the stationary formula for the scattering matrix,*

$$S(\lambda; H_r, H_0) = 1_\lambda - 2\pi i \mathcal{E}_\lambda(H_0) V_r (1 + R_{\lambda+i0}(H_0) V_r)^{-1} \mathcal{E}_\lambda^\diamondsuit(H_0). \tag{7.6}$$

(The meaning of notation 1_λ is clear, though the subscript λ will often be omitted).

Proof. For $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$, the second resolvent identity

$$R_z(H_r) - R_z(H_0) = -R_z(H_r) V_r R_z(H_0) = -R_z(H_0) V_r R_z(H_r)$$

implies that the stationary formula can be written as

$$S(\lambda; H_r, H_0) = 1 - 2\pi i \mathcal{E}_\lambda(H_0) V_r (1 - R_{\lambda+i0}(H_r) V_r) \mathcal{E}_\lambda^\diamondsuit(H_0). \tag{7.7}$$

It follows that it is enough to prove the equality

$$w_+^*(\lambda; H_r, H_0) w_-(\lambda; H_r, H_0) = 1 - 2\pi i \mathcal{E}_\lambda(H_0) V_r (1 - R_{\lambda+i0}(H_r) V_r) \mathcal{E}_\lambda^\diamondsuit(H_0).$$

Since $\mathcal{E}_\lambda(H_0)\mathcal{H}_1$ is dense in $\mathfrak{h}_\lambda^{(0)} = \mathfrak{h}_\lambda(H_0)$, it is enough to show that for any $f, g \in \mathcal{H}_1$,

$$\begin{aligned}&\langle \mathcal{E}_\lambda(H_0) f, w_+^*(\lambda; H_r, H_0) w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle_{\mathfrak{h}_\lambda^{(0)}} \\ &\qquad = \langle \mathcal{E}_\lambda f, (1 - 2\pi i \mathcal{E}_\lambda V_r (1 - R_{\lambda+i0}(H_r) V_r) \mathcal{E}_\lambda^\diamondsuit) \mathcal{E}_\lambda g \rangle_{\mathfrak{h}_\lambda^{(0)}}.\end{aligned}$$

In other words, using Lemma 7.2.1 and (5.5), it is enough to show that

$$\begin{aligned}(E) &:= \langle w_+(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) f, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle_{\mathfrak{h}_\lambda^{(r)}} \\ &= \left\langle f, (1 + R_{\lambda-i0}(H_0) V_r) \frac{1}{\pi} \operatorname{Im} R_{\lambda+i0}(H_r)(1 + V_r R_{\lambda-i0}(H_0)) g \right\rangle_{1,-1}.\end{aligned} \tag{7.8}$$

Let $\varepsilon > 0$. Since $\mathcal{E}_\lambda(H_r)\mathcal{H}_1$ is dense in $\mathfrak{h}_\lambda^{(r)}$ (see (3.2)), there exists $h \in \mathcal{H}_1$ such that the vector

$$a := w_+(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) f - \mathcal{E}_\lambda(H_r) h \in \mathfrak{h}_\lambda^{(r)} \tag{7.9}$$

has norm less than ε. The definition (5.6) of $w_-(\lambda; H_r, H_0)$ implies that

$$\begin{aligned}(E) &= \langle w_+(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) f, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle_{\mathfrak{h}_\lambda^{(r)}} \\ &= \langle \mathcal{E}_\lambda(H_r) h + a, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle_{\mathfrak{h}_\lambda^{(r)}} \\ &= \langle h, \mathfrak{a}_-(\lambda; H_r, H_0)(\lambda) g \rangle_{1,-1} + \langle a, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle_{\mathfrak{h}_\lambda^{(r)}}.\end{aligned}$$

So, by the second equality of (5.4),

$$(E) = \left\langle h, \frac{1}{\pi} \operatorname{Im} R_{\lambda+i0}(H_r)[1 + V_r R_{\lambda-i0}(H_0)] g \right\rangle + \langle a, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle.$$

Further, by (5.5) and (7.9),

$$\begin{aligned}(E) &= \langle \mathcal{E}_\lambda(H_r) h, \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)] g \rangle \\ &\quad + \langle a, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle \\ &= \langle w_+(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) f - a, \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)] g \rangle \\ &\quad + \langle a, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle \\ &= \langle \mathcal{E}_\lambda(H_0) f, w_+(\lambda; H_0, H_r) \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)] g \rangle \\ &\quad - \langle a, \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)] g \rangle + \langle a, w_-(\lambda; H_r, H_0) \mathcal{E}_\lambda(H_0) g \rangle.\end{aligned}$$

By the definition (5.6) of $w_+(\lambda; H_r, H_0)$, it follows that

$$(E) = \langle f, \mathfrak{a}_+(\lambda; H_0, H_r)[1 + V_r R_{\lambda-i0}(H_0)]g\rangle + \text{remainder},$$

where

$$\text{remainder} := \langle a, w_-(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0)g - \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)]g\rangle.$$

By the first equality of (5.4),

$$(E) = \left\langle f, [1 + R_{\lambda-i0}(H_0)V_r]\frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_r)[1 + V_r R_{\lambda-i0}(H_0)]g\right\rangle + \text{remainder}.$$

Since the norm of the remainder term can be made arbitrarily small, it follows that

$$(E) = \left\langle f, [1 + R_{\lambda-i0}(H_0)V_r]\frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_r)[1 + V_r R_{\lambda-i0}(H_0)]g\right\rangle. \ \blacksquare$$

As can be seen from the proof, the remainder term in the last proof is actually zero and so it does not depend on the choice of the vector $h \in \mathcal{H}_1$; that is, for any $f, g \in \mathcal{H}$,

$$\langle w_+(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0)f, w_-(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0)g - \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)]g\rangle = 0.$$

Since the set $w_+(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0)\mathcal{H}_1$ is dense in $\mathfrak{h}_\lambda(H_r)$, we obtain

Corollary 7.2.3. *For any* $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$,

$$w_-(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0) = \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda-i0}(H_0)].$$

From this equality and (7.8) it also follows that

$$w_+(\lambda; H_r, H_0)\mathcal{E}_\lambda(H_0) = \mathcal{E}_\lambda(H_r)[1 + V_r R_{\lambda+i0}(H_0)].$$

These equalities are analogues of Lippmann-Schwinger equations for scattering states (see e.g. [T]).

Corollary 7.2.4. *If* $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$, *then* $S(\lambda; H_r, H_0) \in 1 + \mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$.

Proof. Since $\mathcal{E}_\lambda^\diamondsuit \in \mathcal{L}_2(\mathfrak{h}_\lambda^{(0)}, \mathcal{H}_{-1})$, $V \in \mathcal{B}(\mathcal{H}_{-1}, \mathcal{H}_1)$, $R_{\lambda+i0}(H_0) \in \mathcal{L}_\infty(\mathcal{H}_1, \mathcal{H}_{-1})$ and $\mathcal{E}_\lambda \in \mathcal{L}_2(\mathcal{H}_1, \mathfrak{h}_\lambda^{(0)})$, this follows from (7.7). $\blacksquare$

Physicists (see e.g. [T]) write the stationary formula as in (7.6). As is often the case, the stationary formula, as written by physicists, does not have a rigorous mathematical sense.

M. Sh. Birman and S. B. Èntina [BE] created a mathematically rigorous stationary scattering theory for trace-class perturbations. In order to give the stationary formula a rigorous meaning, they factorized the perturbation V as G^*JG with a Hilbert–Schmidt operator $G\colon \mathcal{H} \to \mathcal{K}$ and a bounded operator $J\colon \mathcal{K} \to \mathcal{K}$, and rewrote the stationary formula for the scattering matrix in the form (see also [Y])

$$S(\lambda; H_0 + V, H_0) = 1 - 2\pi i Z(\lambda; G)(1 + JT_{\lambda+i0}(H_0))^{-1} J_r Z^*(\lambda; G), \tag{7.10}$$

where

$$Z(\lambda; G)f = \mathcal{F}(G^*f)(\lambda), \qquad T_z(H_0) = GR_z(H_0)G^*,$$

and where $\mathcal{F}$ is an isomorphism of the absolutely continuous (with respect to H_0) subspace of $\mathcal{H}$ to a direct integral of Hilbert spaces

$$\int_{\hat{\sigma}}^{\oplus} \mathfrak{h}_\lambda \, d\rho(\lambda)$$

such that

$$\mathcal{F}(H_0 f)(\lambda) = \lambda \mathcal{F}(f)(\lambda) \quad \text{a.e. } \lambda \in \mathbb{R}.$$

Existence of such an isomorphism is a consequence of the spectral theorem. The stationary formula can be rewritten in the form (7.10), since all ingredients of this formula can be given a rigorous sense (see [BE, Y]): $T_{\lambda+i0}(H_0)$ exists for a.e. λ by Theorem 1.9.2, and, while the operator $\mathcal{F}$ does not make sense at a given point λ of the spectral line, combined with a Hilbert–Schmidt operator G^* in $Z(\lambda; G)$, it defines a bounded operator for a.e. λ. In this way, the stationary formula is given a rigorous meaning for a.e. λ. One drawback of the classical approach of [BE] to stationary scattering theory is that it is impossible to keep track of the set of full Lebesgue measure for which the stationary formula holds (already because the isomorphism $\mathcal{F}$ is intrinsically defined for a.e. λ, but it cannot be defined at a given point λ).

In the approach to stationary scattering theory given in this paper, all the ingredients of the stationary formula—as written by physicists—are given a rigorous meaning; as a consequence, there is no need to consider operators such as $Z(\lambda; G)$. The role of these operators is taken over by the frame operator F.

One can also note here that, while factorizations such as $V = G^*JG$ have no physical meaning (at least I am not aware of any), the background frame operator F may have a physical meaning, since, as discussed in Subsection 2.1, in the case of the Hilbert space $L_2(M, g)$ with (M, g) a Riemannian manifold, F bears the same information as the Laplace operator Δ, which in its turn is determined by the metric, that is, by gravitation ([1]).

Proposition 7.2.5. *The scattering matrix $S(\lambda; H_r, H_0)$ is a meromorphic function of r with values in $1 + \mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$, which admits analytic continuation to all resonance points of the path $\{H_r\}$.*

Proof. Since $R_{\lambda+i0}(H_0)$ is compact, the function

$$\mathbb{R} \ni r \mapsto S(\lambda; H_r, H_0) \in 1 + \mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$$

admits meromorphic continuation to $\mathbb{C}$ by (7.6) and the analytic Fredholm alternative (see Theorem 1.8.3). As $S(\lambda; H_r, H_0)$ is also bounded (unitary-valued) on the set $\{r \in \mathbb{R} : \lambda \in \Lambda(H_r; F)\}$, which by Theorem 4.1.9 has discrete complement in $\mathbb{R}$, it follows that $S(\lambda; H_r, H_0)$ has analytic continuation to $\mathbb{R} \subset \mathbb{C}$, that is, the Laurent expansion of $S(\lambda; H_r, H_0)$ (as a function of the coupling constant r) in a neighbourhood of any resonance point $r_0 \in R(\lambda; \{H_r\}, F)$ does not have negative powers of $r - r_0$. ■

Though this proposition is quite straightforward, it seems to be new (to the best knowledge of the author). Proposition 7.2.5 asserts that the scattering matrix, in a sense,

([1]) I am not a physicist, and this is a purely speculative remark.

ignores resonance points. There is a modified “scattering matrix”

$$\widetilde{S}(\lambda+i0;H_r,H_0)=1-2ir\sqrt{\operatorname{Im}T_{\lambda+i0}(H_0)}J(1+rT_{\lambda+i0}(H_0)J)^{-1}\sqrt{\operatorname{Im}T_{\lambda+i0}(H_0)},$$

introduced in [Pu], which does notice resonance points. This has some implications discussed in [Az_2]; in the setting of this paper, they will be discussed in Section 9.

7.3. Infinitesimal scattering matrix. Let $\{H_r\}$ be a path of operators which satisfies Assumption 4.1.1.

If $\lambda \in \Lambda(H_0;F)$, then, by 2.15(vi), the Hilbert–Schmidt operator $\mathcal{E}_\lambda\colon \mathcal{H}_1 \to \mathfrak{h}_\lambda$ is well defined. Hence, for any $\lambda \in \Lambda(H_0;F)$, it is possible to introduce the *infinitesimal scattering matrix*

$$\Pi_{H_0}(\dot H_0)(\lambda)\colon \mathfrak{h}_\lambda^{(0)} \to \mathfrak{h}_\lambda^{(0)}$$

by the formula

$$\Pi_{H_0}(\dot H_0)(\lambda)=\mathcal{E}_\lambda(H_0)\dot H_0\mathcal{E}_\lambda^{\diamondsuit}(H_0), \tag{7.11}$$

where $\mathcal{E}_\lambda^{\diamondsuit}\colon \mathfrak{h}_\lambda \to \mathcal{H}_{-1}$ is a Hilbert–Schmidt operator as well (see Subsection 2.6.1). Here by $\dot H_0$ we mean the value of the trace-class derivative $\dot H_r$ at $r=0$. Since $\mathcal{E}_\lambda(H_0)$ and $\mathcal{E}_\lambda^{\diamondsuit}(H_0)$ are Hilbert–Schmidt operators, and $\dot H_0\colon \mathcal{H}_{-1}\to\mathcal{H}_1$ is bounded, it follows that $\Pi_{H_0}(\dot H_0)(\lambda)$ is a self-adjoint trace-class operator on the fiber Hilbert space $\mathfrak{h}_\lambda^{(0)}$.

The notion of infinitesimal scattering matrix was introduced in [Az_1].

We note the following simple property of $\Pi_H(V)(\lambda)$.

LEMMA 7.3.1. *The operator (transformator)*

$$\mathcal{A}(F)\ni V\mapsto \Pi_H(V)(\lambda)\in\mathcal{L}_1(\mathfrak{h}_\lambda(H_0))$$

is bounded.

