# The singular spectral shift function for relatively trace class perturbations

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A thesis presented for the degree of Doctor of Philosophy

September 2018

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# Abstract

Recently discovered is a natural decomposition of the Lifshitz-Kreĭn spectral shift function (SSF) à la Lebesgue into the sum of absolutely continuous and singular SSF's. The latter part represents the flow of singular spectrum and takes integer values even within the essential spectrum. The singular SSF may be alternatively characterised as the either of the so-called total resonance index or singular $\mu$-invariant. The first of these measures the total number of poles of the sandwiched resolvent, considered as a function of the coupling parameter, which split from the unit interval as the spectral parameter is perturbed off of the real axis, counting the poles that move into the upper half-plane with a positive sign and those that move to the lower half-plane with a negative sign. The second measures the sum of winding numbers of the eigenvalues of the scattering matrix as it is continuously deformed to the identity in two different ways: by shrinking the coupling parameter to 0 and by sending the imaginary part of the spectral parameter to $\infty$. This document is in part a review of these facts, which were first established by N. Azamov under the assumption of a trace class perturbation, and also generalises their proofs to the case of relatively trace class perturbations, thereby making them applicable for instance to Schrödinger operators with bounded potentials undergoing integrable perturbations.

# Declaration

I certify that this thesis does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any university; and that to the best of my knowledge and belief it does not contain any material previously published or written by another person except where due reference is made in the text.

Tom Daniels

# Acknowledgements

I would like to thank Flinders University and everyone who contributed to provide me with the opportunity to undertake this research. I thank my friend Yohei Tanaka for his advice and many useful discussions and also for translating parts of some modern Japanese textbooks for me. My greatest thanks goes to my supervisor Nurulla Azamov whose creative ideas form a basis of the results presented here and without whose generous and patient guidance this would certainly not have been possible.

CHAPTER 1

# Introduction

The major themes of this document belong to the broad subject of perturbation theory for self-adjoint operators on a Hilbert space $\mathcal{H}$, in which the general scheme is to relate the spectral properties of two self-adjoint operators $H_0$ and $H_1$. The operator $H_1$ is considered to be the result of a slight perturbation of the 'initial' operator $H_0$ and the theory makes requirements on the 'size' of the perturbation $V := H_1 - H_0$. Two important examples of this type of condition which appear regularly herein are for $V$ to be 'relatively compact,' and further 'relatively trace class,' with respect to $H_0$. Exactly what is meant here will be clarified later; still the latter is a significant restriction of the former. Also important for the purposes of this introduction is the even more stringent condition that the perturbation $V$ belongs to the trace class $\mathcal{L}_1(\mathcal{H})$ of compact operators with summable $s$-numbers.

The key theorems presented here are generalisations of recently discovered results from the case of trace class perturbations to the case of relatively trace class perturbations. This widening of the allowable size of a perturbation passes a threshold in the applicability of the theory to physics. In the context of quantum mechanics the operators $H_0$ and $H_1$ are Schrödinger operators. For example, on the Hilbert space $L_2(\mathbb{R}^3)$, consider the initial Hamiltonain $H_0 = -\Delta + V_0$, where $\Delta$ is the Laplacian and $V_0$ is an operator of multiplication by a bounded function $V_0 \in L_\infty(\mathbb{R}^3)$ (denoted by the same symbol). Then a perturbation of multiplication by some other function $V$ can never be trace class or even compact, but it is relatively trace class if it is integrable $V \in L_1(\mathbb{R}^3)$.

The closed subset $\sigma(H)$ of the real line $\mathbb{R}$ forming the spectrum of an arbitrary self-adjoint operator $H$ can be deconstructed in a few different ways. One is to separate the discrete spectrum $\sigma_d(H)$, consisting of isolated eigenvalues of finite multiplicity, from its closed complement the essential spectrum $\sigma_{ess}(H)$. There is also the measure-theoretic (non-disjoint) decomposition into absolutely continuous $\sigma_{ac}(H)$ and singular $\sigma_s(H)$ spectra, the latter admitting further decomposition into pure-point $\sigma_{pp}(H)$ and singular continuous $\sigma_{sc}(H)$ parts. This describes the finer structure of the essential spectrum, since the simpler discrete spectrum is entirely pure-point. The discrete spectrum is rarely stable under small perturbations; the eigenvalues can shift around and trace out continuous, possibly overlapping paths (see e.g. [Kat84, Chapter II]). (Although the perturbation of isolated eigenvalues is essentially a finite dimensional problem described by linear algebra, it is hardly a trivial problem on which the last words have been said.) On the other hand, it is a classical result of perturbation theory due to H. Weyl (Theorem 2.18) that the essential spectrum as a whole is left unchanged by relatively compact perturbations. Another finer classical result due to T. Kato and M. Rosenblum (Theorem 7.24) assures a similar stability of the absolutely continuous spectrum under trace class perturbations. This result has since been generalised with the help of M. Sh. Birman and M. G. Kreĭn to the relatively trace class case and much weaker conditions of trace class type. Nevertheless it depends crucially on a condition 'of trace class type' in the sense that it fails for a perturbation of arbitrarily small norm taken from any larger Schatten class of compact operators (see e.g. [Yaf92, Part 2 of §6.2] and references therein). These two stability theorems are global in the sense that there is still likely to be turbulent movement within these masses of spectra.

Under a condition of trace class type an important object of perturbation theory can be defined, namely the *spectral shift function (SSF),* which is denoted by the symbol $\xi$ and is uniquely associated to a pair of self-adjoint operators $H_0$ and $H_1$. The SSF $\xi(H_1, H_0)$ (by convention the order of the operators is reversed to match the trace formula (1.2) below) is a locally integrable real-valued function of the spectral parameter $\lambda \in \mathbb{R}$ and its value $\xi(\lambda) = \xi(\lambda; H_1, H_0)$ indicates the shift which is undergone at the point $\lambda$ as the spectrum of $H_0$ is perturbed to that of $H_1$. In this sense the SSF extends the intuitive idea of the flow of discrete spectrum through the point $\lambda$. Indeed if $\lambda$ is outside of the essential spectrum, then $\xi(\lambda)$ is the net number of eigenvalues which cross $\lambda$ in the positive direction. (The flow of isolated eigenvalues, usually called 'spectral flow,' has many guises and has been studied extensively from a geometric perspective. For information about the connection between the SSF and some common definitions of spectral flow see e.g. [Aza17].) Although the SSF is naturally integer-valued outside of the essential spectrum, it may otherwise take any real value. (In fact any real-valued integrable function is the SSF of some pair of self-adjoint operators with trace class difference, see e.g. [BY93, §3.6].)

The SSF first appeared in the work of I. M. Lifshitz ([Lif52]), where it is formally defined by the heuristic

$$\xi(\lambda; H_1, H_0) = \mathrm{Tr}\,(E_0(\lambda) - E_1(\lambda))\,, \tag{1.1}$$

where $E_j$, $j = 0, 1$, denotes the spectral measure of $H_j$. This makes sense in the special case that the Hilbert space $\mathcal{H}$ has finite dimension, but requires some regularisation before it makes sense in much more generality. Lifshitz also noticed that the SSF should satisfy the trace formula

$$\mathrm{Tr}\,(\varphi(H_1) - \varphi(H_0)) = \int_{\mathbb{R}} \varphi'(\lambda)\xi(\lambda; H_1, H_0)\,d\lambda, \tag{1.2}$$

which for test functions $\varphi \in C_c^\infty(\mathbb{R})$ determines the generalised derivative of the SSF.

For a trace class perturbation $V \in \mathcal{L}_1(\mathcal{H})$, the SSF was famously made rigorous in [Kre53] by M. G. Kreĭn. He showed that in this case there is a unique integrable function $\xi$ which satisfies (1.2) for all functions $\varphi$ from a large class including the test functions $C_c^\infty(\mathbb{R})$. A necessary condition and a sufficient condition on $\varphi$, which ensure the validity of the trace formula (1.2) for all trace class perturbations, were later obtained by V. V. Peller in [Pel85]. What's more, Peller's recent work [Pel16] provides a condition both necessary and sufficient, clarifying this class as the operator Lipschitz functions. We won't in any case pay much attention to the extent of the class of functions $\varphi$ for which (1.2) holds; it should at least include test functions and as a rule of thumb it shrinks as the size of the perturbation grows.