Proof. This follows from the estimate

$$\|\mathcal{E}_\lambda(H_0)V\mathcal{E}_\lambda^{\diamondsuit}(H_0)\|_{\mathcal{L}_1(\mathfrak{h}_\lambda)}\le\|\mathcal{E}_\lambda\|_{\mathcal{L}_2(\mathcal{H}_1,\mathfrak{h}_\lambda)}\,\|V\|_{\mathcal{B}(\mathcal{H}_{-1},\mathcal{H}_1)}\,\|\mathcal{E}_\lambda^{\diamondsuit}\|_{\mathcal{L}_2(\mathfrak{h}_\lambda,\mathcal{H}_{-1})}. \ \blacksquare$$

The dependence of $\Pi_H(V)(\lambda)$ on H does not make an exact sense, since for different H the infinitesimal scattering matrix acts in different Hilbert spaces $\mathfrak{h}_\lambda(H)$. But given an analytic path $\{H_r\}$ of operators, we can identify the Hilbert spaces $\mathfrak{h}_\lambda(H_r)$ and $\mathfrak{h}_\lambda(H_s)$ in a natural way via the unitary operator $w_\pm(\lambda;H_r,H_s)$. So, one can ask how the operator-function

$$\mathbb{R}\ni r\mapsto w_\pm(\lambda;H_0,H_r)\Pi_{H_r}(V)(\lambda)w_\pm(\lambda;H_r,H_0)\in\mathcal{L}_1(\mathfrak{h}_\lambda(H_0))$$

depends on r. It turns out that it is very regular.

As for dependence on λ, in the context of arbitrary self-adjoint operators, the dependence of $\Pi_H(V)(\lambda)$ on λ has to be very bad.

LEMMA 7.3.2. *Let $\{H_r\}$ be a path as above. Let r_0 be a point of analyticity of H_r. If $\lambda\in\Lambda(H_{r_0};F)$, then $\lambda\in\Lambda(H_r;F)$ for all r close enough to r_0 and*

$$\frac{d}{dr}S(\lambda;H_r,H_{r_0})\bigg|_{r=r_0}=-2\pi i\Pi_{H_{r_0}}(\dot H_{r_0})(\lambda),$$

where the derivative is taken in the $\mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$-topology.

Proof. By Theorem 4.1.9, if $\lambda \in \Lambda(H_{r_0}; F)$, then $\lambda \in \Lambda(H_r; F)$ for all r from some neighbourhood of r_0. Without loss of generality we can assume that $r_0 = 0$. We have

$$\begin{aligned} &\frac{d}{dr} V_r(1 + R_{\lambda+i0}(H_0)V_r)^{-1} \\ &\qquad = \dot{V}_r(1 + R_{\lambda+i0}(H_0)V_r)^{-1} \\ &\qquad\quad - V_r(1 + R_{\lambda+i0}(H_0)V_r)^{-1} R_{\lambda+i0}(H_0)\dot{V}_r(1 + R_{\lambda+i0}(H_0)V_r)^{-1}, \end{aligned} \tag{7.12}$$

where the derivative is taken in $\mathcal{B}(\mathcal{H}_{-1}, \mathcal{H}_1)$. Since $V_0 = 0$ and $\dot{H}_r = \dot{V}_r$, this and Theorem 7.2.2 imply that

$$\begin{aligned} &\frac{d}{dr} S(\lambda; H_r, H_0)\Big|_{r=0} \\ &\qquad = \frac{d}{dr}(1_\lambda - 2\pi i \mathcal{E}_\lambda(H_0)V_r(1 + R_{\lambda+i0}(H_0)V_r)^{-1}\mathcal{E}_\lambda^\diamondsuit(H_0))\Big|_{r=0} \\ &\qquad = -2\pi i \mathcal{E}_\lambda(H_0) \cdot \frac{d}{dr}(V_r(1 + R_{\lambda+i0}(H_0)V_r)^{-1})\Big|_{r=0} \cdot \mathcal{E}_\lambda^\diamondsuit(H_0) \\ &\qquad = -2\pi i \mathcal{E}_\lambda(H_0)\dot{H}(0)\mathcal{E}_\lambda^\diamondsuit(H_0). \end{aligned} \tag{7.13}$$

This and (7.11) complete the proof. ■

THEOREM 7.3.3. *If $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$, then*

$$\frac{d}{dr} S(\lambda; H_r, H_0) = -2\pi i w_+(\lambda; H_0, H_r)\Pi_{H_r}(\dot{H}_r)(\lambda)w_+(\lambda; H_r, H_0)S(\lambda; H_r, H_0), \tag{7.14}$$

where the derivative is taken in the trace-class norm.

Proof. By Theorem 4.1.9, $\lambda \in \Lambda(H_{r+h}; F)$ for all h small enough. It follows from Theorem 7.1.2(iii) and unitarity of $w_\pm(\lambda; H_r, H_0)$ (Corollary 5.3.8) that

$$\begin{aligned} &S(\lambda; H_{r+h}, H_0) - S(\lambda; H_r, H_0) \\ &\qquad = w_+(\lambda; H_0, H_r)(S(\lambda; H_{r+h}, H_r) - 1_\lambda)w_+(\lambda; H_r, H_0)S(\lambda; H_r, H_0). \end{aligned}$$

Dividing this equality by h and taking the trace-class limit $h \to 0$ we get

$$\begin{aligned} &\frac{d}{dh} S(\lambda; H_{r+h}, H_0)\Big|_{h=0} \\ &\qquad = w_+(\lambda; H_0, H_r)\frac{d}{dh} S(\lambda; H_{r+h}, H_r)\Big|_{h=0} w_+(\lambda; H_r, H_0)S(\lambda; H_r, H_0). \end{aligned}$$

So, Lemma 7.3.2 completes the proof. ■

The definition of the chronological exponential Texp, used in the next theorem, is given in Appendix 9.7.

THEOREM 7.3.4. *Let $\{H_r\}$ be a path of operators which satisfies Assumption 4.1.1. If $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$, then*

$$S(\lambda; H_r, H_0) = \mathrm{Texp}\left(-2\pi i \int_0^r w_+(\lambda; H_0, H_s)\Pi_{H_s}(\dot{H}_s)(\lambda)w_+(\lambda; H_s, H_0)\, ds\right), \tag{7.15}$$

where the chronological exponential is taken in the trace-class norm.

Proof. By Theorem 4.1.9, the definition (7.11) of the infinitesimal scattering matrix and Proposition 5.2.2, the integral in (7.15) makes sense for all s except the discrete resonance set $R(\lambda; \{H_r\}, F)$. By Proposition 7.2.5 and (7.12), the derivative $\frac{d}{dr} S(\lambda; H_r, H_0)$ is piecewise $\mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$-analytic. Since $\mathbb{R} \ni r \mapsto S(\lambda; H_r, H_0)$ is also piecewise $\mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$-analytic, by (7.14) the function

$$\begin{aligned} r \mapsto w_+(\lambda; H_0, H_r)\Pi_{H_r}(\dot H_r)(\lambda) w_+(\lambda; H_r, H_0) \\ = -\frac{1}{2\pi i}\left[\frac{d}{dr} S(\lambda; H_r, H_0)\right] S(\lambda; H_r, H_0)^{-1} \qquad (7.16) \end{aligned}$$

is also piecewise $\mathcal{L}_1(\mathfrak{h}_\lambda^{(0)})$-analytic. Hence, integration of the equation (7.14) by Lemma A.1.1 gives (7.15). ∎

COROLLARY 7.3.5. *Let $\{H_r\}$ be a path of operators which satisfies Assumption* 4.1.1 *and let $\lambda \in \Lambda(H_0; F)$. The function*

$$\mathbb{R} \ni r \mapsto \operatorname{Tr}(\Pi_{H_r}(\dot H_r)(\lambda))$$

is piecewise analytic (not necessarily continuous). Analyticity of this path may fail only at those points where $r \mapsto S(\lambda; H_r, H_0)$ is not analytic.

Proof. This follows from (7.16), unitarity of the wave matrix $w_+(\lambda; H_0, H_r)$ (Corollary 5.3.8) and unitarity and analyticity of the scattering matrix $S(\lambda; H_r, H_0)$ as a function of r (Proposition 7.2.5). ∎

One can also prove the following formula:

$$S(\lambda; H_r, H_0) = \overrightarrow{\exp}\left(-2\pi i \int_0^r w_-(\lambda; H_0, H_s)\Pi_{H_s}(\dot H_s)(\lambda) w_-(\lambda; H_s, H_0)\, ds\right), \qquad (7.17)$$

where the right chronological exponential $\overrightarrow{\exp}$ is defined by

$$\overrightarrow{\exp}\left(\frac{1}{i}\int_a^t A(s)\, ds\right) = 1 + \sum_{k=1}^\infty \frac{1}{i^k}\int_a^t dt_k \int_a^{t_k} dt_{k-1} \ldots \int_a^{t_2} dt_1 A(t_1)\ldots A(t_k).$$

8. Absolutely continuous and singular spectral shift functions

8.1. Infinitesimal spectral flow. In this subsection we prove that the trace of the infinitesimal scattering matrix is a density of the absolutely continuous part of the infinitesimal spectral flow.

We recall that if $A\colon \mathcal{H} \to \mathcal{K}$ and $B\colon \mathcal{K} \to \mathcal{H}$ are bounded operators such that AB and BA are trace-class operators in the Hilbert spaces $\mathcal{K}$ and $\mathcal{H}$ respectively, then

$$\operatorname{Tr}_{\mathcal{K}}(AB) = \operatorname{Tr}_{\mathcal{H}}(BA). \qquad (8.1)$$

Let $\{H_r\}$ be a path of self-adjoint operators which satisfies Assumption 4.1.1. In addition, we will use the condition

$$\sum_{j,k=1}^\infty \kappa_j \kappa_k J_{jk}^r \quad \text{is absolutely convergent,} \qquad (8.2)$$

where $V_r = F^* J_r F$, and (J_{jk}^r) is the matrix of J_r in the basis (ψ_k), i.e., $J_{jk}^r = \langle \psi_j, J_r \psi_k\rangle$.

Obviously, for a straight line path $H_r = H_0 + rV$, there exists a frame F such that this additional condition holds.

REMARK. V. V. Peller constructed an example of a trace-class operator $A = (a_{ij})$ and a bounded operator $B = (b_{ij})$ on ℓ_2 such that the double series $\sum_{i,j=1}^{\infty} |a_{ij} b_{ij}|$ diverges ([1]).

LEMMA 8.1.1. *Let F be a frame operator on a Hilbert space $\mathcal{H}$. Let $\{H_r\}$ be a path of operators on $\mathcal{H}$ such that Assumption* 4.1.1 *and* (8.2) *hold. For any r the double series*

$$\sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \kappa_j \kappa_k J_{jk}^r \langle \phi_j(\lambda), \phi_k(\lambda) \rangle$$

is absolutely convergent for a.e. $\lambda \in \Lambda(H_0; F)$ and the function

$$\Lambda(H_0; F) \ni \lambda \mapsto \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \kappa_j \kappa_k |J_{jk}^r \langle \phi_j(\lambda), \phi_k(\lambda) \rangle|$$

is integrable.

Proof. It follows from the assumption (8.2) and Corollary 3.1.4 that it is enough to prove the following assertion.

If a non-negative series $\sum_{j=1}^{\infty} a_n$ is convergent (to A) and if a sequence of integrable functions $f_1, f_2, \ldots$ is such that $\|f_j\|_{L_1} \le 1$ for all $j = 1, 2, \ldots$, then the series

$$\sum_{j=1}^{\infty} a_j f_j$$

is absolutely convergent a.e. and its sum is integrable.

The series $g(x) := \sum_{j=1}^{\infty} a_j |f_j|(x)$ is convergent (so far, possibly to $+\infty$) a.e. Since

$$\int \sum_{j=1}^{N} a_j |f_j|(x)\, dx \le A$$

for all N, the series $\sum_{j=1}^{\infty} a_j |f_j|$ is absolutely convergent a.e. and its sum $g(x)$ is integrable. Since

$$\sum_{j=1}^{N} a_j |f_j|(x) \le g(x),$$

it follows, by the Lebesgue dominated convergence theorem, that the series above is absolutely convergent and its sum is integrable. ■

PROPOSITION 8.1.2. *Let H_0 be a self-adjoint operator on a framed Hilbert space $(\mathcal{H}, F)$. The non-negative function*

$$\Lambda(H_0; F) \ni \lambda \mapsto \operatorname{Tr} \phi(\lambda) = \frac{1}{\pi} \operatorname{Tr}(F \operatorname{Im} R_{\lambda+i0}(H_0) F^*)$$

is summable and

$$\int_{\Lambda(H_0;F)} \operatorname{Tr} \phi(\lambda)\, d\lambda = \operatorname{Tr}(F E^{(a)} F^*).$$

([1]) Private communication.

Proof. Using (3.8), we have

$$\begin{aligned}\int \operatorname{Tr} \phi(\lambda)\, d\lambda &= \frac{1}{\pi} \int \sum_{j=1}^{\infty} \kappa_j^2 \langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\phi_j \rangle \, d\lambda \\ &= \frac{1}{\pi} \sum_{j=1}^{\infty} \int \kappa_j^2 \langle \phi_j, \operatorname{Im} R_{\lambda+i0}(H_0)\phi_j \rangle \, d\lambda \\ &= \frac{1}{\pi} \sum_{j=1}^{\infty} \int \langle F^*\psi_j, \operatorname{Im} R_{\lambda+i0}(H_0) F^*\psi_j \rangle \, d\lambda \\ &= \sum_{j=1}^{\infty} \langle \psi_j, F E^{(a)} F^* \psi_j \rangle = \operatorname{Tr}(F E^{(a)} F^*). \ \blacksquare\end{aligned}$$

THEOREM 8.1.3. *Let H_0 be a self-adjoint operator on a Hilbert space with a frame F. Let V be a trace-class operator such that for $V_r = rV$ the condition* (4.2) *holds. Then for any bounded measurable function h,*

$$\operatorname{Tr}(V h(H_0^{(a)})) = \int_{\Lambda(H_0;F)} h(\lambda) \operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V)(\lambda))\, d\lambda.$$

Proof. (A) First we prove the claim assuming (8.2). Since V satisfies (4.2), it has the representation

$$V = F^* J F, \tag{8.3}$$

where $J \colon \mathcal{K} \to \mathcal{K}$ is a bounded self-adjoint operator (not necessarily invertible). We recall that the frame operator F is given by (2.3). Let (J_{jk}) be the matrix of J in the basis (ψ_j) (see (2.3)), i.e.

$$J\psi_j = \sum_{k=1}^{\infty} J_{jk} \psi_k. \tag{8.4}$$

Using (8.1) and (8.3), we have

$$\operatorname{Tr}_{\mathcal{H}}(V h(H_0^{(a)})) = \operatorname{Tr}_{\mathcal{K}}(J F h(H_0^{(a)}) F^*).$$

Calculation of the trace on the right hand side of this formula in the orthonormal basis (ψ_j) of $\mathcal{K}$, together with (8.4) and (2.4), gives

$$\begin{aligned}\operatorname{Tr}_{\mathcal{H}}(V h(H_0^{(a)})) &= \sum_{j=1}^{\infty} \langle J F h(H_0^{(a)}) F^* \psi_j, \psi_j \rangle = \sum_{j=1}^{\infty} \langle h(H_0^{(a)}) F^* \psi_j, F^* J \psi_j \rangle \\ &= \sum_{j=1}^{\infty} \Big\langle h(H_0^{(a)}) F^* \psi_j, F^* \sum_{k=1}^{\infty} J_{jk} \psi_k \Big\rangle = \sum_{j=1}^{\infty} \kappa_j \Big\langle h(H_0^{(a)}) \phi_j, \sum_{k=1}^{\infty} J_{jk} \kappa_k \phi_k \Big\rangle \\ &= \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \kappa_j \kappa_k J_{jk} \langle h(H_0^{(a)}) \phi_j, \phi_k \rangle.\end{aligned}$$

This double sum is absolutely convergent by (8.2) and since $|\langle h(H_0^{(a)})\phi_j, \phi_k\rangle| \le \|h\|_\infty$.