As an aside, when $V \in \mathcal{L}_1(\mathcal{H})$ the formula (1.1) can be seen as an instance of (1.2) for the step function $\varphi$ for which $\varphi(x) = -1$ or $\varphi(x) = 0$ accordingly if $x < \lambda$ or $x \geq \lambda$ and whose generalised derivative is the delta function $\delta_\lambda$ at $\lambda$. Although this step function does not belong to the class of functions for which (1.2) holds, it can be approximated by such functions and a rigorous interpretation of (1.1) can thus be attained ([BP98]).

Using a limiting argument, Kreĭn built up the SSF for a trace class perturbation from the simpler case of finite rank perturbations, beginning with the rank-one case. In essence his method (reviewed in Section 5.1) was to investigate the SSF through its Cauchy-Stieltjes transform

$$\xi(R_z) = \int_{\mathbb{R}} \frac{\xi(\lambda)}{\lambda - z}\, d\lambda, \quad z \in \mathbb{C} \setminus \mathbb{R}, \tag{1.3}$$

where $R_z(\lambda) := (\lambda - z)^{-1}$ is the resolvent function. He found an alternative definition of this function (via its exponential, the so-called perturbation determinant) and was able to show that it satisfies certain conditions (Theorem 2.9) which ensure it to be the Cauchy-Stieltjes transform of a unique function $\xi$. Although this method is effective in the case of trace class perturbations, it begins to break down under 'larger' perturbations in which case the SSF is no longer integrable and the integral (1.3) might be divergent. Despite this, Kreĭn later established the existence of the SSF for relatively trace class perturbations too ([Kre62]), which he achieved by transformation from the case of unitary pairs of operators with trace class differences. In this context the SSF is integrable with the weight $(1+\lambda^2)^{-1}$ and only determined up to an additive constant (which can usually be adequately specified by a normalisation condition). Note that the trace formula (1.2) can in general only specify a locally integrable function $\xi$ up to an additive constant.

Kreĭn's paper [Kre53] brought a lot of attention to the SSF and before long it found a surprising connection to scattering theory. If perturbation theory is divided in accordance with the structure of the spectrum of a self-adjoint operator, then to a reasonable approximation scattering theory is the subdivision concerned with the perturbation of the absolutely continuous part. It is from another point of view the mathematical framework for quantum physical scattering phenomena and is concerned with the behaviour at large times $t$ of solutions $u(t) = e^{-itH_1}f$ of the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}u(t) = H_1 u(t), \quad u(0) = f \in \mathcal{H}.$$

With a trace class type restriction on the size of the perturbation, solutions for $f$ from the absolutely continuous subspace $\mathcal{H}^{(a)}(H_1)$ asymptotically approach solutions to the Schrödinger equation for the initial or 'free' operator $H_0$, which are explicitly known in many applications. That is, $u(t) = e^{-itH_1}f \to e^{-itH_0}f_\pm$ for some free states $f_\pm \in \mathcal{H}^{(a)}(H_0)$ as $t \to \pm\infty$. Of course in an experimental setting, information about the initial $f_-$ and final $f_+$ free states is available while very little is known about the scattering state $f$. One of the key objects in scattering theory is the scattering matrix $S(\lambda; H_1, H_0)$, which is a unitary operator relating the initial and final free eigenstates with energy $\lambda$.

In [BK62], assuming $V \in \mathcal{L}_1(\mathcal{H})$, M. Sh. Birman and M. G. Kreĭn prove the following elegant formula which expresses the SSF as the scattering phase shift. For almost every $\lambda \in \mathbb{R}$,

$$\det S(\lambda; H_1, H_0) = e^{-2\pi i \xi(\lambda; H_1, H_0)}, \tag{1.4}$$

where the scattering matrix belongs to $1 + \mathcal{L}_1(\mathcal{H})$ and the determinant calculates the product of its eigenvalues. This deep result is now known to hold under much broader assumptions of trace class type (see e.g. [Yaf92, Chapter 8]). Note that the scattering matrix is related only to the absolutely continuous spectrum, while the SSF also detects singular spectrum. Quoting the survey paper [BP98], "this is reflected in the fact that the SSF can be determined from (1.4) only up to a singular term which takes integer values almost everywhere." The nature of this missing singular term is a focus of this document.

Serving to further illuminate the connection between the SSF and the scattering matrix is a new proof of the Birman-Kreĭn formula (1.4) due to my supervisor N. A. Azamov ([Aza11a]). Its generalisation to relatively trace class perturbations will be presented in Chapter 8. The proof turns on a representation of the scattering matrix as a type of exponential and while its method is fairly simple, its justification takes some work (undertaken in Chapter 7). Before discussing these matters further let's return to the history of the SSF.

Another celebrated development in the theory of the SSF appeared in [BS75]. There, M. Sh. Birman and M. Z. Solomyak prove that if $V \in \mathcal{L}_1(\mathcal{H})$ then the SSF is the density of an absolutely continuous measure, the *spectral shift measure* (for which we use the same symbol $\xi$), given by the formula

$$\xi(\varphi; H_1, H_0) = \int_0^1 \operatorname{Tr}\left(V\varphi(H_r)\right)\, dr, \quad \varphi \in C_c(\mathbb{R}), \tag{1.5}$$

where $H_r = H_0 + rV$. (Here and in what follows we are identifying locally finite Borel measures with continuous linear functionals on $C_c(\mathbb{R})$, as discussed in Section 2.1). This is achieved using their theory of double operator integrals (see e.g. [BS03] where the original Russian references can also be found), which allows a proof of a version of the trace formula:

$$\operatorname{Tr}(\varphi(H_1) - \varphi(H_0)) = \int_{\mathbb{R}} \varphi'(\lambda)\, d\xi(\lambda),$$

where $\xi$ is the measure defined by (1.5). By comparison with Kreĭn's formula (1.2) they conclude that $d\xi(\lambda) = \xi(\lambda)d\lambda$, i.e. the measure $\xi$ is absolutely continuous and can be identified with the SSF.

Of the formulas involving the SSF mentioned so far, we give logical precedence to the Birman-Solomyak formula (1.5). Although $\xi$ appears in isolation, this formula does not yet define the SSF, since the measure $\xi$ is not a priori absolutely continuous. Nevertheless, Kreĭn's result can be considered as a proof of the absolute continuity and we adopt this point of view. In this regard we mention the recent work [MNP18] which proves the absolute continuity by means of double operator integrals.

An indication of the fundamental nature of the Birman-Solomyak formula is that it represents the spectral shift measure as an integral of the generalised 1-form

$$V \mapsto \Phi_H(V)(\varphi) := \operatorname{Tr}(V\varphi(H)), \quad \varphi \in C_c(\mathbb{R}), \tag{1.6}$$

on some real affine space $\mathcal{A}$ of self-adjoint operators. This 1-form $\Phi$ is called the *infinitesimal spectral shift measure.* In the paper [AS08] (set in an abstract semifinite von-Neumann algebra), $\Phi$ is shown using double operator integral techniques to be exact on the corresponding affine space $\mathcal{A}$ as long as $V\varphi(H) \in \mathcal{L}_1(\mathcal{H})$ for test functions $\varphi$. Then the independence of the spectral shift measure $\xi = \int_{H_r} \Phi$ from the path $H_r$ is used (via the so-called invariance principle) to reduce its absolute continuity to the case of a trace class perturbation. This method defines the SSF uniquely (unlike the trace formula; there is no uncertain additive constant here) and quite comprehensively and it is adapted in Chapter 5.

Although the spectral shift measure $\xi$ is absolutely continuous, the same cannot be said of the infinitesimal spectral shift measure $\Phi$. It turns out that its Lebesgue decomposition $\Phi = \Phi^{(a)} + \Phi^{(s)}$ results in a natural decomposition of the SSF, which was studied in [Aza11a] under the assumption of a trace class perturbation and appears here in the relatively trace class case.