Now, combining the last equality with Theorem 3.4.1 and Corollary 3.3.4 implies

$$\operatorname{Tr}_{\mathcal{H}}(V h(H_0^{(a)})) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \kappa_j \kappa_k J_{jk} \int_{\Lambda(H_0;F)} h(\lambda) \langle \phi_j(\lambda), \phi_k(\lambda) \rangle_{\mathfrak{h}_\lambda} \, d\lambda.$$

It follows from Lemma 8.1.1 that the integral and summations can be interchanged:

$$\operatorname{Tr}_{\mathcal{H}}(Vh(H_0^{(a)})) = \int_{\Lambda(H_0;F)} h(\lambda) \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \kappa_j\kappa_k J_{jk}\langle \phi_j(\lambda), \phi_k(\lambda)\rangle_{\mathfrak{h}_\lambda}\, d\lambda. \tag{8.5}$$

On the other hand, by (8.1) and (8.3), for any $\lambda \in \Lambda(H_0; F)$,

$$\operatorname{Tr}_{\mathfrak{h}_\lambda}(\mathcal{E}_\lambda V \mathcal{E}_\lambda^{\diamondsuit}) = \operatorname{Tr}_{\mathcal{K}}(JF\mathcal{E}_\lambda^{\diamondsuit}\mathcal{E}_\lambda F^*).$$

Similarly, evaluation of the last trace in the orthonormal basis (ψ_j) of $\mathcal{K}$ gives

$$\begin{aligned}\operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V)(\lambda)) &= \operatorname{Tr}_{\mathfrak{h}_\lambda}(\mathcal{E}_\lambda V\mathcal{E}_\lambda^{\diamondsuit}) = \sum_{j=1}^{\infty}\langle \mathcal{E}_\lambda^{\diamondsuit}\mathcal{E}_\lambda F^*\psi_j, F^*J\psi_j\rangle_{-1,1} \\ &= \sum_{j=1}^{\infty}\langle \mathcal{E}_\lambda F^*\psi_j, \mathcal{E}_\lambda F^* J\psi_j\rangle_{\mathfrak{h}_\lambda} = \sum_{j=1}^{\infty}\kappa_j \Big\langle \mathcal{E}_\lambda\phi_j, \mathcal{E}_\lambda \sum_{k=1}^{\infty} J_{jk}\kappa_k\phi_k\Big\rangle_{\mathfrak{h}_\lambda} \\ &= \sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\kappa_j\kappa_k J_{jk}\langle \mathcal{E}_\lambda\phi_j, \mathcal{E}_\lambda\phi_k\rangle_{\mathfrak{h}_\lambda}.\end{aligned}$$

(The last equality holds, since $\sum_{k=1}^{\infty}$ converges absolutely.) Combining this equality with (8.5) completes the proof of (A).

(B) Plainly, the set of operators J which satisfy (8.2) is dense in $\mathcal{B}(\mathcal{K})$ in the strong operator topology. So, let $J \in \mathcal{B}(\mathcal{K})$ and let $J_1, J_2, \ldots$ be a sequence of operators converging to J in the strong operator topology and such that all J_n satisfy (8.2). Convergence in the strong operator topology implies that $J_1, J_2, \ldots$ are uniformly bounded. We have

$$\begin{aligned}\operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V)(\lambda)) &= \operatorname{Tr}_{\mathcal{H}_1}(V\mathcal{E}_\lambda^{\diamondsuit}\mathcal{E}_\lambda) = \operatorname{Tr}_{\mathcal{H}_1}\Big(V\frac{1}{\pi}\operatorname{Im} R_{\lambda+i0}(H_0)\Big) \\ &= \operatorname{Tr}_{\mathcal{H}}\Big(J\frac{1}{\pi}F\operatorname{Im} R_{\lambda+i0}(H_0)F^*\Big).\end{aligned}$$

It now follows from Lemma 1.6.2 that for all $\lambda \in \Lambda(H_0; F)$,

$$\operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V_n)(\lambda)) \to \operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V)(\lambda))$$

as $n \to \infty$, where $V_n = F^*J_nF$. Since the norms of the operators $J_1, J_2, \ldots$ are uniformly bounded (by, say, $C > 0$), the summable functions $\lambda \mapsto \operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V_n)(\lambda))$ are dominated by a single summable (by Proposition 8.1.2) function $C\operatorname{Tr}_{\mathcal{H}}(\frac{1}{\pi}F\operatorname{Im}R_{\lambda+i0}(H_0)F^*)$.

It now follows from the Lebesgue dominated convergence theorem that

$$\|\operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V_n)(\cdot)) - \operatorname{Tr}_{\mathfrak{h}_\lambda}(\Pi_{H_0}(V)(\cdot))\|_1 \to 0.$$

(C) Combining (A), (B) and Lemma 1.6.2 completes the proof. ∎

The *infinitesimal spectral flow* $\Phi_{H_0}(V)$ is the distribution on $\mathbb{R}$ defined by the formula

$$\Phi_{H_0}(V)(\phi) = \operatorname{Tr}(V\phi(H_0)).$$

This notion was introduced in [ACS] and developed in [AS, Az$_1$]. The terminology is justified by the following classical formula from formal perturbation theory (see e.g. [LL, (38.6)]):

$$E_n^{(1)} = V_{nn},$$

where $V_{nn} = \langle n|V|n\rangle$ is the matrix element of the perturbation V, and $E_n^{(1)}$ denotes the first correction term for the nth eigenvalue $E_n^{(0)}$ (corresponding to $|n\rangle$) of the unperturbed operator H_0 perturbed by V. If the support of ϕ contains only the eigenvalue $E_n^{(0)}$ and $\phi(E_n^{(0)}) = 1$, then $\operatorname{Tr}(V\phi(H_0)) = V_{nn}$. So, $\Phi_{H_0}(V)(\phi)$ measures the shift of eigenvalues of H_0. Another justification is that, according to the Birman–Solomyak formula (1) (see Introduction), the spectral shift function is the integral of the infinitesimal spectral flow $\Phi_{H_r}(V)(\delta)$.

Remark 8.1.4. From now on, for an absolutely continuous measure μ we denote its density by the same symbol. So, in $\mu(\phi)$, $\phi \in C_c(\mathbb{R})$, μ is a measure, while in $\mu(\lambda)$, $\lambda \in \mathbb{R}$, μ is a function.

Actually, $\Phi_{H_0}(V)$ is a measure [AS]. So, one can introduce the absolutely continuous and singular parts of the infinitesimal spectral flow:

$$\Phi_{H_0}^{(a)}(V)(\phi) = \operatorname{Tr}(V\phi(H_0^{(a)})), \quad \Phi_{H_0}^{(s)}(V)(\phi) = \operatorname{Tr}(V\phi(H_0^{(s)})).$$

Recall (see (7.11)) that for every $\lambda \in \Lambda(H_0; F)$ and any $V \in \mathcal{A}(F)$ (see (4.1) for the definition of $\mathcal{A}(F)$), we have a trace class operator

$$\Pi_{H_0}(V)(\lambda) \colon \mathfrak{h}_\lambda^{(0)} \to \mathfrak{h}_\lambda^{(0)}.$$

We define the *standard density* function of the absolutely continuous infinitesimal spectral flow by the formula

$$\Phi_{H_0}^{(a)}(V)(\lambda) := \operatorname{Tr}(\Pi_{H_0}(V)(\lambda)) \quad \text{for all } \lambda \in \Lambda(H_0; F), \tag{8.6}$$

where $V \in \mathcal{A}(F)$, and where, allowing a little abuse of notation ([2]), we denote the density of the infinitesimal spectral flow $\Phi_{H_0}^{(a)}(V)$ by the same symbol $\Phi_{H_0}^{(a)}(V)(\cdot)$. Since $\Phi_{H_0}^{(a)}(V)$ is absolutely continuous, the usage of this notation should not cause any problems. This terminology and notation are justified by Theorem 8.1.3.

The absolutely continuous part $\Phi_{H_0}^{(a)}(\cdot)(\lambda)$ of the infinitesimal spectral flow can be viewed as a one-form on the affine space of operators

$$H_0 + \mathcal{A}(F),$$

where $\mathcal{A}(F)$ is defined by (4.1).

The standard density $\Phi_{H_0}^{(a)}(V)(\cdot)$ of the absolutely continuous part of the infinitesimal spectral flow may depend on the frame operator F. But, as Theorem 8.1.3 shows, for any two frames the corresponding standard densities are equal a.e.

Corollary 8.1.5. *Let H_0 be a self-adjoint operator and let V be a trace-class self-adjoint operator. For any two frame operators F_1 and F_2 such that $V \in \mathcal{A}(F_1) \cap \mathcal{A}(F_2)$, the standard densities* (8.6) *of the absolutely continuous part of the infinitesimal spectral flow coincide a.e.*

Proof. Indeed, the left hand side of the formula in Theorem 8.1.3 does not depend on F. ■

Recall that $\mathcal{A}(F)$ is the vector space of trace-class self-adjoint operators, associated with a given frame F (see (4.1)).

([2]) See Remark 8.1.4.

LEMMA 8.1.6. *Let H be a self-adjoint operator on a Hilbert space with frame F and let $V \in \mathcal{A}(F)$. The function $\Lambda(H,F) \ni \lambda \mapsto \Phi_H^{(a)}(V)(\lambda)$ is summable and its L_1-norm is $\leq \|V\|_1$.*

Proof. By Theorem 8.1.3, this function is a density of an absolutely continuous finite measure $\phi \mapsto \Phi_H^{(a)}(V)(\phi)$. By the same theorem, its L_1-norm is $\leq \|V\|_1$. ■

One can consider the resonance set as a set-function of two variables r and λ:

$$\gamma(\{H_r\}; F) := \{(\lambda, r) \in \mathbb{R}^2 : \lambda \in \Lambda(H_r; F)\}.$$

LEMMA 8.1.7. *Let $\{H_r\}$ be a path of self-adjoint operators which satisfies Assumption 4.1.1. The set $\gamma(\{H_r\}; F) \subset \mathbb{R}^2$ is Borel measurable and the function (see (8.6))*

$$\gamma(\{H_r\}; F) \ni (\lambda, r) \mapsto \Phi_{H_r}^{(a)}(\dot{H}_r)(\lambda) \tag{8.7}$$

is also measurable. Moreover, the complement of $\gamma(\{H_r\}; F)$ is a null set in $\mathbb{R}^2$.

Proof. The set $\gamma(\{H_r\}; F)$ is Borel measurable since it is the set of points of convergence of two families of continuous functions

$$T_z(H_r) = F R_z(H_r) F^* \quad \text{and} \quad \operatorname{Im} T_z(H_r)$$

of two variables r and $z = \lambda + iy$ (see Definition 2.4.1), as $y \to 0^+$.

The function $(\lambda, r) \mapsto \Phi_{H_r}^{(a)}(\dot{H}_r)(\lambda)$ is measurable since

$$\begin{aligned}\Phi_{H_r}^{(a)}(\dot{H}_r)(\lambda) &= \operatorname{Tr}(\Pi_{H_r}(\dot{H}_r)(\lambda)) = \operatorname{Tr}(\mathcal{E}_\lambda(H_r)\dot{H}_r\mathcal{E}_\lambda^\diamondsuit(H_r)) \\ &= \lim_{y\to 0^+} \operatorname{Tr}(\mathcal{E}_{\lambda+iy}(H_r)\dot{H}_r\mathcal{E}_{\lambda+iy}^\diamondsuit(H_r)),\end{aligned}$$

where the last equality follows from the fact that $\mathcal{E}_{\lambda+iy}^\diamondsuit(H_r) \colon \mathfrak{h}_\lambda^{(r)} \to \mathcal{H}_{-1}$ is Hilbert–Schmidt (see Subsection 2.15), $\dot{H}_r \colon \mathcal{H}_{-1} \to \mathcal{H}_1$ is bounded and $\mathcal{E}_{\lambda+iy}(H_r) \colon \mathcal{H}_1 \to \mathfrak{h}_\lambda^{(r)}$ is also Hilbert–Schmidt, and the operators $\mathcal{E}_{\lambda+iy}^\diamondsuit(H_r)$, $\mathcal{E}_{\lambda+iy}(H_r)$ converge to $\mathcal{E}_{\lambda+i0}^\diamondsuit(H_r)$, $\mathcal{E}_{\lambda+i0}(H_r)$ in the Hilbert–Schmidt norm, so that the product $\mathcal{E}_{\lambda+iy}(H_r)\dot{H}_r\mathcal{E}_{\lambda+iy}^\diamondsuit(H_r)$ converges to $\mathcal{E}_\lambda(H_r)\dot{H}_r\mathcal{E}_\lambda^\diamondsuit(H_r)$ in the trace-class norm, as $y \to 0^+$.

That the complement of $\gamma(\{H_r\}; F)$ is a null set in $\mathbb{R}^2$ now follows from Fubini's theorem, from the discreteness property of the resonance set with respect to r (Theorem 4.1.9) and from the fact that $\Lambda(H_r; F)$ is a full set (Proposition 2.4.2). ■

8.2. Absolutely continuous and singular spectral shift functions. Let

$$\gamma = \{H_r : r \in [0,1]\}$$

be a continuous piecewise real-analytic path of operators.

For the given path γ, we define the spectral shift function ξ and its absolutely continuous $\xi^{(a)}$ and singular $\xi^{(s)}$ parts as distributions by the formulae

$$\xi_\gamma(\phi; H_1, H_0) = \xi(\phi; H_1, H_0) = \int_0^1 \Phi_{H_r}(\dot{H}_r)(\phi)\, dr, \quad \phi \in C_c^\infty(\mathbb{R}), \tag{8.8}$$

$$\xi_\gamma^{(a)}(\phi; H_1, H_0) = \int_0^1 \Phi_{H_r}^{(a)}(\dot{H}_r)(\phi)\, dr, \quad \phi \in C_c^\infty(\mathbb{R}), \tag{8.9}$$

$$\xi_\gamma^{(s)}(\phi; H_1, H_0) = \int_0^1 \Phi_{H_r}^{(s)}(\dot{H}_r)(\phi)\, dr, \quad \phi \in C_c^\infty(\mathbb{R}). \tag{8.10}$$

For the straight line path $\{H_r = H_0 + rV\}$, the first of these formulae is the Birman–Solomyak spectral averaging formula [BS$_2$], which shows that the definition of the spectral shift function, given above, coincides with the classical definition of M. G. Kreĭn [Kr]. It was shown in [AS] that the integral in (8.8) is the same for all continuous piecewise analytic paths connecting H_0 and H_1.

While ξ does not depend on the path γ connecting H_0 and H_1, the distributions $\xi^{(a)}$ and $\xi^{(s)}$ depend on the path (see Subsection 8.3).

Lemma 8.2.1. *Let $\gamma = \{H_r\}$ be a path which satisfies Assumption 4.1.1. The distribution $\xi_\gamma^{(a)}$ is a finite absolutely continuous measure with density* ([3])

$$\xi_\gamma^{(a)}(\lambda; H_1, H_0) := \int_0^1 \Phi_{H_r}^{(a)}(\dot H_r)(\lambda)\,dr, \qquad \lambda \in \Lambda(H_0; F). \tag{8.11}$$

Proof. (A) The function $\Phi_{H_r}^{(a)}(\dot H_r)(\lambda)$ is summable on $[0,1]\times\mathbb{R}$. Indeed, by Lemma 8.1.7 this function is measurable and by Lemma 8.1.6 the L_1-norm of $\Phi_{H_r}^{(a)}(V)(\lambda)$ is uniformly bounded (by $\|V\|_1$) with respect to $r \in [0,1]$.

(B) It follows from (A) and Fubini's theorem that for any bounded measurable function h, one can interchange the order of integrals in the iterated integral

$$\int_0^1 \int_{\mathbb{R}} h(\lambda)\Phi_{H_r}^{(a)}(\dot H_r)(\lambda)\,d\lambda\,dr.$$

It now follows from (8.9) and Theorem 8.1.3 that for any $\phi \in C_c(\mathbb{R})$,

$$\begin{aligned}\xi_\gamma^{(a)}(\phi) &= \int_0^1 \Phi_{H_r}^{(a)}(\dot H_r)(\phi)\,dr = \int_0^1 \int_{\mathbb{R}} \Phi_{H_r}^{(a)}(\dot H_r)(\lambda)\phi(\lambda)\,d\lambda\,dr \\ &= \int_{\mathbb{R}} \phi(\lambda) \int_0^1 \Phi_{H_r}^{(a)}(\dot H_r)(\lambda)\,dr\,d\lambda = \int_{\mathbb{R}} \phi(\lambda)\xi_\gamma^{(a)}(\lambda)\,d\lambda.\end{aligned}$$

It follows that $\xi_\gamma^{(a)}$ is absolutely continuous. Lemma 8.1.6 implies that $\xi_\gamma^{(a)}$ is a finite measure. ■

Corollary 8.2.2. *The measure $\xi^{(s)}$ is also absolutely continuous and finite.*

Proof. Since ξ and $\xi^{(a)}$ are finite and absolutely continuous, the claim follows from $\xi^{(s)} = \xi - \xi^{(a)}$. ■

In the last lemma we again denote by the same symbol $\xi_\gamma^{(a)}$ an absolutely continuous measure and its density. We call the function $\xi_\gamma^{(a)}(\lambda)$ the standard density of $\xi_\gamma^{(a)}$ with respect to the frame F. Note that $\xi_\gamma^{(a)}$ is explicitly defined for all $\lambda \in \Lambda(H_0; F)$. It is not difficult to see that, for the straight line path $H_r = H_0 + rV$, the function $\xi_\gamma^{(a)}(\lambda)$ thus defined coincides a.e. with the right hand side of the formula (3) of the Introduction.

Definition (8.11) of the value $\xi_\gamma^{(a)}(\lambda; H_1, H_0)$ of the absolutely continuous spectral shift function at a fixed point λ obviously implies that $\xi_\gamma^{(a)}(\lambda; H_1, H_0)$ is *path additive*, that is, if $\gamma_1 = \{H_r : r \in [a,b]\}$, $\gamma_2 = \{H_r : r \in [b,c]\}$ and $\gamma = \{H_r : r \in [a,c]\}$ are piecewise analytic paths satisfying Assumption 4.1.1, then

$$\xi_\gamma^{(a)}(\lambda; H_c, H_a) = \xi_{\gamma_1}^{(a)}(\lambda; H_b, H_a) + \xi_{\gamma_2}^{(a)}(\lambda; H_c, H_b). \tag{8.12}$$

([3]) See Remark 8.1.4.

Also, it is not difficult to see that $\xi^{(a)}_\gamma(\lambda; H_1, H_0)$ does not depend on an analytic parametrization of the curve γ as a set of operators.

For further use, we note the following

PROPOSITION 8.2.3. *Let λ be an essentially regular point. Let $\gamma = \{H_r : r \in [a,b]\}$ be an analytic path regular at λ which satisfies Assumption* 4.1.1. *The function $[a,b] \ni r \mapsto \xi^{(a)}_\gamma(\lambda; H_r, H_0)$ is analytic in a neighbourhood of $[a,b]$.*

Proof. The function $r \mapsto \Phi^{(a)}_{H_r}(\dot H_r)(\lambda)$ is analytic as the trace of the analytic function $r \mapsto \Pi_{H_r}(\dot H_r)(\lambda)$ (see Corollary 7.3.5). Therefore, $r \mapsto \xi^{(a)}_\gamma(\lambda; H_r, H_0)$ is analytic as the definite integral of the analytic function $r \mapsto \Phi^{(a)}_{H_r}(H_r)(\lambda)$. ■

This proposition implies that, for a given essentially regular point λ, as long as an analytic path γ of operators which satisfies Assumption 4.1.1 contains at least one operator regular at λ, the function $\xi^{(a)}_\gamma(\lambda; H_r, H_0)$ is or can be defined for all values of r, including resonant ones, by analytic continuation. This also shows that, given an analytic path $\{H_r\}$ of operators, the condition $\lambda \in \Lambda(H_0; F)$ is not essential as long as λ is a regular point for at least one operator from the path.

If T is a trace-class operator, then by $\det(1+T)$ we denote the classical Fredholm determinant of $1+T$ (see Subsection 1.6.4). Since, by Corollary 7.2.4, the scattering matrix $S(\lambda; H_r, H_0)$ takes values in $1 + \mathcal{L}_1(\mathfrak{h}^{(0)}_\lambda)$, the determinant $\det S(\lambda; H_r, H_0)$ makes sense.

Let $\lambda \in \Lambda(H_0; F)$. Note that, by Proposition 7.2.5, the function

$$\mathbb{R} \ni r \mapsto S(\lambda; H_r, H_0) \in 1 + \mathcal{L}_1(\mathfrak{h}^{(0)}_\lambda)$$

is continuous in $\mathcal{L}_1(\mathfrak{h}^{(0)}_\lambda)$. Hence, the function

$$\mathbb{R} \ni r \mapsto \det S(\lambda; H_r, H_0) \in \mathbb{T}$$

is also continuous (see (1.18)), where $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$. So, it is possible to define a continuous function

$$\mathbb{R} \ni r \mapsto -\frac{1}{2\pi i} \log\det S(\lambda; H_r, H_0) \in \mathbb{R}$$

with zero value at 0.

THEOREM 8.2.4. *Let F be a frame operator on $\mathcal{H}$ and let $\gamma = \{H_r\}_{r\in[0,1]}$ be a path of operators which satisfies Assumption* 4.1.1. *For all $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$,*

$$\xi^{(a)}_\gamma(\lambda; H_r, H_0) = -\frac{1}{2\pi i} \log\det S(\lambda; H_r, H_0), \tag{8.13}$$

where the logarithm is defined in such a way that the function

$$[0,r] \ni s \mapsto \log\det S(\lambda; H_s, H_0)$$

is continuous.

Proof. By the definitions (8.11) and (8.6) of $\xi^{(a)}$ and $\Phi^{(a)}$ we have

$$\xi^{(a)}_\gamma(\lambda; H_r, H_0) = \int_0^r \Phi^{(a)}_{H_s}(\dot H_r)(\lambda)\, ds = \int_0^r \operatorname{Tr}_{\mathfrak{h}^{(s)}_\lambda}(\Pi_{H_s}(\dot H_r)(\lambda))\, ds. \tag{8.14}$$

By Theorem 4.1.9 and by the definition (7.11) of the infinitesimal scattering matrix $\Pi_{H_s}(V)(\lambda)$, the last integrand is defined for all $s \in [0, r]$ except the *discrete* resonance set $R(\lambda; \{H_r\}, F)$ (see (4.5)). Moreover, by Corollary 7.3.5, the function

$$\mathbb{R} \ni s \mapsto \operatorname{Tr}_{\mathfrak{h}_\lambda^{(s)}}(\Pi_{H_s}(V)(\lambda))$$

is piecewise analytic. Consequently, the integral (8.14) is well defined.

Since, by Corollary 5.3.8, the operator $w_+(\lambda; H_s, H_0)\colon \mathfrak{h}_\lambda^{(0)} \to \mathfrak{h}_\lambda^{(s)}$ is unitary for all $s \notin R(\lambda; \{H_r\}, F)$, it follows from (8.14) that

$$\xi_\gamma^{(a)}(\lambda; H_r, H_0) = \int_0^r \operatorname{Tr}_{\mathfrak{h}_\lambda^{(0)}}(w_+(\lambda; H_0, H_s)\Pi_{H_s}(V)(\lambda)w_+(\lambda; H_s, H_0))\, ds.$$

Theorem 7.3.4 and Lemma A.1.3 now imply

$$-2\pi i \xi_\gamma^{(a)}(\lambda; H_r, H_0) = \log\det S(\lambda; H_r, H_0),$$

where the branch of the logarithm is chosen as in the statement of the theorem. ■

Corollary 8.2.5. *Let F be a frame operator on $\mathcal{H}$, and let $\gamma = \{H_r\}_{r\in[0,1]}$ be a path of operators which satisfies Assumption* 4.1.1. *If $\lambda \in \Lambda(H_r; F) \cap \Lambda(H_0; F)$, then*

$$e^{-2\pi i \xi_\gamma^{(a)}(\lambda; H_r, H_0)} = \det S(\lambda; H_r, H_0).$$

Let $\xi_\gamma^{(s)}(\lambda; H_r, H_0)$ (respectively, $\xi(\lambda; H_r, H_0)$) be the density of the absolutely continuous measure ([4]) $\xi_\gamma^{(s)}(\phi; H_r, H_0)$ (respectively, $\xi(\phi; H_r, H_0)$). Since V is trace-class, Corollary 8.2.5 and the Birman–Kreĭn formula (2) (see Introduction)

$$e^{-2\pi i \xi(\lambda)} = \det S(\lambda; H_r, H_0) \qquad \text{a.e. } \lambda \in \mathbb{R}$$

imply the following result.

Theorem 8.2.6. *For any path of operators $\gamma = \{H_r\}_{r\in[0,1]}$ which satisfies Assumption* 4.1.1, *the singular part $\xi_\gamma^{(s)}(\lambda; H_0 + V, H_0)$ of the spectral shift function is an a.e. integer-valued function.*

Theorem 8.2.6 suggests that the singular part of the spectral shift function measures the "spectral flow" of the singular spectrum regardless of its position with respect to the absolutely continuous spectrum.

The following corollary is the result mentioned in the introduction.

Corollary 8.2.7. *Let H_0 be a self-adjoint operator and V a self-adjoint trace-class operator. Let $H_r = H_0 + rV$. The density $\xi^{(s)}(\lambda; H_1, H_0)$ of the absolutely continuous measure*

$$\xi_{H_1,H_0}^{(s)}(\phi) = \int_0^1 \operatorname{Tr}(V\phi(H_r^{(s)}))\, dr$$

is an a.e. integer-valued function.

Proof. By Lemma 4.1.2, for the straight line path $\{H_r = H_0 + rV : r \in [0, 1]\}$ which connects H_0 and $H_0 + V$, there exists a frame F such that Assumption 4.1.1 holds. So, Theorem 8.2.6 completes the proof. ■

([4]) See Remark 8.1.4.

8.3. Non-additivity of the singular spectral shift function. In the previous version of this paper (in arXiv) and in [Az$_4$] I mistakenly claimed that the singular part of the spectral shift function was additive. I have found a contradiction in development of an example of a non-trivial singular spectral shift function given in [Az$_5$]. Looking for its source I found a gap in the proof of additivity of the singular part of the spectral shift function. Since the example was based on the additivity, it is also wrong, but it allows one to give a counter-example to additivity of the singular spectral shift function. An example of a non-trivial singular spectral shift function will be given in [Az$_7$].

THEOREM 8.3.1. *The singular part of the spectral shift function is not additive. That is, there exist self-adjoint operators H_0, H_1, H_2 with trace-class differences such that*

$$\xi^{(s)}_{H_2,H_0} \neq \xi^{(s)}_{H_2,H_1} + \xi^{(s)}_{H_1,H_0},$$

where the paths connecting the operators are assumed to be straight lines. As a consequence, the absolutely continuous part of the spectral shift function is not additive either:

$$\xi^{(a)}_{H_2,H_0} \neq \xi^{(a)}_{H_2,H_1} + \xi^{(a)}_{H_1,H_0}.$$

The rest of this subsection is devoted to the proof of this theorem.

LEMMA 8.3.2. *Let $\mathcal{H}$ a Hilbert space, $v \in \mathcal{H}$ and D a self-adjoint operator on $\mathcal{H}$. If*

$$H = \begin{pmatrix} D & v \\ \langle v, \cdot\rangle & \alpha \end{pmatrix}$$

is a self-adjoint operator on $\mathcal{H} \oplus \mathbb{C}$, where $\alpha \in \mathbb{R}$, then the resolvent of H is

$$R_z(H) = (H-z)^{-1} = \begin{pmatrix} R_z(D) + A\langle R_{\bar z}(D)v, \cdot\rangle R_z(D)v & -AR_z(D)v \\ -A\langle R_{\bar z}(D)v, \cdot\rangle & A \end{pmatrix},$$

where $A = (\alpha - z - \langle v, R_z(D)v\rangle)^{-1}$.