The absolutely continuous $\Phi^{(a)}$ and singular $\Phi^{(s)}$ parts are given by the formula

$$\Phi_H^{(\cdot)}(V)(\varphi) = \operatorname{Tr}\left(V\varphi(H)P^{(\cdot)}(H)\right), \quad \varphi \in C_c(\mathbb{R}),$$

where $(\cdot)$ stands for $(a)$ or $(s)$ and $P^{(\cdot)}(H)$ denotes the orthogonal projection onto the absolutely continuous or singular subspace $\mathcal{H}^{(\cdot)}(H)$ of the self-adjoint operator $H$. The absolutely continuous component $\Phi^{(a)}$ can only be nonzero in the presence of absolutely continuous spectrum, where in general $\Phi^{(a)}$ and $\Phi^{(s)}$ individually fail to be exact (see Section 5.6). Still, their integrals along a piecewise analytic path $H_r$ in the affine space $\mathcal{A}$, chosen for now to be a straight line $H_r = H_0 + rV$, give rise to absolutely continuous measures

$$\xi^{(\cdot)}(\varphi; H_1, H_0) := \int_0^1 \operatorname{Tr}\left(V\varphi(H_r)P^{(\cdot)}(H_r)\right) dr, \quad \varphi \in C_c(\mathbb{R}), \tag{1.7}$$

whose sum is the spectral shift measure $\xi = \xi^{(a)} + \xi^{(s)}$. Since both measures (1.7) are absolutely continuous, they can be identified with their density functions; $\xi^{(a)}$ is the *absolutely continuous SSF* and $\xi^{(s)}$ is the *singular SSF*. As proved in [Aza11a] for trace class perturbations and in Chapter 8 for relatively trace class perturbations, it is the absolutely continuous SSF which is responsible for the Birman-Kreĭn formula.

N. Azamov noticed that the combination of (1.4) and (1.5), which looks something like

$$\det S(\lambda; H_1, H_0) = \exp\left(-2\pi i \int_0^1 \operatorname{Tr}(V\delta_\lambda(H_r))\, dr\right), \tag{1.8}$$

suggests an exponential form of the scattering matrix. This is made clear by comparing (1.8) with the formula $\det(e^A) = \exp \operatorname{Tr}(A)$, or rather with the formula (2.34) below, in which $A$ is replaced by a noncommutative integral $\int A(r)\, dr$. Proving such an 'ordered exponential representation' of the scattering matrix reduces to showing that it satisfies a differential equation of the form

$$\frac{d}{dr} S(r) = A(r)S(r), \tag{1.9}$$

where $A(r)$ takes values in the trace class. In this case $r$ should be the path variable, or *coupling parameter*, of $H_r = H_0 + rV$. That is, we need to consider the scattering matrix $S(\lambda; H_r, H_0)$ as a function of $r$ for fixed $\lambda$, which seems to be a new idea; the scattering matrix is only defined for almost every spectral value $\lambda$ and the null set of exceptional values is often not specified, let alone tracked as $r$ varies, no doubt because there is usually little reason to consider more than a fixed pair of operators $H_0$ and $H_1$. This poses a problem, since a continuous collection of these null sets might accumulate significantly. Apart from this problem, it happens that an equation (1.9) can be quite easily obtained by formally differentiating the well-known stationary formula for the scattering matrix ((1.13) below). In order to properly discuss the resulting equation and its implications for the SSF, we digress into stationary scattering theory and related topics.

Instead of large time limits, the 'stationary' approach to scattering theory involves limits with respect to the off-axis spectral parameter $\lambda + iy$ as $y \to 0^+$. The absolutely continuous part $\mu^{(a)}$ of a real-valued measure $\mu$ on $\mathbb{R}$ is expressible in terms of such limits, or boundary values, of its Cauchy-Stieltjes transform

$$\mu(R_{\lambda+iy}) = \int_{\mathbb{R}} \frac{1}{x - \lambda - iy}\, d\mu(x).$$

In particular, as $y \to 0^+$,

$$\pi^{-1} \operatorname{Im} \mu(R_{\lambda+iy}) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{y}{(x-\lambda)^2 + y^2} \, d\mu(x) \;\to\; \mu^{(a)}(\lambda) \tag{1.10}$$

for a.e. $\lambda \in \mathbb{R}$ (Theorem 2.4). To some extent, the same analysis can be applied to the spectral measure of a self-adjoint operator $H$. The resolvent $R_{\lambda+iy}(H)$ itself cannot be expected to converge as $y \to 0^+$ when $\lambda$ is within the spectrum $\sigma(H)$, but suppose that for some closed operator $F$, the *sandwiched resolvent*

$$T_z(H) := F R_z(H) F^* \tag{1.11}$$

is bounded for $z = \lambda + iy$, $y > 0$, and let $\Lambda(H, F)$ denote the set of points $\lambda \in \mathbb{R}$ at which the limit $T_{\lambda+i0}(H)$ exists as a bounded operator. It is important that the boundary values of the imaginary part $\operatorname{Im} T_z(H)$ often exist in a stronger topology than those of $T_z(H)$. The fact that for an appropriate choice of $F$ the set $\Lambda(H, F)$ has full measure is known as the (abstract) *Limiting Absorption Principle (LAP)*.

The LAP, in its connection with the investigation of the absolutely continuous part of a self-adjoint operator, is the key to stationary scattering theory and plays a significant role in this document. (Worth mentioning in this regard is Corollary 7.13, which derives from the LAP a diagonalisation of the absolutely continuous part of the self-adjoint operator $H$. This result and its importance for the approach we will take to stationary scattering theory is discussed in the introduction to Chapter 7, which can be read in conjunction with this digression for a more detailed account.) Given that the resolvents of two self-adjoint operators $H_0$ and $H_1 = H_0 + V$ are formally related by the identity

$$R_z(H_0) - R_z(H_1) = R_z(H_0) V R_z(H_1), \tag{1.12}$$

we might hope that the operator $F$ is related to the perturbation $V$. In fact it is a common technique in perturbation theory to suppose that $V$ can be factorised as $V = F^* J F$ for some bounded self-adjoint operator $J$. We will assume in addition that either the closed operator $F$ is bounded or the initial operator $H_0$ is bounded below. Then if $F$ is relatively compact with respect to $|H_0|^{1/2}$, one of the famous Kato-Rellich or KLMN Theorems on the stability of self-adjointness (numbered 2.28 and 2.29 below) can be used to interpret the perturbed operator $H_1 = H_0 + V$.

For our purposes the premise that $F$ is relatively compact with respect to $|H_0|^{1/2}$ (in the usual sense reviewed in Section 2.8) defines the 'relative compactness' of the perturbation $V = F^* J F$ with respect to $H_0$. An affine space of self-adjoint operators, over the real vector space of such relatively compact perturbations, can be defined by

$$\mathcal{A} = \{H_0 + V \,:\, V = F^* J F,\ J = J^*,\ \|J\| < \infty\}$$

(see Section 3.3) and will be called a *rigged affine space*. It happens that for any $H \in \mathcal{A}$ and $z \in \mathbb{C} \setminus \mathbb{R}$ the sandwiched resolvent $T_z(H)$ is compact.

A perturbation $V = F^*JF$ will be considered 'relatively trace class' with respect to $H_0$, if, in addition to being relatively compact, it happens that the imaginary part $\operatorname{Im} T_z(H_0)$ belongs to the trace class (which holds for any $z \in \mathbb{C} \setminus \mathbb{R}$ as long as it holds for one). The same is then true for any $H \in \mathcal{A}$. Under this assumption the rigged affine space $\mathcal{A}$ will be called *resolvent comparable*. This terminology comes from the fact that the difference of resolvents $R_z(H_1) - R_z(H_0)$ belongs to $\mathcal{L}_1(\mathcal{H})$ for any $H_0, H_1 \in \mathcal{A}$ and such a pair of operators is called *resolvent comparable* following [Yaf92].

A resolvent comparable rigged affine space $\mathcal{A}$ is the basic context for the main results presented in this document. The setting is conducive to the (trace class) techniques of stationary scattering theory, which will be discussed in more detail in Chapter 7. For now we state two important results, both of which can be found in the paper [BE67] (also see [Yaf92, Section 6.1 and Theorem 5.7.1′]). First, for any self-adjoint operator $H$ from such an affine space $\mathcal{A}$, the LAP holds in the sense that the set $\Lambda(H, F)$ has full measure. Moreover, by omitting a null set it can be assumed that for any $\lambda \in \Lambda(H, F)$ the limit $\operatorname{Im} T_{\lambda+i0}(H)$ exists in the trace class. Second, for any pair of self-adjoint operators $H_0$ and $H_1 = H_0 + V$ from $\mathcal{A}$, where $V = F^*JF$, and for a.e. $\lambda \in \mathbb{R}$, the scattering matrix $S(\lambda; H_1, H_0)$ has the 'stationary' representation

$$S(\lambda; H_1, H_0) = 1 - 2\pi i Z(\lambda; H_0)(1 + JT_{\lambda+i0}(H_0))^{-1} J Z^*(\lambda; H_0), \tag{1.13}$$

where the operator $Z(\lambda; H_0)$ is such that

$$Z^*(\lambda; H_0) Z(\lambda; H_0) = \frac{1}{\pi} \operatorname{Im} T_{\lambda+i0}(H_0). \tag{1.14}$$

A standard proof of the stationary formula (1.13) leaves significant uncertainty in the set of exceptional points $\lambda$ for which it fails. Assuming the scattering matrix is defined by (1.13), the uncertainty is mainly the fault of the operator $Z(\lambda; H_0)$, which also depends on $F$ and is usually denoted $Z_0(\lambda, F)$ but the change of notation indicates our change of focus; for a fixed $F$ we wish to consider its dependence on $H_0$. The problem is in the definition of this operator (see Chapter 7); it is defined for every $\lambda$ from some set of full measure, but nothing much is certain about this set apart from its existence. The point is that it's difficult to say which values of $\lambda$ satisfy the stationary formula and their dependence on $H_0$ is completely obscured.