Proof. Direct calculation. ■

Note also that if $V = \langle v, \cdot\rangle v$, then (see e.g. [Y, (6.7.3)])

$$R_z(D + rV) = R_z(D) - \frac{r}{1 + r\langle v, R_z(D)v\rangle}\langle R_{\bar z}(D)v, \cdot\rangle R_z(D)v. \tag{8.15}$$

LEMMA 8.3.3. *Let*

$$H_{r,\alpha} := \begin{pmatrix} D + r\langle v, \cdot\rangle v & rv \\ r\langle v, \cdot\rangle & \alpha \end{pmatrix}$$

be a self-adjoint operator on the Hilbert space $L_2(\mathbb{R}) \oplus \mathbb{C}$, where $r, \alpha \in \mathbb{R}$ and

$$D = \frac{1}{i}\frac{d}{dx} \quad \text{and} \quad v = \frac{1}{\sqrt[4]{\pi}}e^{-x^2/2}.$$

If $r \neq 0$, then the operator $H_{r,\alpha}$ is absolutely continuous.

Proof. (A) First we show that the pure point part of $H_{r,\alpha}$ is zero. Assume that there is a non-zero vector $\mathbf{f} = \binom{f}{f_0} \in \mathcal{H}$ such that $H_{r,\alpha}\mathbf{f} = \lambda\mathbf{f}$ for some $\lambda \in \mathbb{R}$. This implies that f belongs to the domain of D. Further, we have

$$H_{r,\alpha}\mathbf{f} = \begin{pmatrix} Df + r\langle v, f\rangle v + rf_0 v \\ r\langle v, f\rangle + \alpha f_0 \end{pmatrix} = \begin{pmatrix} \lambda f \\ \lambda f_0 \end{pmatrix}.$$

This implies that $Df = \lambda f - r\langle v, f\rangle v - rf_0 v$, so that $f' \in L_2(\mathbb{R})$. Taking the Fourier transform of the last equality gives

$$\xi \hat{f}(\xi) = \lambda \hat{f}(\xi) - r\langle v, f\rangle \hat{v}(\xi) - r f_0 \hat{v}(\xi).$$

Since $\hat{v} = v$, it follows that

$$\hat{f}(\xi) = -r(\langle v, f\rangle + f_0) \cdot \frac{v(\xi)}{\xi - \lambda}.$$

Since $\frac{v(\xi)}{\xi-\lambda}$ is not in L_2, it follows that $f = 0$ and $f_0 = 0$; that is, $\mathbf{f} = 0$. This contradiction completes the proof of (A).

(B) It remains to show that the singular continuous part of $H_{r,\alpha}$ is also zero. Let (ϕ_j, κ_j) be a frame in $L_2(\mathbb{R})$ consisting of, say, Hermite functions ϕ_j; the numbers $\kappa_1, \kappa_2, \ldots$ can be chosen arbitrarily as long as they satisfy the definition of the frame. Using Lemma 8.3.2 and (8.15) one can show that the set $\mathbb{R} \setminus \Lambda_0(H_{r,\alpha}, F)$, given by (2.6), is empty. By Proposition 2.5.2, the singular continuous part of the operator $H_{r,\alpha}$ is also zero. ■

Proof of Theorem 8.3.1. In the notation of Lemma 8.3.3, let $H_0 = H_{0,-1}$, $H_1 = H_{1,0}$ and $H_2 = H_{0,1}$. It is easy to see that $\xi^{(s)}_{H_2,H_0} = \chi_{[-1,1]}$. At the same time, by Lemma 8.3.3, the operators which connect H_0 to H_1 and H_1 to H_2 have zero singular parts. Hence, $\xi^{(s)}_{H_2,H_1} = \xi^{(s)}_{H_1,H_0} = 0$. ■

This proof also shows that the pure point part of the spectral shift function (defined in an obvious way) is not additive either.

9. Pushnitski μ-invariant and singular spectral shift function

Though Theorem 8.2.6 shows that $\xi^{(s)}(\lambda)$ is a.e. integer-valued, it leaves a feeling of dissatisfaction, since the set of full measure on which $\xi^{(s)}$ is defined is not explicitly indicated.

In fact, it is possible to give another proof of Theorem 8.2.6, which uses a natural decomposition of the Pushnitski μ-invariant $\mu(\theta, \lambda)$ (cf. [Pu], cf. also [Az$_2$]) into absolutely continuous $\mu^{(a)}(\theta, \lambda)$ and singular $\mu^{(s)}(\theta, \lambda)$ parts, so that the Birman–Kreĭn formula becomes a corollary of this result and Theorem 8.2.4, rather than the other way round.

In this section it will be shown that $\mu^{(s)}(\theta, \lambda)$ does not depend on the angle variable θ and coincides with $-\xi^{(s)}(\lambda)$. Since the μ-invariant is integer-valued (it measures the spectral flow of partial scattering phase shifts), it follows that $\xi^{(s)}(\lambda)$ is integer-valued. The invariants $\mu(\theta, \lambda)$, $\mu^{(a)}(\theta, \lambda)$ and $\mu^{(s)}(\theta, \lambda)$ can be explicitly defined on $\Lambda(H_r; F) \cap \Lambda(H_0; F)$.

9.1. Spectral flow for unitary operators. Spectral flow for unitary operators of the class $1 + \mathcal{L}_\infty(\mathcal{H})$ was studied in [Pu]. Here we suggest a different approach. It is based on the following intuitively obvious theorem, the proof of which is nevertheless lengthy and tedious.

We denote by $\{a, b, \ldots\}^*$ sets in which elements may appear more than once, and these multiple appearances are counted, so that, say, $\{7, 7\}^* \neq \{7\}^*$, unlike usual sets. We call such sets *rigged sets*.

For $p \in [1, \infty]$, let

$$\mathcal{U}_p(\mathcal{H}) = \{U \in 1 + \mathcal{L}_p(\mathcal{H}) : U \text{ is unitary}\}$$

with the topology of convergence in the $\mathcal{L}_p(\mathcal{H})$-norm.

THEOREM 9.1.1. *Let $-\infty \le a < b \le +\infty$. Let $U\colon [a, b] \to \mathcal{U}_1(\mathcal{H})$ be a continuous path of unitary operators. There exists a sequence of continuous functions*

$$\theta_j\colon [a, b] \to \mathbb{R}, \qquad j = 1, 2, \dots,$$

such that for any $r \in [a, b]$ the rigged set

$$\{e^{i\theta_1(r)}, e^{i\theta_2(r)}, \dots\}^* \tag{9.1}$$

coincides with the spectrum of $U(r)$ (counting multiplicities), except possibly the point 1. In particular, if $U(a) = 1$, then the functions $\theta_j\colon [a, b] \to \mathbb{R}$, $j = 1, 2, \dots$, can be chosen so that additionally $\theta_j(a) = 0$ for all $j = 1, 2, \dots$.

DEFINITION 9.1.2. The *μ-invariant* of the path U is the function

$$\mu(\cdot; U)\colon (0, 2\pi) \to \mathbb{Z} \cup \frac{1}{2}\mathbb{Z}, \qquad \mu(\theta; U) = \sum_{j=1}^{\infty} [\theta; \theta_j(a), \theta_j(b)],$$

where

$$[\theta; \theta_1, \theta_2] = \frac{1}{2}\big(\#\{k \in \mathbb{Z} : \theta_1 < \theta + 2\pi k < \theta_2\} + \#\{k \in \mathbb{Z} : \theta_1 \le \theta + 2\pi k \le \theta_2\}\big).$$

If $U(a) = 1$, so that $\theta_j(a) = 0$ for all $j = 1, 2, \dots$, the last formula can be written as

$$\mu(\theta; U) = -\sum_{j=1}^{\infty} \left[\frac{\theta - \theta_j(b)}{2\pi}\right].$$

The μ-invariant $\mu(\theta, U)$ counts the number of times the eigenvalues of $U(r)$ cross a point $e^{i\theta} \in \mathbb{T}$ in anticlockwise direction as r moves from a to b. In other words, the μ-invariant is the spectral flow of a path of unitary operators.

THEOREM 9.1.3.

(1) *The μ-invariant is correctly defined, that is, it does not depend on the choice of continuous enumeration from Theorem* 9.1.1.
(2) *The μ-invariant is a homotopy invariant: if two continuous paths $U_1, U_2\colon [a, b] \to 1 + \mathcal{L}_1(\mathcal{H})$ of unitary operators with the same endpoints are homotopic, then $\mu(\theta; U_1) = \mu(\theta; U_2)$ for all $\theta \in (0, 2\pi)$.*
(3) *If two continuous paths $U_1\colon [a, b] \to \mathcal{U}_1(\mathcal{H})$ and the $U_2\colon [a, b] \to \mathcal{U}_1(\mathcal{K})$ are such that $U_1(a) = 1_{\mathcal{H}}$ and $U_2(a) = 1_{\mathcal{K}}$ and spectra of $U_1(b)$ and $U_2(b)$ coincide (counting multiplicities, and possibly excepting* 1*), then the difference $\mu(\theta; U_1) - \mu(\theta; U_2)$ is constant (does not depend on θ).*
(4) *If $U(a) = 1$, then*

$$\int_0^{2\pi} \mu(\theta; U)\, d\theta = \sum_{j=1}^{\infty} \theta_j(b).$$

In particular, the right hand side does not depend on the choice of continuous enumeration (9.1).

We introduce the following definition.

Definition 9.1.4. Let $U\colon [a,b] \to \mathcal{U}_1(\mathcal{H})$ be a continuous path of unitary operators such that $U(a) = 1$. The *ξ-invariant* of this path is the number

$$\xi(U) = -\frac{1}{2\pi}\int_0^{2\pi} \mu(\theta; U)\,d\theta = -\frac{1}{2\pi}\sum_{j=1}^{\infty}\theta_j(b).$$

It follows from Theorem 9.1.3 that the ξ-invariant is a homotopy invariant.

Proposition 9.1.5. *Let U be as in Theorem 9.1.1. The function*

$$[a,b] \ni r \mapsto \xi(U_r) \in \mathcal{U}_1(\mathcal{H})$$

is continuous, where U_r is the restriction of the path U to the interval $[a,r]$.

The proofs of Theorems 9.1.1 and 9.1.3 and of Proposition 9.1.5 can be found in [Az$_3$].

9.2. Absolutely continuous part of the Pushnitski μ-invariant. Let $\lambda \in \Lambda(H_0;F)$. Let $\gamma = \{H_r\}$ be a path of operators which satisfies Assumption 4.1.1.

We denote by

$$e^{i\theta_1^*(\lambda,r)}, e^{i\theta_2^*(\lambda,r)}, \ldots \in \mathbb{T}$$

the eigenvalues of the scattering matrix $S(\lambda; H_r, H_0)$. Since, by Proposition 7.2.5, $\lambda \to S(\lambda; H_r, H_0)$ is a meromorphic function which is analytic for real r's, by Theorem 9.1.1 for a given path $\{H_r\}$ the arguments $\theta_1^*(\lambda,r), \theta_2^*(\lambda,r), \ldots$ may and will be chosen to be continuous functions of r such that $\theta_j^*(\lambda,0) = 0$.

Definition 9.2.1. Let $\lambda \in \Lambda(H_0;F)$. Let $\gamma = \{H_r\}$ be a path of operators which satisfies Assumption 4.1.1. The absolutely continuous part $\mu^{(a)}(\theta,\lambda; H_r, H_0)$ of the Pushnitski μ-invariant is the μ-invariant of the path

$$[0,1] \ni r \mapsto S(\lambda; H_r, H_0). \tag{9.2}$$

In other words,

$$[0,2\pi) \times \Lambda(H_0;F) \ni (\theta,\lambda) \mapsto \mu^{(a)}(\theta,\lambda; H_r, H_0) = -\sum_{j=1}^{\infty}\left[\frac{\theta - \theta_j^*(\lambda,r)}{2\pi}\right]. \tag{9.3}$$

Recall that the vector space $\mathcal{A}(F)$ is defined in (4.1).

Theorem 9.2.2. *Let $\gamma = \{H_r\}$ be a path of operators which satisfies Assumption 4.1.1. For every $\lambda \in \Lambda(H_0;F)$,*

$$\xi_\gamma^{(a)}(\lambda; H_1, H_0) = -\frac{1}{2\pi}\int_0^{2\pi} \mu^{(a)}(\theta,\lambda; H_1, H_0)\,d\theta, \tag{9.4}$$

where $H_1 = H_0 + V$. That is, $\xi_\gamma^{(a)}(\lambda; H_1, H_0)$ is equal to the ξ-invariant of the path (9.2).

Recall that $\xi_\gamma^{(a)}(\lambda; H_1, H_0)$ is defined by (8.11).

Proof. By the Lidskii theorem (see (1.19))

$$\det S(\lambda; H_r, H_0) = \prod_{j=1}^{\infty} e^{i\theta_j^*(\lambda,r)} = \exp\Big(i\sum_{j=1}^{\infty}\theta_j^*(\lambda,r)\Big).$$

It follows from Proposition 9.1.5 and Theorem 9.1.3(4) that

$$-\frac{1}{2\pi i}\log\det S(\lambda; H_r, H_0) = -\frac{1}{2\pi}\sum_{j=1}^{\infty}\theta_j^*(\lambda, r) = -\frac{1}{2\pi}\int_0^{2\pi}\mu^{(a)}(\theta,\lambda; H_r, H_0)\,d\theta,$$

where all functions of r are continuous. Now, Theorem 8.2.4 completes the proof. ∎

9.3. Pushnitski μ-invariant. Let H_0 be a self-adjoint operator on $\mathcal{H}$, let F be a frame operator on $\mathcal{H}$, let

$$V_r \in F^* J_r F,$$

where $J_r \in \mathcal{B}(\mathcal{K})$, and let $\{H_r = H_0 + V_r\}$ satisfy Assumption 4.1.1.

Let $z \in \mathbb{C}$ with $\operatorname{Im} z > 0$. Following [Pu], we define the *$\tilde{S}$-function* by

$$\begin{aligned}\tilde{S}(z,r) &= \tilde{S}(z; H_r, H_0; F)\\ &= 1 - 2i\sqrt{\operatorname{Im} T_z(H_0)}J_r(1 + T_z(H_0)J_r)^{-1}\sqrt{\operatorname{Im} T_z(H_0)} \in 1 + \mathcal{L}_1(\mathcal{K}),\end{aligned} \tag{9.5}$$

where

$$T_z(H_0) = FR_z(H_0)F^*.$$

It is not difficult to verify that $\tilde{S}(z; H_r, H_0; F)$ is a unitary operator, so that

$$\tilde{S}(z; H_r, H_0; F) \in \mathcal{U}_1(\mathcal{K}).$$

Lemma 9.3.1. *Let $\{H_r\}$ be a path which satisfies Assumption* 4.1.1. *The function*

$$(z, r) \mapsto \tilde{S}(z; H_r, H_0; F)$$

is $\mathcal{L}_1$-continuous on $\mathbb{C}_+ \times \mathbb{R}$.