In the case of trace class perturbations, this uncertainty was overcome in [Aza11a] by a new constructive approach. N. Azamov later generalised and simplified this approach, which appears with some minor tweaks in Chapter 7 (an overview is provided in the beginning of the chapter, but also see the introduction to [Aza16]). It turns out that we can simply define

$$Z(\lambda, H_0) := \sqrt{\pi^{-1} \operatorname{Im} T_{\lambda+i0}(H_0)}, \tag{1.15}$$

for any $\lambda$ from the full set $\Lambda(H_0, F)$, and the stationary formula can be shown to hold for any $\lambda$ from the intersection $\Lambda(H_0, F) \cap \Lambda(H_1, F)$. Then the question of its dependence on the operators $H_0, H_1 \in \mathcal{A}$ can be reduced to a consideration of the sandwiched resolvent (1.11) and found to be quite simple thanks to the resolvent identity (1.12).

In fact in the framework of the affine space $\mathcal{A}$, with $H_r = H_0 + rV$ and $V = F^*JF$, there is a sandwiched version of (1.12) which implies

$$T_z(H_r) = T_z(H_0)(1 + rJT_z(H_0))^{-1}. \tag{1.16}$$

Then as a result of the analytic Fredholm alternative (Theorem 2.17), the inverted factor on the right hand side must depend meromorphically on the coupling parameter $r$. In this way the sandwiched resolvent $T_z(H_r)$ can be considered as a meromorphic function of $r$. Its poles, which will be called *resonance points* corresponding to $z$ and are usually denoted $r_z$, occur when $-r_z^{-1}$ is an eigenvalue of the compact operator $JT_z(H_0)$. Moreover, by considering the limit $z = \lambda + i0$, it can be inferred from (1.16) that if $\lambda$ belongs to $\Lambda(H_0, F)$, then it also belongs to $\Lambda(H_r, F)$ for all real numbers $r$ except the discrete set of real resonance points $r_\lambda$ corresponding to $\lambda$. These facts appear in more detail in Chapter 4. The phenomenon of real resonance points is intimately connected with the singular SSF and will be revisited in that context at the end of this introduction. Given the stationary formula, the scattering matrix $S(\lambda; H_r, H_0)$ can also be considered as a meromorphic function of $r$, which looks like it might have poles at real resonance points. However, since it is unitary and thus bounded for any non-resonant real $r$, it must admit analytic continuation to all of $\mathbb{R}$.

Returning to the exponential representation of the scattering matrix, the plan for obtaining a differential equation (1.9) is to use the stationary formula to differentiate $S(r) := S(\lambda; H_r, H_0)$ with respect to $r$, where $H_r = H_0 + rV$, $V = F^*JF$, and $r \in \mathbb{R}$. Formally, the derivative of (1.13) at the initial operator $H_0$ can be easily calculated to be

$$S'(0) = -2\pi i Z(\lambda; H_0) J Z^*(\lambda; H_0),$$

and this calculation can be conveniently combined with a well-known multiplicative identity for the scattering matrix (specifically (7.37)) to obtain the desired differential equation (1.9), in which the $\mathcal{L}_1$-valued function $A(r)$ is unitarily equivalent (pointwise, via a wave matrix $w_+(\lambda; H_r, H_0)$) to

$$\tilde{A}(r) := -2\pi i Z(\lambda; H_r) J Z^*(\lambda; H_r). \tag{1.17}$$

Therefore, specifying the initial condition $S(0) = 1$, the scattering matrix must coincide with the unique ordered exponential solution to the resulting initial value problem (see Section 8.1).

From this result, suppose we attempt to recover the Birman-Kreĭn formula (1.4). Applying the determinant to the unique ordered exponential $S(r)$ which satisfies (1.9) with the initial condition $S(0) = 1$ returns the formula (see Proposition 2.22)

$$\det S(r) = \exp \int_0^r \operatorname{Tr}(A(s))\, ds.$$

In this case with $A(r)$ unitarily equivalent to $\tilde{A}(r)$ given by (1.17), after using the cyclic property of the trace and the equality (1.14), we find that

$$\det S(\lambda; H_1, H_0) = \exp\left(-2i \int_0^1 \operatorname{Tr}(J \operatorname{Im} T_{\lambda+i0}(H_r))\, dr\right). \tag{1.18}$$

Interestingly, it is not the SSF which appears in the exponent on the right hand side, but instead the absolutely continuous SSF.

Indeed, by expressing the absolutely continuous part $\Phi^{(a)}$ of the infinitesimal spectral shift measure in terms of the boundary values of its Poisson integral according to (1.10) (Theorem 2.4), it is shown in Section 5.5 that the absolutely continuous SSF $\xi^{(a)}$ defined by (1.7) can be represented as

$$\xi^{(a)}(\lambda; H_1, H_0) = \frac{1}{\pi} \int_0^1 \operatorname{Tr}(J \operatorname{Im} T_{\lambda+i0}(H_r))\, dr. \tag{1.19}$$

From (1.18) and (1.19) we conclude that the Birman-Kreĭn formula (1.4) holds if the SSF is replaced by the absolutely continuous SSF:

$$\det S(\lambda; H_1, H_0) = e^{-2\pi i \xi^{(a)}(\lambda; H_1, H_0)}. \tag{1.20}$$

It turns out that it is also possible to express the so-called off-axis scattering matrix $S(\lambda + iy; H_1, H_0)$ as an ordered exponential, from which the Birman-Krein formula itself can be recovered in the limit $y \to 0^+$ (see Chapter 8). Comparing the original Birman-Kreĭn formula (1.4) with its variant (1.20), it follows that the singular SSF $\xi^{(s)}$ must be an integer-valued function.

Assume for simplicity that the perturbation $V$ belongs to the trace class, in which case the singular SSF is integrable. Then since its values $\xi^{(s)}(\lambda)$ can be obtained by differentiating the measure (1.7) (see e.g. [Rud87, Theorem 7.11]), for almost every $\lambda$ it must be that

$$\xi^{(s)}(\lambda; H_1, H_0) = \frac{d}{d\lambda} \int_0^1 \operatorname{Tr}\left(V E_r^{(s)}(\lambda)\right) dr \quad \in \mathbb{Z}. \tag{1.21}$$

It is a remarkable fact that this complicated formula should result in an integer, even when $\lambda$ is within the essential spectrum. At a point $\lambda$ outside of the essential spectrum, the absolutely continuous SSF $\xi^{(a)}(\lambda)$ is zero and the singular SSF $\xi^{(s)}(\lambda) = \xi(\lambda)$ is understood to be the integer number of discrete eigenvalues which flow through the point $\lambda$. The singular SSF is naturally interpreted as measuring this flow of singular spectrum within the essential spectrum as well.

Through the application of this result to a pair of Schrödinger operators of the form $H_0 = -\Delta + V_0$, where $V_0 \in L_\infty(\mathbb{R}^\nu)$, and $H_1 = H_0 + V$, where $V \in L_1(\mathbb{R}^\nu)$, we believe we are observing a novel property of Schrödinger operators in physical dimensions $\nu = 1, 2$, or 3. If it is assumed that the initial operator $H_0$ has no absolutely continuous spectrum in an interval $I$, then the integrality of the singular SSF $\xi^{(s)}(\lambda)$ in $I$ follows easily from two powerful results: the stability of the absolutely continuous spectrum (Kato-Rosenblum Theorem) and the Birman-Kreĭn formula (1.4). Indeed if the absolutely continuous spectrum is absent, then its stability implies that the singular SSF is equal to the SSF itself, while the Birman-Krein formula implies that the SSF is integer-valued since in this case the scattering matrix reduces to the identity. For example this situation can occur for Schrödinger operators $H_0 = -\Delta + V_0$, with random bounded potentials $V_0$ (a phenomenon known as Anderson localisation, see e.g. [Pas80; Kir08; AW15], and references therein) and integrable perturbations $V$. However, if $H_0$ does have absolutely continuous spectrum, then the integrality of the singular SSF does not that easily follow from any known results.

There is more to say about the singular SSF than just the fact that it takes integer values. Like the SSF itself, it is multifaceted. In particular, there are at least two other spectral invariants which can be associated to a path of operators $H_r$ in the affine space $\mathcal{A}$, whose definitions are quite independent and yet both of which coincide with the singular SSF. These are namely the singular $\mu$-invariant [Aza11a] and the total resonance index [Aza16], which are discussed in turn below.

Additional light was shed on the connection between the SSF and the scattering matrix by A. B. Pushnitski in [Pus01], where her presents yet another representation of the SSF. Because the (off-axis) scattering matrix $S(\lambda + iy; H_1, H_0)$, $y \geq 0$, is unitary and differs from the identity by a compact operator, its spectrum lies on the unit circle $\mathbb{T}$ with essential spectrum concentrated at 1. Moreover, by sending the imaginary part of the spectral parameter $y$ from 0 to $\infty$, the scattering matrix is continuously deformed to the identity and therefore all of its eigenvalues converge to 1. In [Pus01], Pushnitski proves that the SSF is equal to the average flow of these eigenvalues: for a.e. $\lambda$,

$$\xi(\lambda; H_1, H_0) = -\frac{1}{2\pi} \int_0^{2\pi} \mu(\theta, \lambda; H_1, H_0)\, d\theta, \tag{1.22}$$

where the so-called *$\mu$-invariant* $\mu(\theta, \lambda; H_1, H_0)$ is defined as the spectral flow of the path

$$t \mapsto S(\lambda + iy(t); H_1, H_0), \quad y(t) := (1-t)t^{-1},$$

that is, the net number of eigenvalues which cross a point $e^{i\theta} \in \mathbb{T}$, $\theta \in (0, 2\pi)$, in the anticlockwise direction as the path is traversed. In Section 8.2 this fact is derived from the ordered exponential representation of the off-axis scattering matrix mentioned above (thereby avoiding the transition to a modified scattering matrix with identical spectrum).

Another natural way to connect the scattering matrix with the identity, which is considered in [Aza11a], is to send $H_1$ to $H_0$ along the path $H_r = H_0 + rV$ in the affine space $\mathcal{A}$. It turns out that the absolutely continuous SSF is for a.e. $\lambda$ given by the average

$$\xi^{(a)}(\lambda; H_1, H_0) = -\frac{1}{2\pi} \int_0^{2\pi} \mu^{(a)}(\theta, \lambda; H_1, H_0)\, d\theta, \tag{1.23}$$

where $\mu^{(a)}(\theta, \lambda; H_1, H_0)$, the *absolutely continuous $\mu$-invariant*, denotes the spectral flow of the path $r \mapsto S(\lambda; H_r, H_0)$. This fact is derived from the ordered exponential representation of the scattering matrix itself and also appears in Section 8.2.

The *singular $\mu$-invariant* is by definition the difference

$$\mu^{(s)}(\lambda; H_1, H_0) := \mu(\theta, \lambda; H_1, H_0) - \mu^{(a)}(\theta, \lambda; H_1, H_0),$$

which is the spectral flow of a loop based at 1 and hence does not depend on the angle $\theta$. It follows from the equalities (1.22) and (1.23) that the singular SSF and the singular $\mu$-invariant are negatives of one another:

$$\xi^{(s)}(\lambda; H_1, H_0) = -\mu^{(s)}(\lambda; H_1, H_0), \qquad \text{for a.e. } \lambda \in \mathbb{R}.$$

In other words, the singular SSF can be realised as the (necessarily finite) sum of winding numbers of the eigenvalues of the scattering matrix $S(y, r) := S(\lambda + iy; H_r, H_0)$ as it is deformed along the path which results as $(y, r)$ goes from $(0, 0)$ to $(0, 1)$ to $(\infty, 1)$. Note that unlike the singular SSF itself, the singular $\mu$-invariant is clearly an integer-valued function.

The spectral flow is well-known to be homotopically invariant and this property can be used to obtain some insight into the behaviour of the singular SSF $\xi^{(s)}(\lambda; H_r, H_0)$ as a function of the coupling parameter $r$. The notion of a resonant value of the coupling parameter was briefly mentioned above; a resonance point $r_z$ is a pole of the meromorphic function $r \mapsto (1 + rJT_z(H_0))^{-1}$ and corresponds to an eigenvalue $-r_z^{-1}$ of the compact operator $JT_z(H_0)$. It can be deduced from the stationary formula that $S(y, r)$ is continuous on compact subsets of $[0, \infty] \times \mathbb{C}$ which do not contain pairs $(y, r_z)$ where $r_z$ is a resonance point corresponding to $z = \lambda + iy$. Since it happens that $r_z$ cannot be real if $y > 0$, it follows that for any interval $[0, r]$ which does not contain real resonance points, there exists a homotopy between the paths formed as $(0, 0) \to (0, r)$ and $(0, r) \to (\infty, r)$. Thus in this case by the homotopy invariance of spectral flow, the $\mu$-invariant and absolutely continuous $\mu$-invariant coincide and hence $\xi^{(s)}(\lambda; H_r, H_0) = 0$. Although the singular SSF is path-dependent, it is additive along a given path $H_r$ in the sense that

$$\xi^{(s)}(\lambda; H_r, H_t) = \xi^{(s)}(\lambda; H_r, H_s) + \xi^{(s)}(\lambda; H_s, H_t), \quad r > s > t,$$

and we therefore conclude that the singular SSF is a locally constant function of the coupling parameter whose points of discontinuity are resonance points.

By analysing the definition of a resonance point, it can be determined that each integer jump of the singular SSF should only depend on the triple $(\lambda, H_{r_\lambda}, V)$ consisting of a point $\lambda$ which belongs to the set $\Lambda(H, F)$ for some $H \in \mathcal{A}$; a self-adjoint operator $H_{r_\lambda} \in \mathcal{A}$ such that $\lambda \notin \Lambda(H_{r_\lambda}, F)$; and a perturbation $V$ such that $\lambda \in \Lambda(H_r, F)$ for some $H_r$ on the line determined by $H_{r_\lambda}$ and $V$. In [Aza16] it is shown that this integer, called the *resonance index* and denoted by $\operatorname{ind}_{res}(\lambda, H_{r_\lambda}, V)$, can be quite easily calculated.

Suppose the spectral parameter $\lambda$ is perturbed to $\lambda + iy$ for small $y$. Then the real resonance point $r_\lambda$ must move of off the real axis. In general it may have a multiplicity greater than one in which case it may split into finitely many resonance points $r^j_{\lambda+iy}$, $j = 1, 2 \ldots, N$, none of which can remain on the real axis. If $N_+$ is the number of resonance points counting multiplicities which move into the upper complex half-plane $\mathbb{C}_+$ and likewise $N_-$ is the number which move into the lower half-plane $\mathbb{C}_-$, then the resonance index is their difference

$$\operatorname{ind}_{res}(\lambda, H_{r_\lambda}, V) = N_+ - N_-.$$

This definition is reviewed in more detail in Chapter 4 and in Chapter 6 it is confirmed to be the integer jump of the singular SSF. Further information about the resonance index can be found in the detailed study [Aza16] (also see [Aza17]).