Proof. By Lemma 4.1.4, the operator $1 + J_r T_z(H_0)$ is invertible on $\mathbb{C}_+ \times \mathbb{R}$. Since, by Lemma 1.6.5, $\sqrt{\operatorname{Im} T_z(H_0)}$ is $\mathcal{L}_2$-continuous, it follows from Hölder's inequality (1.12) that $\tilde{S}(z; H_r, H_0; F)$ is $\mathcal{L}_1$-continuous $\mathbb{C}_+ \times \mathbb{R}$. ∎

Lemma 9.3.2. *If $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_r, F)$, then the limit*

$$\begin{aligned}\tilde{S}(\lambda + i0, r) &= \tilde{S}(\lambda + i0; H_r, H_0; F)\\ &= 1 - 2i\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}J_r(1 + T_{\lambda+i0}(H_0)J_r)^{-1}\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)} \in \mathcal{U}_1(\mathcal{K})\end{aligned} \tag{9.6}$$

exists in the $\mathcal{L}_1(\mathcal{K})$-norm.

Proof. Since $\lambda \in \Lambda(H_0; F)$, the limit $\operatorname{Im} T_{\lambda+i0}(H_0)$ exists in the $\mathcal{L}_1(\mathcal{H})$. By Lemma 1.6.5, the limit $\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}$ exists in the $\mathcal{L}_2(\mathcal{K})$-norm and from $\lambda \in \Lambda(H_r; F)$ it follows that the operator $(1 + T_{\lambda+i0}(H_0)J_r)^{-1}$ is invertible. So, again Hölder's inequality (1.12) completes the proof. ∎

When $y \to +\infty$, the operator $\tilde{S}(\lambda + iy, r)$ goes to 1. So, we have a continuous (in fact, real-analytic) path of unitary operators in $\mathcal{U}_1(\mathcal{K})$:

$$[-\infty, 0] \ni y \to \tilde{S}(\lambda - iy; H_r, H_0) \in \mathcal{U}_1(\mathcal{K}). \tag{9.7}$$

Definition 9.3.3. Let $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_r; F)$. The *Pushnitski μ-invariant* of the pair (H_0, H_r) is the μ-invariant of the continuous path (9.7).

The Pushnitski μ-invariant will be denoted by $\mu(\theta, \lambda; H_r, H_0)$.

9.4. M-function. Let $z \in \mathbb{C} \setminus \mathbb{R}$ and let H_0, H_1 be two self-adjoint operators on $\mathcal{H}$ with bounded difference $V = H_1 - H_0$. Following [Pu, (4.1)], we define the *M-function* by

$$M(z; H_1, H_0) = (H_1 - \bar{z})R_z(H_1)(H_0 - z)R_{\bar{z}}(H_0) \in \mathcal{B}(\mathcal{H}). \tag{9.8}$$

The M-function can be considered as the product of the Cayley transforms of the operators H_1 and H_0, and its values are unitary operators.

Let $\gamma = \{H_r\}$, $H_r = H_0 + V_r$, be a continuous piecewise real-analytic path.

Evidently, we have the multiplicative property

$$M(z; H_{r_2}, H_{r_0}) = M(z; H_{r_2}, H_{r_1})M(z; H_{r_1}, H_{r_0}). \tag{9.9}$$

One can also easily check that (see [Pu, (4.4)])

$$M(z; H_r, H_0) = 1 - 2iyR_z(H_r)V_rR_{\bar{z}}(H_0). \tag{9.10}$$

This equality, the estimate $\|R_z(H)\| \le 1/|\operatorname{Im} z|$ and the norm continuity of the function $\mathbb{C}_+ \times \mathbb{R} \ni (z, r) \mapsto R_z(H_r)$ imply the following lemma.

Lemma 9.4.1.

(i) *The function*

$$(z, r) \in \mathbb{C}_+ \times \mathbb{R} \mapsto M(z; H_r, H_0)$$

takes values in $1 + \mathcal{L}_1(\mathcal{H})$ and is continuous in the $\mathcal{L}_1(\mathcal{H})$-norm.

(ii) *When $y \to +\infty$,*

$$\|M(\lambda + iy, H_r, H_0) - 1\|_1 \to 0$$

locally uniformly with respect to $r \in \mathbb{R}$.

Indeed, it follows from (9.10) that

$$\|M(\lambda + iy, H_r, H_0) - 1\|_1 \le 2\|V_r\|_1/y.$$

Since $\|V_r\|_1$ is locally bounded, the claim follows.

Theorem 9.4.2 ([Pu, Theorem 4.1]). *The spectral measures of the operators $M(z; H_r, H_0)$ and $\widetilde{S}(z; H_r, H_0; F)$ coincide.*

This proposition means that in the definition of the Pushnitski μ-invariant one can replace the $\tilde{S}$-function by the M-function.

Corollary 9.4.3. *The μ-invariant (and, consequently, the ξ-invariant as well) of the path*

$$[-\infty, 0] \ni y \mapsto M(\lambda - iy; H_r, H_0) \in \mathcal{U}_1(\mathcal{K}) \tag{9.11}$$

coincides with the μ-invariant (respectively, the ξ-invariant) of the path (9.7)*. This also holds if the interval $[-\infty, 0]$ is replaced by $[-\infty, y_0]$ with $y_0 > 0$.*

Proof. This follows immediately from Theorem 9.4.2 and Lemmas 9.4.1 and 9.3.1. ∎

The following formula is taken from [Az$_2$].

Theorem 9.4.4. *Let $\{H_r\}$ be a continuous piecewise analytic path of operators and let $z \in \mathbb{C}_+$. Then*

$$M(z; H_r, H_{r_0}) = \operatorname{Texp}\Big(-2iy\int_{r_0}^{r} R_z(H_s)\dot{V}_rR_{\bar{z}}(H_s)\,ds\Big). \tag{9.12}$$

Proof. It follows from (9.10) that in $\mathcal{L}_1(\mathcal{H})$,

$$\frac{d}{dr}M(z;H_r,H_s)\bigg|_{r=s} = -2iyR_z(H_s)\dot V_s R_{\bar z}(H_s).$$

This equality and the multiplicative property (9.9) of the M-function imply that

$$\frac{d}{dr}M(z;H_r,H_s) = -2iyR_z(H_r)\dot V_r R_{\bar z}(H_r)M(z;H_r,H_s).$$

Combining this with Lemma A.1.1 we obtain (9.12). ■

9.5. Smoothed spectral shift function. We define the *smoothed spectral shift function* $\xi(\lambda+iy;H_1,H_0)$ of a pair of operators H_1 and H_0 as the ξ-invariant of the path

$$[-\infty,-y] \ni \tilde y \mapsto \tilde S(\lambda - i\tilde y;H_1,H_0) \in \mathcal{U}_1(\mathcal{K}). \tag{9.13}$$

This means by definition that (for $z \in \mathbb{C}_+$)

$$\xi(z;H_1,H_0) = -\frac{1}{2\pi}\sum_{j=1}^{\infty}\theta_j(z) = -\frac{1}{2\pi i}\log\det\tilde S(z;H_1,H_0), \tag{9.14}$$

where the functions $\theta_1(z),\theta_2(z),\ldots$ are chosen as in Theorem 9.1.1 for the continuous path (9.13).

PROPOSITION 9.5.1. *Let $\{H_r\}$ be a continuous path which connects H_0 and H_1. The smoothed spectral shift function $\xi(z;H_1,H_0)$ is equal to the ξ-invariant of the path*

$$[0,1] \ni r \mapsto M(z;H_r,H_0).$$

Proof. Let $z_0 = \lambda + iy_0$ and let $y_0 < y_1$. Consider a path which connects $M(\lambda+iy_0;H_r,H_0)$ to 1 and which consists of two arcs: the first arc connects $M(\lambda+iy_0;H_r,H_0)$ to $M(\lambda+iy_1;H_r,H_0)$ as y changes from y_0 to y_1, and the second arc connects $M(\lambda+iy_1;H_r,H_0)$ to 1 as r changes from 1 to 0. Now we let y_1 move from y_0 to $+\infty$. It follows from Lemma 9.4.1 that this gives a homotopy of the two paths connecting $M(\lambda+iy_0;H_r,H_0)$ to the identity operator, where in the first path y goes from y_0 to $+\infty$ and in the second path r goes from 1 to 0. It follows from Theorem 9.1.3 that the ξ-invariants of these two paths coincide. ■

LEMMA 9.5.2. *If $\lambda \in \Lambda(H_0;F)\cap\Lambda(H_1,F)$, then the limit*

$$\xi(\lambda+i0;H_1,H_0) := \lim_{y\to 0^+}\xi(\lambda+iy;H_1,H_0)$$

exists and

$$\xi(\lambda+i0;H_1,H_0) = -\frac{1}{2\pi}\int_0^{2\pi}\mu(\theta,\lambda;H_1,H_0)\,d\theta. \tag{9.15}$$

Proof. Existence of $\xi(\lambda+i0)$ follows from Lemma 9.3.2 and Proposition 9.1.5. Proposition 9.1.5 also implies that $\xi(\lambda+i0)$ is the ξ-invariant of the path (9.7), so that equality (9.15) holds by Definitions 9.3.3 and 9.1.4. ■

Theorem 9.4.2 and the proof of Proposition 9.5.1 imply the following

COROLLARY 9.5.3. *Let $\lambda \in \Lambda(H_0;F) \cap \Lambda(H_1;F)$. The number $\xi(\lambda+i0;H_1,H_0)$ is the ξ-invariant of a continuous path of unitary operators which consists of two pieces:*

$$[0,1] \ni r \mapsto \tilde S(\lambda+iy_0;H_r,H_0) \quad \textit{and} \quad [-y_0,0] \ni y \mapsto \tilde S(\lambda - iy;H_1,H_0).$$

The meaning of this corollary is simple: we cannot directly connect the unitary operator $\tilde S(\lambda+i0;H_1,H_0)$ to the identity operator by varying r from 1 to 0 because of possible resonance points in $[0,1]$, but we can do this after shifting the point $\lambda+i0$ out of the real axis.

PROPOSITION 9.5.4. *We have*

$$\xi(\lambda+iy;H_1,H_0) = \int_0^1 \operatorname{Tr}\Big[V\frac{1}{\pi}\operatorname{Im} R_{\lambda+iy}(H_s)\Big]\,ds. \tag{9.16}$$

Proof. It follows from (9.14), Corollary 9.4.3, Theorem 9.4.4 and Lemma A.1.3 that

$$\begin{aligned}\xi(\lambda+iy;H_1,H_0) &= -\frac{1}{2\pi i}\log\det M(\lambda+iy;H_1,H_0)\\ &= \frac{y}{\pi}\int_0^1 \operatorname{Tr}(R_{\lambda+iy}(H_s)VR_{\lambda-iy}(H_s))\,ds\\ &= \int_0^1 \operatorname{Tr}\Big[V\frac{1}{\pi}\operatorname{Im} R_{\lambda+iy}(H_s)\Big]\,ds. \ \blacksquare\end{aligned}$$

9.6. Pushnitski formula. The following theorem was proved in [Pu]. Here we give another simpler proof, following that from [Az$_2$].

THEOREM 9.6.1 (Pushnitski formula). *For a.e. $\lambda \in \Lambda(H_0;F) \cap \Lambda(H_r;F)$,*

$$\xi(\lambda;H_r,H_0) = -\frac{1}{2\pi}\int_0^{2\pi} \mu(\theta,\lambda;H_r,H_0)\,d\theta.$$

Proof. By Lemma 9.5.2, it is enough to show that for a.e. $\lambda \in \Lambda(H_0;F) \cap \Lambda(H_r;F)$,

$$\xi(\lambda+i0;H_1,H_0) = \xi(\lambda;H_1,H_0). \tag{9.17}$$

The trace on the right hand side of (9.16) is the Poisson integral of the measure $\Delta \mapsto \operatorname{Tr}(VE_\Delta^{H_s})$. It follows from (9.16) and Fubini's theorem (see e.g. [Ja, VI.2] or [ACS, Lemma 2.4]) that $\xi(\lambda+iy;H_1,H_0)$ is the Poisson integral of the measure

$$\Delta \mapsto \int_0^1 \operatorname{Tr}(VE_\Delta^{H_s})\,ds,$$

which is the absolutely continuous spectral shift measure ξ (see (8.8)). Hence, by Theorem 1.3.3, (9.17) holds for a.e. $\lambda \in \mathbb{R}$. $\blacksquare$

This theorem allows us to define explicitly the spectral shift function on the full set $\Lambda(H_0;F)$.

DEFINITION 9.6.2. Let $\lambda \in \Lambda(H_0;F) \cap \Lambda(H_1;F)$. The *Lifshits–Kreĭn spectral shift function* $\xi(\lambda)$ is by definition

$$\xi(\lambda;H_1,H_0) = -\frac{1}{2\pi}\int_0^{2\pi} \mu(\theta,\lambda;H_1,H_0)\,d\theta.$$

In other words, $\xi(\lambda)$ is the ξ-invariant of the path (9.7). The advantage of this definition is that it gives explicit values of ξ on an explicit set of full Lebesgue measure.

REMARK 9.6.3. The functions ξ and $\xi^{(a)}$ are summable. Hence one can consider the full sets $\Lambda(\xi)$ and $\Lambda(\xi^{(a)})$ and standard values of ξ and $\xi^{(a)}$ on these sets. However, the above definitions of $\xi(\lambda)$ and $\xi^{(a)}(\lambda)$ and of the corresponding sets of full Lebesgue measure differ from the standard definition of $f(\lambda)$ for a general summable function f. In particular, it may happen that $\xi(\lambda) \neq 0$ at some regular point λ, while $\xi = 0$ as an element of $L_1(\mathbb{R})$.

It is known that ξ is additive in the sense that

$$\xi(\lambda; H_2, H_0) = \xi(\lambda; H_2, H_1) + \xi(\lambda; H_1, H_0) \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Definition 9.6.2 prompts the question of whether this equality holds for *every* λ in $\Lambda(H_0; F) \cap \Lambda(H_1; F) \cap \Lambda(H_2; F)$. The answer is affirmative.

LEMMA 9.6.4. *If $U, V\colon [a,b] \to \mathcal{U}_1(\mathcal{H})$ are two continuous paths such that $U(a)=V(a)=1$, then*

$$\xi(UV) = \xi(U) + \xi(V).$$

Proof. By (1.14), for every $r \in [a,b]$,

$$\det(U(r)V(r)) = \det(U(r)) \det(V(r)).$$

Also, by Proposition 9.1.5 and (1.18),

$$\det(U(r)) = e^{-2\pi i \xi(U(r))}.$$

It follows that

$$\xi(U(r)V(r)) = \xi(U(r)) + \xi(V(r)) \bmod \mathbb{Z}.$$

Since both sides are continuous functions of r and $\xi(U(0)V(0)) = \xi(U(0)) + \xi(V(0)) = 0$, the claim follows. ∎

THEOREM 9.6.5. *Let $H_1, H_2 \in H_0 + \mathcal{A}(F)$. For every $\lambda \in \Lambda(H_0; F) \cap \Lambda(H_1; F) \cap \Lambda(H_2; F)$,*

$$\xi(\lambda; H_2, H_0) = \xi(\lambda; H_2, H_1) + \xi(\lambda; H_1, H_0).$$

Proof. Since the M-function is multiplicative (9.9), the claim follows from Lemma 9.6.4 and Corollary 9.4.3. ∎

This theorem implies that the value $\xi(\lambda; H_1, H_0)$ of the spectral shift function at a point can be formally considered as path additive (formally, since the definition of $\xi(\lambda; H_1, H_0)$ does not involve a path of operators connecting H_0 and H_1).

9.7. Singular part of μ-invariant. Let $\gamma = \{H_r : r \in [0,1]\}$ be a continuous piecewise analytic path of operators which satisfies Assumption 4.1.1. Let λ be an essentially regular point. We assume that each analytic arc of the path γ contains at least one operator which is regular at λ. In this case we also say that each arc is regular at λ. By Theorem 4.1.11 and Lemma 4.1.7, this plainly implies that all operators of the path, except a finite number, are regular at λ.

DEFINITION 9.7.1. The *singular part of the Pushnitski μ-invariant* is the function

$$\mu_\gamma^{(s)}(\theta, \lambda; H_r, H_0) := \mu(\theta, \lambda; H_r, H_0) - \mu_\gamma^{(a)}(\theta, \lambda; H_r, H_0).$$

Note that while $\mu(\theta,\lambda;H_r,H_0)$ and $\mu_\gamma^{(a)}(\theta,\lambda;H_r,H_0)$ are the μ-invariants of some paths of unitary operators, the singular part $\mu_\gamma^{(s)}(\theta,\lambda;H_r,H_0)$ of the μ-invariant is not.

Also, for every $\lambda \in \Lambda(H_0;F)\cap\Lambda(H_r;F)$ we define the standard density $\xi_\gamma^{(s)}(\lambda)$ of the singular part of the spectral shift function $\xi_\gamma^{(s)}$ by the formula

$$\xi_\gamma^{(s)}(\lambda;H_r,H_0) = \xi(\lambda;H_r,H_0) - \xi_\gamma^{(a)}(\lambda;H_r,H_0),$$

where $\xi(\lambda;H_r,H_0)$ is defined by (9.6.2) and $\xi_\gamma^{(a)}(\lambda;H_r,H_0)$ is defined by (8.14).

Lemma 9.7.2 ([Pu]). *Let $\lambda \in \Lambda(H_0;F)\cap\Lambda(H_r;F)$. The eigenvalues of $\tilde S(\lambda+i0;H_r,H_0)$ coincide with the eigenvalues of the scattering matrix $S(\lambda;H_r,H_0)$ (counting multiplicities); that is, the spectral measures of these operators coincide.*

Proof. The stationary formula for the scattering matrix (Theorem 7.2.2), the definition (9.5) of $\tilde S(\lambda+i0;H_1,H_0)$ and the equality (5.5), combined with (1.6), imply that the spectra of $S(\lambda;H_r,H_0)$ and $\tilde S(\lambda;H_r,H_0;F)$ coincide counting multiplicities. ∎

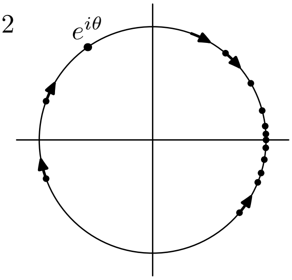
Theorem 9.7.3. *Let $\lambda\in\mathbb R$ be an essentially regular point. Let $\gamma=\{H_r : r\in[0,1]\}$ be a continuous piecewise analytic path of operators which satisfies Assumption 4.1.1, and such that each analytic arc of γ is regular at λ. The singular part of the Pushnitski μ-invariant $\mu_\gamma^{(s)}(\theta,\lambda)$ does not depend on the angle variable θ. As a function of λ, it is equal to minus the density $\xi_\gamma^{(s)}(\lambda)$ of the singular part of the spectral shift function. That is, for all $\lambda\in\Lambda(H_0;F)$ and all $r\notin R(\lambda;\{H_r\},F)$,*

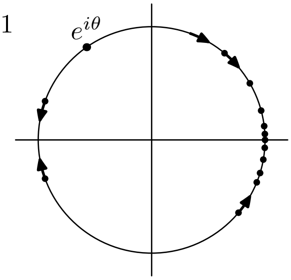
$$\xi_\gamma^{(s)}(\lambda;H_r,H_0) = -\mu_\gamma^{(s)}(\lambda;H_r,H_0). \tag{9.18}$$

Consequently, $\xi_\gamma^{(s)}(\lambda)$ is integer-valued.

Proof. It follows from Lemma 9.7.2 and Theorem 9.1.3(3) that the singular part of the μ-invariant does not depend on θ. The equality (9.18) now follows from (9.4) and Definition 9.6.2. ∎

The last theorem deserves some comment. The scattering matrix $S(\lambda;H_r,H_0)$ for $\lambda\in\Lambda(H_0;F)\cap\Lambda(H_r;F)$ is a unitary operator in the class $1+\mathcal L_1(\mathfrak h_\lambda)$. So, its spectrum is a discrete subset of the unit circle $\mathbb T$ with only one possible accumulation point at 1. The eigenvalues of $S(\lambda;H_r,H_0)$ (called scattering phases) can be send to 1 in two essentially different ways. The first way is to connect $S(\lambda;H_r,H_0)$ to the identity operator by letting the coupling constant r vary from 1 to 0. This is possible, since $S(\lambda;H_r,H_0)$ is continuous for all $r\in\mathbb R$. Now, $S(\lambda;H_r,H_0)$ and $\tilde S(\lambda+i0;H_r,H_0)$ have the same eigenvalues (counting multiplicities). So, the second way to send scattering phases to 1 is to vary y from 0 to $+\infty$ in $\tilde S$. In both ways, scattering phases go to 1 continuously. However, it is possible that these two ways are not homotopic; that is, some eigenvalue can make a different number of windings around the unit circle as it is sent to 1 (see picture below). The Pushnitski μ-invariant $\mu(\theta,\lambda;H_r,H_0)$ and its absolutely continuous part $\mu_\gamma^{(a)}(\theta,\lambda;H_r,H_0)$ measure the spectral flow of the scattering phases through $e^{i\theta}$ in two different ways, corresponding to the above mentioned two ways of connecting the scattering phases to 1, and the difference $\mu(\theta,\lambda;H_r,H_0)-\mu_\gamma^{(a)}(\theta,\lambda;H_r,H_0)$ does not depend on θ. This difference measures the difference of winding numbers.





Combined with Corollary 8.2.5, Theorem 9.7.3 gives a proof of

THEOREM 9.7.4 (Birman–Kreĭn formula). *Let H_0 be a self-adjoint operator and V be a trace-class self-adjoint operator. Then for a.e. $\lambda \in \mathbb{R}$,*

$$e^{-2\pi i \xi(\lambda; H_1, H_0)} = \det S(\lambda; H_1, H_0),$$

where $H_1 = H_0 + V$.

This theorem holds for all λ from the set $\Lambda(H_0; F) \cap \Lambda(H_1; F)$ of full Lebesgue measure, provided that there is some fixed frame F such that $V \in \mathcal{A}(F)$. By Lemma 4.1.2, for every trace-class operator V such a frame exists, and consequently the Birman–Kreĭn formula holds for a.e. $\lambda \in \mathbb{R}$. Also, in this theorem the scattering matrix $S(\lambda; H_1, H_0)$ is defined by (7.1), but as is shown in Section 6, this definition coincides with the classical definition of the scattering matrix via the direct integral decomposition of the scattering operator.

Let λ be a fixed essentially regular point. We consider the singular spectral shift function $\xi^{(s)}(r) = \xi^{(s)}(\lambda; H_r, H_0)$ as a function of r. Theorem 9.7.3 tells us that $\xi^{(s)}(r)$ is an integer. It turns out that $\xi^{(s)}(r)$ is a locally constant function, and it can jump only at resonance points of the path $\{H_r\}$. In the rest of this section we prove this assertion.

LEMMA 9.7.5. *If $\lambda \in \Lambda(H_0; F)$, then $\tilde{S}(\lambda + iy; H_r, H_0)$ converges to $\tilde{S}(\lambda + i0; H_r, H_0)$ in $\mathcal{L}_1(\mathcal{H})$ locally uniformly with respect to r outside of the resonance set $R(\lambda; H_0, V; F)$ as $y \to 0$.*

Proof. (A) If I is a closed interval which does not contain resonance points of the path $\{H_r\}$, then the function

$$[0,1] \times I \ni (y, r) \mapsto (1 + T_{\lambda+iy}(H_0)J_r)^{-1}$$

is bounded. Indeed, since λ is regular, $T_{\lambda+iy}(H_0)$ is continuous on $[0,1]$ and so $1 + T_{\lambda+iy}(H_0)J_r$ is continuous on $[0,1] \times I$. Since the map $A \mapsto A^{-1}$ is also continuous, the image of the function $(1 + T_{\lambda+iy}(H_0)J_r)^{-1}$ on the compact rectangle $[0,1] \times I$ is bounded.

(B) We have

$$\begin{aligned}(1 + T_{\lambda+iy}(H_0)J_r)^{-1} &- (1 + T_{\lambda+i0}(H_0)J_r)^{-1} \\ &= (1 + T_{\lambda+iy}(H_0)J_r)^{-1} \cdot [T_{\lambda+i0}(H_0) - T_{\lambda+iy}(H_0)]J_r \cdot (1 + T_{\lambda+i0}(H_0)J_r)^{-1}.\end{aligned}$$

Since, by (A), $(1 + T_{\lambda+iy}(H_0)J_r)^{-1}$ is locally uniformly bounded outside $R(\lambda, H_0, V; F)$ times $\{y \in [0,1]\}$, it follows from the last equality that

$$(1 + T_{\lambda+iy}(H_0)J_r)^{-1} \to (1 + T_{\lambda+i0}(H_0)J_r)^{-1} \quad \text{as } y \to 0$$

in $\|\cdot\|$ locally uniformly with respect to $r \notin R(\lambda; H_0, V; F)$. Since by Lemma 1.6.5, $\sqrt{\operatorname{Im} T_{\lambda+iy}(H_0)}$ converges to $\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}$ in $\mathcal{L}_2(\mathcal{H})$, the claim follows from the definition (9.5) of $\tilde{S}(\lambda + iy, r)$ and the Hölder inequality (1.12). ∎

Theorem 9.7.6. *Let λ be a fixed essentially regular point. Let $\gamma = \{H_r\}$ be a path of operators which satisfies Assumption* 4.1.1 *and such that each arc of γ is regular at λ. The singular spectral shift function $\xi_\gamma^{(s)}(\lambda; H_r, H_0)$ is a locally constant function of r and the discontinuity points of this function of r are resonance points of the path $\gamma = \{H_r\}$.*

Proof. Since both ξ and $\xi_\gamma^{(a)}$ are path additive (see (8.12)), we can assume that γ is analytic. Further, for the same reason, it is enough to show that if there are no resonance points, then ξ and $\xi_\gamma^{(a)}$ coincide as functions of r for fixed λ. In this case, it follows from Lemma 9.7.5 that the function $[0,\infty) \times [0,1] \ni (y,r) \mapsto \tilde{S}(\lambda + iy; H_r, H_0)$ is continuous. It follows from Corollary 9.5.3 and Theorem 9.1.3(2) that $\xi(\lambda)$ is equal to the ξ-invariant of the continuous path

$$[0,1] \ni r \mapsto \tilde{S}(\lambda + i0; H_r, H_0).$$

By Lemma 9.7.2, this path and the continuous path

$$[0,1] \ni r \mapsto S(\lambda; H_r, H_0)$$

have the same spectral measures. It follows that they have the same ξ-invariants. ∎

Corollary 9.7.7. *Let λ be a fixed essentially regular point. Let $\gamma = \{H_r\}$ be a real-analytic path which satisfies Assumption* 4.1.1 *and such that each arc of γ is regular at λ. The value $\xi(\lambda; H_r, H_0)$ of the spectral shift function at λ as a function of $r \in \mathbb{R}$ is a locally analytic function, with (necessarily integer) jumps only at resonance points of the path γ.*

Corollary 9.7.8. *Let λ be an essentially regular point. If a path $\gamma = \{H_r\}$ which satisfies Assumption* 4.1.1 *does not intersect the resonance set $R(\lambda; \mathcal{A}, F)$, then $\xi(\lambda; H_1, H_0) = \xi_\gamma^{(a)}(\lambda; H_1, H_0)$.*

Using pointwise additivity of $\xi(\lambda; H_1, H_0)$ (Theorem 9.6.5) and the last corollary, it can be shown that for a fixed essentially regular point λ the one-forms $\Phi_H(\cdot)(\lambda)$ and $\Phi_H^{(a)}(\cdot)(\lambda)$ are locally exact and, as a consequence, are also closed on the manifold $\Gamma(\lambda; \mathcal{A}, F)$.

Appendix. Chronological exponential

In this appendix an exposition of the chronological exponential is given. See e.g. [AgG, G] and [BSh, Chapter 4].