The singular SSF $\xi^{(s)}(\lambda; H_1, H_0)$ is in other words equal to the finite sum of resonance indices at those resonance points $r_\lambda$ from the interval $[0, 1]$. This *total resonance index* is a surprisingly tangible characterisation of the singular SSF. It generalises a simple representation of the SSF valid outside of the essential spectrum, which is closely related to the so-called Birman-Schwinger principle (see e.g. [Sim05, Proposition 7.9; Sim79, Theorem 8.1]). Specifically, if the perturbation $V$ is assumed to have a definite sign – suppose $V \geq 0$, $F = V^{1/2}$, and $H_\pm = H_0 \pm V$, then for any $\lambda$ outside of the spectra of $H_0$ and $H_\pm$, the SSF is given by (see e.g. [BP98])

$$\xi(\lambda; H_\pm, H_0) = \pm\, n(1, \mp F R_\lambda(H_0) F),$$

where $n(1, T)$ denotes the total number of eigenvalues of a self-adjoint operator $T$ which are greater than 1. It is shown in [Pus11] that this principle can be extended into the essential spectrum under the assumption that there is an interval within which $\lambda \mapsto T_{\lambda+i0}(H_0)$ is continuous. The total resonance index is another extension in the same spirit, which makes use of the regularity of the sandwiched resolvent as a function of the coupling parameter and requires only for the limit $T_{\lambda+i0}(H_0)$ to exist at a single point $\lambda$.

To summarise, we present what can be considered as the main theorem to be found within the following pages. (The case that the rigging operator $F$ is bounded can be found in the paper [AD18], which is in essence a condensed version of this document.)

THEOREM 1.1. *Let $H_0$ and $H_1 = H_0 + V$ be self-adjoint operators and suppose that the perturbation admits a decomposition $V = F^* J F$ for some closed operator $F$ for which the products $F(|H_0| + 1)^{-1/2}$ and $F(|H_0| + 1)^{-1}$ respectively belong to the compact and Hilbert-Schmidt classes. Suppose in addition that either $F$ is bounded or $H_0$ is bounded below. Let $H_r = H_0 + rV$, $r \in [0, 1]$. Then the formula*

$$\xi^{(s)}(\varphi; H_1, H_0) = \int_0^1 \operatorname{Tr}\left(\varphi(H_r) V P_r^{(s)}\right) dr, \quad \varphi \in C_c(\mathbb{R}),$$

*where* $P_r^{(s)}$ *denotes the projection onto the singular subspace of* $H_r$, *defines an absolutely continuous real measure whose density function, namely the singular SSF* $\xi^{(s)}(\lambda; H_1, H_0)$, *is integer-valued for a.e.* $\lambda \in \mathbb{R}$.

*Moreover, for a.e.* $\lambda$ *the singular SSF coincides with the total resonance index*

$$\xi^{(s)}(\varphi; H_1, H_0) = \sum_{r_\lambda \in [0,1]} \operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V),$$

*which is by definition the integer* $N_+^{[0,1]} - N_-^{[0,1]}$, *where* $N_\pm^{[0,1]}$ *is the total number of poles of the sandwiched resolvent*

$$T_{\lambda+iy}(H_r) = F R_{\lambda+iy}(H_r) F^*,$$

*considered as a function of the coupling parameter* $r$, *which converge to the unit interval* $[0,1]$ *from the half-plane* $\mathbb{C}_\pm$ *as* $y \to 0^+$.

*It also coincides with (the negative of) the singular* $\mu$*-invariant*

$$\xi^{(s)}(\varphi; H_1, H_0) = -\mu^{(s)}(\lambda; H_1, H_0), \quad \forall \text{ a.e. } \lambda \in \mathbb{R},$$

*which is by definition (the negative of) the sum of winding numbers of the eigenvalues of the (off-axis) scattering matrix* $S(\lambda + iy; H_r, H_0)$ *as it is continuously deformed along the loop*

$$1 \xrightarrow[y=0]{r=0 \to r=1} S(\lambda; H_1, H_0) \xrightarrow[y=0 \to y=\infty]{r=1} 1.$$

Proof. The premise is expanded on in Chapter 3 (also see Section 5.2), while the conclusion can be broken into the following three main parts. The singular spectral shift measure is absolutely continuous, by Corollary 5.32. The singular SSF coincides with the total resonance index, by Theorem 6.1. The singular SSF coincides with the singular $\mu$-invariant, by Theorem 8.11. □

CHAPTER 2

# Preliminaries

Some relevant preliminary material is collected here, with selected proofs. Most of what appears here can be found in standard books from the appropriate literature. A reference to a proof should be found wherever one is omitted.

## 2.1. Measures

Let $X$ be a locally compact Hausdorff space. A positive measure $\mu$ defined on the Borel $\sigma$-algebra generated by the topology of $X$ will be called *locally finite* if $\mu(K) < \infty$ for any compact $K \subset X$. For our purposes $X$ will usually be a Euclidean space, most often $X = \mathbb{R}$, so it is safe to assume there is a countable base for the topology of $X$. In this context a locally finite Borel measure is automatically regular in the sense that it is approximable from within by compact sets and from without by open sets (see e.g. [Rud87, Theorem 2.18]). Such measures are also known as Radon measures and the Riesz representation theorem characterises them as linear functionals on the space $C_c(X)$ of compactly supported continuous functions $X \to \mathbb{C}$ ([Rud87, Theorem 2.14; BC10, Theorem 7.3.4]).

THEOREM 2.1. *Let $X$ be a second countable locally compact Hausdorff space. To any linear functional $\mu$ on $C_c(X)$ which is positive in the sense that $f \geq 0 \implies \mu(f) \geq 0$, there corresponds a locally finite positive Borel measure (which we denote by the same symbol) $\mu$, such that*

$$\mu(f) = \int_{\mathbb{R}} f \, d\mu \qquad \forall f \in C_c(X).$$

We equip the compactly supported continuous functions $C_c(X)$ with the standard inductive-limit topology, which is the finest locally convex topology making the inclusions of the sup-normed spaces $(C_c(K), \|\cdot\|_\infty) \hookrightarrow C_c(X)$ continuous for any compact $K \subset X$. This topology is finer than the one induced by the supremum norm and with it $C_c(X)$ is a complete locally convex Hausdorff space. As a subspace $C_c(K)$ retains the topology given by the supremum norm. The convergence of a sequence of functions $\varphi_n \to \varphi$ in $C_c(X)$ is characterised by its uniform convergence plus the existence of a compact $K$ containing the support of each $\varphi_n$. Proofs of these facts can be found in [Hor66, 2,§12] (also see [RS72, Section V.4]).

The theorem below appears as Theorem 7.3.8 in [BC10].

THEOREM 2.2. *With $X$ as in Theorem 2.1, any positive linear functional on $C_c(X)$ is continuous and any continuous linear functional $\mu \in (C_c(X))'$ can be decomposed into a linear combination $\mu = \mu_1 - \mu_2 + i\mu_3 - i\mu_4$ of positive linear functionals $\mu_j$, $j = 1, \ldots, 4$.*

Any element of the dual space $(C_c(X))'$ will be referred to as a (complex valued, possibly unbounded) *measure.* Although locally finite, these measures may not be defined on unbounded sets. An example of such an unbounded measure on $\mathbb{R}$ is $d\mu = \sin x \, dx$.

For a brief note on generalised functions, we put $X = \mathbb{R}$. This information can be found in most standard texts, e.g. [Rud91]. The space of smooth functions $\mathbb{R} \to \mathbb{C}$ with compact support, i.e. test functions, is denoted $C_c^\infty(\mathbb{R})$. This complete locally convex space has the inductive-limit topology coming from the subspaces $C_c^\infty(K)$ for compact $K \subset \mathbb{R}$, which themselves have the Fréchet topology induced by the norms

$$\|\varphi\|_{N,K} = \max_{x \in K} \left\{ \left|\varphi^{(n)}(x)\right| : n \leq N \right\}, \quad N = 1, 2, \ldots.$$

Convergence of a sequence of functions $\varphi_n \to \varphi$ in $C_c^\infty(\mathbb{R})$ is characterised by the existence of a compact set $K$ such that the convergence $\varphi_n \to \varphi$ holds in $C_c^\infty(K)$. Distributions are by definition continuous linear functionals on $C_c^\infty(\mathbb{R})$. The space of test functions $C_c^\infty(\mathbb{R})$ is continuously and densely embedded in the space $C_c(\mathbb{R})$ of compactly supported continuous functions. Therefore their dual spaces are also continuously and densely embedded $(C_c(\mathbb{R}))' \hookrightarrow (C_c^\infty(\mathbb{R}))'$ and measures can be seen as those distributions which continuously extend to $C_c(\mathbb{R})$. Positive distributions and positive measures are in fact the same things, yet the derivative of the delta function is an example of a non-positive distribution which is not a measure.