A.1. Definition and main properties. Let $p \in [1, \infty]$ and let $a < b$. Let $A(\cdot) \colon [a,b] \to \mathcal{L}_p(\mathcal{H})$ be a piecewise continuous path of self-adjoint operators from $\mathcal{L}_p(\mathcal{H})$. Consider the equation

$$\frac{dX(t)}{dt} = \frac{1}{i} A(t) X(t), \qquad X(a) = 1, \tag{A.1}$$

where the derivative is taken in $\mathcal{L}_p(\mathcal{H})$. Let $0 \le t_1 \le \cdots \le t_k \le t$. By definition, the *left chronological exponent* $\mathrm{Texp} = \overleftarrow{\exp}$ is

$$\mathrm{Texp}\Big(\frac{1}{i}\int_a^t A(s)\,ds\Big) = 1 + \sum_{k=1}^{\infty} \frac{1}{i^k}\int_a^t dt_k \int_a^{t_k} dt_{k-1} \ldots \int_a^{t_2} dt_1 A(t_k)\ldots A(t_1), \quad \text{(A.2)}$$

where the series converges in the $\mathcal{L}_p(\mathcal{H})$-norm.

LEMMA A.1.1. *The equation* (A.1) *has a unique continuous solution* $X(t)$, *given by*

$$X(t) = \mathrm{Texp}\Big(\frac{1}{i}\int_a^t A(s)\,ds\Big).$$

Proof. Substitution shows that (A.2) is a continuous solution of (A.1). Let $Y(t)$ be another continuous solution of (A.1). Taking the integral of (A.1) in $\mathcal{L}_p(\mathcal{H})$, one gets

$$Y(t) = 1 + \frac{1}{i}\int_a^t A(s)Y(s)\,ds.$$

Iteration of this integral and the bound $\sup_{t\in[a,b]} \|A(t)\|_p \le \mathrm{const}$ show that $Y(t)$ coincides with $(A.2)$. ∎

A similar argument shows that $\mathrm{Texp}\big(\frac{1}{i}\int_a^t A(s)\,ds\big)X_0$ is the unique solution of the equation

$$\frac{dX(t)}{dt} = \frac{1}{i}A(t)X(t), \qquad X(a) = X_0 \in 1 + \mathcal{L}_p(\mathcal{H}).$$

LEMMA A.1.2. *We have*

$$\mathrm{Texp}\Big(\int_s^u A(s)\,ds\Big) = \mathrm{Texp}\Big(\int_t^u A(s)\,ds\Big)\mathrm{Texp}\Big(\int_s^t A(s)\,ds\Big).$$

Proof. Using (A.2), it is easy to check that both sides are solutions of the equation

$$\frac{dX(u)}{du} = \frac{1}{i}A(u)X(u)$$

(in $\mathcal{L}_p(\mathcal{H})$) with the initial condition $X(t) = \mathrm{Texp}(\int_s^t A(s)\,ds)$. So, Lemma A.1.1 completes the proof. ∎

By det we denote the classical Fredholm determinant (cf. e.g. [GK, S_3, Y]).

LEMMA A.1.3. *If* $p = 1$ *then*

$$\det \mathrm{Texp}\Big(\frac{1}{i}\int_a^t A(s)\,ds\Big) = \exp\Big(\frac{1}{i}\int_a^t \mathrm{Tr}(A(s))\,ds\Big).$$

Proof. Let $F(t)$ and $G(t)$ be the left and the right hand sides respectively. Then $\frac{d}{dt}G(t) = \frac{1}{i}\,\mathrm{Tr}(A(t))G(t)$, $G(a) = 1$. Further, by Lemma A.1.2 and the product property of det,

$$\frac{d}{dt}F(t) = \lim_{h\to 0}\frac{1}{h}\Big(\det \mathrm{Texp}\Big(\frac{1}{i}\int_t^{t+h} A(s)\,ds\Big) - 1\Big)F(t) = \frac{1}{i}\,\mathrm{Tr}(A(t))F(t),$$

where the last equality follows from the definitions of determinant [S_3, (3.5)], Texp and piecewise continuity of $A(s)$. ∎

References

[Ag] Sh. Agmon, *Spectral properties of Schrödinger operators and scattering theory*, Ann. Scuola Norm. Sup. Pisa Cl. Sci. 2 (1975), 151–218.

[AgG] A. A. Agrachev and R. V. Gamkrelidze, *Exponential representation of flows and a chronological enumeration*, Mat. Sb. (N.S.) 107 (149) (1978), 467–532.

[AhG] N. I. Ahiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space*, F. Ungar, New York, 1963.

[An] T. Ando, *Comparison of norms* $\| \, |f(A) - f(B)| \, \|$ *and* $\|f(|A-B|)\|$, Math. Z. 197 (1988), 403–409.

[Ar] N. Aronszajn, *On a problem of Weyl in the theory of singular Sturm–Liouville equations*, Amer. J. Math. 79 (1957), 597–610.

[AD] N. Aronszajn and W. F. Donoghue, *On exponential representation of analytic functions in the upper half-plane with positive imaginary part*, J. Anal. Math. 5 (1956), 321–388.

[APS] M. Atiyah, V. Patodi and I. M. Singer, *Spectral asymmetry and Riemannian geometry. I*, Math. Proc. Cambridge Philos Soc. 77 (1975), 43–69.

[APS_2] —, —, —, *Spectral asymmetry and Riemannian geometry. III*, ibid. 79 (1976), 71–99.

[Az_1] N. A. Azamov, *Infinitesimal spectral flow and scattering matrix*, arXiv:0705.3282v4.

[Az_2] —, *Pushnitski's μ-invariant and Schrödinger operators with embedded eigenvalues*, arXiv:0711.1190v1.

[Az_3] —, *Singular spectral shift and Pushnitski μ-invariant*, preprint.

[Az_4] —, *Singular spectral shift is additive*, arXiv:1008.2847v1.

[Az_5] —, *Non-trivial singular spectral shift functions exist*, arXiv:1008.4231v1.

[Az_6] —, *On unification of trace-class and smooth scattering theories*, work in progress.

[Az_7] —, *Resonance index and singular spectral shift function*, in preparation.

[Az_8] —, *Spectral Shift Function in von Neumann Algebras*, Verlag Dr Müller, 2010.

[ACDS] N. A. Azamov, A. L. Carey, P. G. Dodds and F. A. Sukochev, *Operator integrals, spectral shift, and spectral flow*, Canad. J. Math. 61 (2009), 241–263.

[ACS] N. A. Azamov, A. L. Carey and F. A. Sukochev, *The spectral shift function and spectral flow*, Comm. Math. Phys. 276 (2007), 51–91.

[AS] N. A. Azamov and F. A. Sukochev, *Spectral averaging for trace compatible operators*, Proc. Amer. Math. Soc. 136 (2008), 1769–1778.

[BW] H. Baumgärtel and M. Wollenberg, *Mathematical Scattering Theory*, Birkhäuser, Basel, 1983.

[BE] M. Sh. Birman and S. B. Èntina, *The stationary approach in abstract scattering theory*, Izv. Akad. Nauk. SSSR Ser. Mat. 31 (1967), 401–430 (in Russian); English transl.: Math. USSR Izv. 1 (1967).

[BKS] M. Sh. Birman, L. S. Koplienko and M. Z. Solomyak, *Estimates for the spectrum of the difference between fractional powers of two self-adjoint operators*, Soviet Math. (Izv. VUZ) 19 (1975), no. 3, 1–6.

[BK] M. Sh. Birman and M. G. Kreĭn, *On the theory of wave operators and scattering operators*, Dokl. Akad. Nauk SSSR 144 (1962), 475–478 (in Russian).

[BP] M. Sh. Birman and A. B. Pushnitski, *Spectral shift function, amazing and multifaceted*, Integral Equations Operator Theory 30 (1998), 191–199.

[BS_1] M. Sh. Birman and M. Z. Solomyak, *Spectral Theory of Self-Adjoint Operators in Hilbert Space*, Reidel, Dordrecht, 1987.

[BS_2] —, —, *Remarks on the spectral shift function*, J. Soviet Math. 3 (1975), 408–419.

[BY] M. Sh. Birman and D. R. Yafaev, *Spectral properties of the scattering matrix*, Algebra i Analiz 4 (1992), no. 5, 1–27 (in Russian); English transl.: St. Petersburg Math. J. 4 (1993), 1055–1079.

[BSh] N. N. Bogolyubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields*, Wiley, New York, 1980.

[B] L. de Branges, *Perturbation of self-adjoint transformations*, Amer. J. Math. 84 (1962), 543–560.

[BF] V. S. Buslaev and L. D. Fadeev, *On trace formulas for a singular differential Sturm–Liouville operator*, Dokl. Akad. Nauk SSSR 132 (1960), 13–16 (in Russian); english transl.: Soviet Math. Dokl. 1 (1960), 451–454.

[CP_1] A. L. Carey and J. Phillips, *Unbounded Fredholm modules and spectral flow*, Canad. J. Math. 50 (1998), 673–718.

[CP_2] —, —, *Spectral flow in Fredholm modules, eta invariants and the JLO cocycle*, K-Theory 31 (2004), 135–194.

[C_1] A. Connes, *Noncommutative Geometry*, Academic Press, San Diego, 1994.

[C_2] —, *Geometry from the spectral point of view*, Lett. Math. Phys. 34 (1995), 203–238.

[DD] P. D. Dodds and T. K. Dodds, *On a submajorization inequality of T. Ando*, in: Oper. Theory Adv. Appl. 15, Birkhäuser, 1992, 942–972.

[G] R. V. Gamkrelidze, *Exponential representation of solutions of ordinary differential equations*, in: Equadiff IV (Praha, 1977), Lecture Notes in Math. 703, Springer, Berlin, 1979, 118–129.

[GM_1] F. Gesztesy and K. A. Makarov, *The Ξ operator and its relation to Kreĭn's spectral shift function*, J. Anal. Math. 81 (2000), 139–183.

[GM_2] —, *$SL_2(\mathbb{R})$, exponential Herglotz representations, and spectral averaging*, Algebra i Analiz 15 (2003), no. 3, 104–144 (in Russian); English transl.: St. Petersburg Math. J. 15 (2004), 393–418.

[Ge] E. Getzler, *The odd Chern character in cyclic homology and spectral flow*, Topology 32 (1993), 489–507.

[GK] I. C. Gohberg and M. G. Kreĭn, *Introduction to the Theory of Non-Selfadjoint Operators*, Transl. Math. Monogr. 18, Amer. Math. Soc., Providence, RI, 1969.

[HPh] E. Hille and R. S. Phillips, *Functional Analysis and Semigroups*, Amer. Math. Soc., Providence, RI, 1957.

[Ja] K. Jacobs, *Measure and Integral*, Academic Press, New York, 1978.

[J] V. A. Javrjan, *A certain inverse problem for Sturm–Liouville operators*, Izv. Akad. Nauk Armjan. SSR Ser. Mat. 6 (1971), 246–251 (in Russian).

[Ka_1] T. Kato, *Perturbation of continuous spectra by trace-class operators*, Proc. Japan Acad. 33 (1957), 260–264.

[Ka_2] —, *Perturbation Theory for Linear Operators*, Springer, Berlin, 1980.

[Ko] S. Kotani, *Lyapunov exponents and spectra for one-dimensional random Schrödinger operators*, in: Contemp. Math. 50, Amer. Math. Soc., 1986, 277–286.

[Kr] M. G. Kreĭn, *On the trace formula in perturbation theory*, Mat. Sb. 33 (75) (1953), 597–626 (in Russian).

[Ku_1] S. T. Kuroda, *An Introduction to Scattering Theory*, Lecture Notes Series 51, Aarhus Universitet, 1976.

[Ku_2] —, *Scattering theory for differential operators, I, operator theory*, J. Math. Soc. Japan 25 (1973), 75–104.

[Ku_3] —, *Scattering theory for differential operators, II, self-adjoint elliptic operators*, ibid. 25 (1973), 222–234.

[LL] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 3rd ed., Pergamon Press, 1977.

[L] I. M. Lifshits, *On a problem in perturbation theory connected with quantum statistics*, Uspekhi Mat. Nauk 7 (1952), no. 1, 171–180 (in Russian).

[N] S. N. Naboko, *Uniqueness theorems for operator-valued functions with positive imaginary part, and the singular spectrum in the Friedrichs model*, Ark. Mat. 25 (1987), 115–140.

[N_2] —, *Boundary values of analytic operator functions with a positive imaginary part*, J. Soviet Math. 44 (1989), 786–795.

[N_3] —, *Non-tangential boundary values of operator-valued R-functions in a half-plane*, Leningrad Math. J. 1 (1990), 1255–1278.

[Nat] I. P. Natanson, *Theory of Functions of a Real Variable*, F. Ungar, 1955.

[Ph_1] J. Phillips, *Self-adjoint Fredholm operators and spectral flow*, Canad. Math. Bull. 39 (1996), 460–467.

[Ph_2] —, *Spectral flow in type I and type II factors—a new approach*, Fields Inst. Comm. 17 (1997), 137–153.

[Pr] I. I. Privalov, *Boundary Properties of Analytic Functions*, GITTL, Moscow, 1950 (in Russian).

[Pu] A. B. Pushnitski, *The spectral shift function and the invariance principle*, J. Funct. Anal. 183 (2001), 269–320.

[RS_1] M. Reed and B. Simon, *Methods of Modern Mathematical Physics: 1. Functional Analysis*, Academic Press, New York, 1972.

[RS_2] —, —, *Methods of Modern Mathematical Physics: 2. Fourier Analysis*, Academic Press, New York, 1975.

[RS_3] —, —, *Methods of Modern Mathematical Physics: 3. Scattering Theory*, Academic Press, New York, 1979.

[Ro] C. A. Rogers, *Hausdorff Measures*, Cambridge Univ. Press, 1970.

[R] M. Rosenblum, *Perturbation of the continuous spectrum and unitary equivalence*, Pacific J. Math. 7 (1957), 997–1010.

[Ru] W. Rudin, *Real and Complex Analysis*, 3rd ed., McGraw-Hill, New York, 1987.

[Sa] S. Saks, *Theory of the Integral*, Hafner, New York, 1961.

[S_1] B. Simon, *Trace Ideals and Their Applications*, London Math. Soc. Lecture Note Ser. 35, Cambridge Univ. Press, Cambridge, 1979.

[S_2] —, *Spectral averaging and the Kreĭn spectral shift*, Proc. Amer. Math. Soc. 126 (1998), 1409–1413.

[S_3] —, *Trace Ideals and Their Applications*, 2nd ed., Math. Surveys Monogr. 120, Amer. Math. Soc., Providence, RI, 2005.

[SW] B. Simon and T. Wolff, *Singular continuous spectrum under rank one perturbations and localization for random Hamiltonians*, Comm. Pure Appl. Math. 39 (1986), 75–90.

[T] J. R. Taylor, *Scattering Theory*, Wiley, New York, 1972.

[Y] D. R. Yafaev, *Mathematical Scattering Theory: General Theory*, Amer. Math. Soc., Providence, RI, 1992.