Lebesgue measure is the unique translation invariant measure on $\mathbb{R}^n$ which assigns 1 to the unit cube. We denote the Lebesgue measure of a Borel set $X \subset \mathbb{R}$ by $|X|$. *Null sets* and *full sets* always refer to Lebesgue measure, as do *absolute continuity, singularity,* and the abbreviation *a.e.* A *support* of a measure $\mu$ is any Borel set whose complement has zero $\mu$-measure. A support $X$ is called *minimal* if for any other support $X'$ the difference $X \setminus X'$ is a null set.

### 2.2. Cauchy-Stieltjes and Poisson transforms

Suppose that $\mu$ is a positive measure (not necessarily finite) on $\mathbb{R}$, which satisfies the condition

$$\int_{\mathbb{R}} (1 + x^2)^{-1} \, d\mu(x) < \infty. \tag{2.1}$$

Then for $z = \lambda + iy$, $y > 0$, the Poisson integral (or Poisson transform) of $\mu$ is defined by the formula

$$\mathcal{P}_\mu(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{y}{(x - \lambda)^2 + y^2} \, d\mu(x), \tag{2.2}$$

which is the convolution $\mu * P_y(\lambda)$ of the measure $\mu$ with the Poisson kernel $P_y(\lambda) = y(\pi(\lambda^2 + y^2))^{-1}$. Since the Poisson kernel converges in the sense of distributions to the delta function as $y \to 0^+$, the Poisson integral $\mu * P_y$ converges in the sense of distributions to $\mu$ :

$$\mu(\varphi) = \lim_{y\to 0^+} \mu * P_y(\varphi) = \lim_{y\to 0^+} \int_{\mathbb{R}} \varphi(\lambda)\mathcal{P}_\mu(\lambda + iy)\, d\lambda, \qquad \varphi \in C_c^\infty(\mathbb{R}).$$

In the case that the measure is finite and absolutely continuous, this convergence holds in $L_1(\mathbb{R})$ as well (see e.g. [Rud87, Theorem 9.10; BC10, Theorem B.3.5]).

THEOREM 2.3. *The Poisson kernel is an approximate identity in $L_1(\mathbb{R})$. In other words, the Poisson integral $f * P_y$ of any $f \in L_1(\mathbb{R})$ converges to $f$ in $L_1(\mathbb{R})$ as $y \to 0^+$.*

On the other hand, taking the pointwise limit of the Poisson integral as $y \to 0^+$ recovers the absolutely continuous part of the measure, according to the following theorem.

THEOREM 2.4. *Let $\mu$ be a positive measure on $\mathbb{R}$ such that $(1 + x^2)^{-1} \in L_1(\mu)$ and let $\mu = \mu^{(a)} + \mu^{(s)}$ be its Lebesgue decomposition, where $d\mu^{(a)} = f d\lambda$. Then the density (Radon-Nikodym derivative) $f$ of its absolutely continuous part is equal a.e. to the limit of its Poisson integral:*

$$f(\lambda) = \lim_{y\to 0^+} \mathcal{P}_\mu(\lambda + iy), \qquad \textit{for a.e } \lambda \in \mathbb{R}.$$

*In other words,*

$$\mu^{(a)}(\varphi) = \int_{\mathbb{R}} \varphi(\lambda) \lim_{y\to 0^+} \mathcal{P}_\mu(\lambda + iy)\, d\lambda, \quad \varphi \in C_c^\infty(\mathbb{R}).$$

*In particular, the Poisson integral of $\mu$ has a finite limit at a.e. $\lambda \in \mathbb{R}$. Moreover, the set of points where the limit fails to exist is a minimal support of the singular part $\mu^{(s)}$.*

PROOF. This theorem can be seen to follow from two facts. Firstly, the density $f$ is equal a.e. to the symmetric derivative

$$(D\mu)(\lambda) = \lim_{\varepsilon\to 0} \frac{\mu(\lambda - \varepsilon, \lambda + \varepsilon)}{2\varepsilon},$$

and the sets

$$\{\lambda : 0 < (D\mu)(\lambda) < \infty\} \quad \text{and} \quad \{\lambda : (D\mu)(\lambda) = \infty\}$$

are minimal supports of the absolutely continuous $\mu^{(a)}$ and singular $\mu^{(s)}$ parts respectively (a summary of this material can be found in [Sch12, Appendix B]). Secondly, the limit $\lim_{y\to 0^+} \mathcal{P}_\mu(\lambda + iy)$ exists and is finite if and only if the same is true of the symmetric derivative $(D\mu)(\lambda)$, in which case these numbers are equal (see e.g. [Don63])

$$(D\mu)(\lambda) = \lim_{y\to 0^+} \mathcal{P}_\mu(\lambda + iy).$$

Also, if $(D\mu)(\lambda) = \infty$, then $\lim_{y\to 0^+} \mathcal{P}_\mu(\lambda + iy) = \infty$, although the converse does not hold in general ([Don63]). □

Theorem 2.4 can be refined. Let $\mathbb{C}_\pm$ denote the open complex half-planes

$$\mathbb{C}_\pm = \{z = \lambda \pm iy \in \mathbb{C} : \lambda \in \mathbb{R}, y \in (0, \infty)\}.$$

Holomorphic functions $\mathbb{C}_+ \to \mathbb{C}_+$ are variously known by the names Herglotz, Nevanlinna, Pick, and $R$–functions. For no special reason we choose the second one. Although it is relevant we only scratch the surface of the rich theory of these functions. For proofs of following results and much more, see e.g. [DK05, Section 1.4; Don74, Chapters II and IV; Sim15a, Chapter 5]. Further information can also be found in the comprehensive paper [GT00] with many more references therein. Finally, alternative summaries of those results we need can be found e.g. in [Sch12, Appendix F; Yaf92, §1.2].

The Poisson transform $v = \mathcal{P}_\mu$ given by (2.2) is a positive harmonic function on $\mathbb{C}_+$ and it turns out that any such function $v$ can be uniquely represented as $v(z) = ay + \mathcal{P}_\mu(z)$ for some $a \geq 0$ and some positive measure $\mu$ satisfying (2.1). These are exactly the imaginary parts of Nevanlinna functions and there is the corresponding (and equivalent) representation theorem:

Theorem 2.5. *Any Nevanlinna function $f$ can be uniquely written as*

$$f(z) = az + b + \int_{\mathbb{R}} \left( \frac{1}{x - z} + \frac{x}{1 + x^2} \right) d\mu(x), \tag{2.3}$$

*for some numbers $a \geq 0$, $b \in \mathbb{R}$, and some positive measure $\mu$ on $\mathbb{R}$ satisfying the condition* (2.1)*.*

The Cauchy-Stieltjes transform of a measure $\mu$ on $\mathbb{R}$ is by definition

$$\mathcal{C}_\mu(z) = \int_{\mathbb{R}} \frac{1}{x - z}\, d\mu(x).$$

Suppose $\mu$ is finite and positive. Then it is easy to see that its Cauchy-Stieltjes transform $f = \mathcal{C}_\mu$ is a Nevanlinna function whose imaginary part is ($\pi$ times) the Poisson integral of $\mu$

$$\frac{1}{\pi} \operatorname{Im} \mathcal{C}_\mu(z) = \mathcal{P}_\mu(z).$$

The following properties of an arbitrary Nevanlinna function will only be needed in this special case $f = \mathcal{C}_\mu$ (in which case a proof of the next theorem can be found e.g. in [Rud87, Theorem 11.32]).

Theorem 2.6. *Suppose $f$ is a Nevanlinna function. Then:*

(i) *the boundary values $f(\lambda + i0) := \lim_{y\to 0^+} f(\lambda + iy)$ exist for a.e. $\lambda \in \mathbb{R}$;*
(ii) *if the boundary values are equal to zero on a set of positive Lebesgue measure, then $f$ is identically zero.*

The following theorem complements Theorem 2.4. (See [Sch12, Theorem F.6] for a proof just for Cauchy-Stieltjes transforms.)

THEOREM 2.7. *Suppose $f$ is a Nevanlinna function with the representation* (2.3)*. Then its boundary values are related to the measure $\mu$ as follows. The absolutely continuous part $\mu^{(a)}$ is given by*

$$d\mu^{(a)}(\lambda) = \frac{1}{\pi} \operatorname{Im} f(\lambda + i0)\, d\lambda,$$

*whereas the singular part $\mu^{(s)}$ is supported by the set*

$$\{\lambda \in \mathbb{R} : \operatorname{Im} f(\lambda + i0) = \infty\}.$$

*A point mass is given by $\mu\{\lambda\} = \lim_{y \to 0^+} y \operatorname{Im} f(\lambda + iy)$.*

The Cauchy-Stieltjes transforms of finite positive measures are characterised among Nevanlinna functions by the following criterion.

THEOREM 2.8. *A Nevanlinna function $f$ is the Cauchy-Stieltjes transform of a finite positive Borel measure on $\mathbb{R}$ if and only if*

$$\sup\{|yf(iy)| : y \geq 1\} < \infty. \tag{2.4}$$

It is apparent from Theorem 2.7 that a sufficient condition for the absolute continuity of the measure $\mu$ is for the imaginary part $\operatorname{Im} f$ to be bounded in $\mathbb{C}_+$. Combining this with the previous theorem:

THEOREM 2.9. *Let $f$ be a Nevanlinna function satisfying* (2.4) *and suppose in addition that its imaginary part* $\operatorname{Im} f(z)$ *is bounded for $z \in \mathbb{C}_+$. Then the function* $\operatorname{Im} f(\lambda + i0)$ *is integrable and*

$$f(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{\operatorname{Im} f(\lambda + i0)}{\lambda - z}\, d\lambda, \quad z \in \mathbb{C}_+.$$

## 2.3. Decomposition of spectrum

The material in this section can be found in books on operator theory such as [Sch12; RS72; Kat84].

By a *Hilbert space* we will mean a complex separable Hilbert space with scalar product $\langle \cdot , \cdot \rangle$ linear in the second argument. The symbols $\mathcal{H}$ and $\mathcal{K}$ will be reserved for Hilbert spaces throughout. As a rule the vectors of $\mathcal{H}$ will be denoted by Roman letters ($f$, $g$, etc.) while Greek letters ($\varphi$, $\psi$, etc.) are reserved for the vectors of $\mathcal{K}$. This is in contrast to the use of these letters to denote functions, in which case we use both Roman and Greek letters with the choice usually meaning little or nothing.

Unless otherwise specified, an *operator* is a densely defined linear operator acting between Hilbert spaces. The domain and range of an operator $F \colon \mathcal{H} \to \mathcal{K}$ are denoted respectively by $\operatorname{dom} F$ and $\operatorname{ran} F$. Since $F$ is assumed to be densely defined, its adjoint $F^* \colon \mathcal{K} \to \mathcal{H}$ is well-defined. The adjoint $F^*$, which is automatically closed, has a dense domain $\operatorname{dom} F^*$ if and only if $F$ is closable. In this case the closure of $F$ satisfies $\overline{F} = F^{**}$ and $(\overline{F})^* = F^*$.

The letter $H$ is reserved for a self-adjoint operator $H^* = H$, while the letter $E$ is reserved for an (orthogonal projection valued) spectral measure.

A version of the spectral theorem (e.g. [Sch12, Theorem 5.7; RS72, Theorem VIII.6]): To any self-adjoint operator $H$, there uniquely corresponds a spectral measure $E$ such that

$$H = \int_{\mathbb{R}} \lambda \, dE(\lambda).$$

Suppose $H$ is a self-adjoint operator on a Hilbert space $\mathcal{H}$. Let $E$ be its spectral measure and let $\mu_{f,g}(\cdot) := \langle f, E(\cdot)g \rangle$, $f, g \in \mathcal{H}$. The absolutely continuous subspace $\mathcal{H}^{(a)}$ of $\mathcal{H}$ with respect to $H$ consists of those vectors $f$ for which $\mu_f := \mu_{f,f}$ is absolutely continuous. The singular subspace $\mathcal{H}^{(s)}$ is defined similarly. The Hilbert space $\mathcal{H}$ decomposes into the direct sum $\mathcal{H}^{(a)} \oplus \mathcal{H}^{(s)}$ of subspaces invariant under $H$. The absolutely continuous $H^{(a)}$ and singular $H^{(s)}$ parts of the operator $H$ are its restrictions to $\mathcal{H}^{(a)}$ and $\mathcal{H}^{(s)}$ respectively. The absolutely continuous spectrum of $H$, denoted $\sigma_{ac}(H)$, is the spectrum of $H^{(a)}$. The singular spectrum $\sigma_s(H)$ is that of $H^{(s)}$. The projections $P^{(a)}$ and $P^{(s)}$ onto $\mathcal{H}^{(a)}$ and $\mathcal{H}^{(s)}$ respectively can be expressed as $P^{(a)} = E(Z_a)$ and $P^{(s)} = E(Z_s)$ for some (non-unique) Borel sets $Z_a$ and $Z_s$. Such a Borel set $Z_a$ is called a support of $\sigma_{ac}(H)$ and likewise for $Z_s$ and the singular spectrum. If $Z_a$ is minimal, in the sense that $|Z_a \setminus Z'_a| = 0$ for any other such $Z'_a$, it is called a core of the absolutely continuous spectrum. Likewise a minimal $Z_s$ is a core of $\sigma_s(H)$. $E^{(a)} = P^{(a)}E$ and $E^{(s)} = P^{(s)}E$ are respectively called the absolutely continuous and singular parts of the spectral measure $E$.

The resolvent of $H$ is the Cauchy-Stieltjes transform of its spectral measure: For any $z$ from the resolvent set $\rho(H) = \mathbb{C} \setminus \sigma(H)$ and any $f, g \in \mathcal{H}$,

$$\langle f, R_z(H)g \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} \, d\langle f, E(\lambda)g \rangle \, .$$

The imaginary part of the resolvent is the Poisson integral

$$\left\langle f, \pi^{-1} \operatorname{Im} R_z(H)g \right\rangle = \frac{1}{\pi} \int_{\mathbb{R}} \frac{y}{(\lambda - x)^2 + y^2} \, d\langle f, E(\lambda)g \rangle \, ,$$

where $z = x + iy$. Theorem 2.4 gives

Corollary 2.10. *For any $f, g \in \mathcal{H}$ the set of points $\lambda$ where there exists a finite limit*

$$\lim_{y \to 0^+} \left\langle f, \pi^{-1} \operatorname{Im} R_{\lambda+iy}(H)g \right\rangle$$

*is a full set and a support of $\mu^{(a)}_{f,g}$, whose complement is a minimal support of $\mu^{(s)}_{f,g}$. For any bounded Borel function $\varphi$, we have*

$$\left\langle f, \varphi(H)P^{(a)}(H)g \right\rangle = \frac{1}{\pi} \int_{\mathbb{R}} \varphi(\lambda) \lim_{y \to 0^+} \langle f, \operatorname{Im} R_{\lambda+iy}(H)g \rangle \, d\lambda.$$

## 2.4. Direct integrals of Hilbert spaces

Direct integrals were introduced by J. von Neumann in his work on (what are now called) von Neumann algebras. On this topic we follow [BS87, §7.1], referring there for all of the proofs (but the same material can be found in books on von Neumann algebras, e.g. [Tak79, Section IV.8]).

A direct integral, for which we will use the notation

$$\mathcal{H} = \int_{\Lambda}^{\oplus} \mathfrak{h}_\lambda \, d\mu(\lambda), \tag{2.5}$$

is roughly speaking a Hilbert space of vector-valued functions (sections) $\Lambda \ni \lambda \mapsto f(\lambda) \in \mathfrak{h}_\lambda$ which take values in a 'field' of Hilbert spaces $\{\mathfrak{h}_\lambda\}_{\lambda\in\Lambda}$ and are square-integrable with respect to a measure $\mu$ on $\Lambda$. If $\Lambda$ is discrete and $\mu$ is counting measure, then this notion reduces to that of a direct sum.

For our purposes it is really only necessary to consider the following case of a direct integral. Let $\Lambda$ be a Borel subset of $\mathbb{R}$ and let $\mu$ be Lebesgue measure. For a.e. $\lambda \in \Lambda$, suppose that $\mathfrak{h}_\lambda$ is a closed subspace of a Hilbert space $\mathcal{K}$. Let $P_\lambda$ be the orthogonal projection onto $\mathfrak{h}_\lambda$ and suppose the field of fibre Hilbert spaces $\{\mathfrak{h}_\lambda\}_{\lambda\in\Lambda}$ is measurable in the sense that $\lambda \mapsto P_\lambda$ is weakly measurable. In this case, the direct integral (2.5) is the closed subspace of $L_2(\Lambda, \mathcal{K})$, which consists of those square-integrable functions $f$ such that $f(\lambda) \in \mathfrak{h}_\lambda$ for a.e. $\lambda \in \Lambda$.

In general a direct integral is allowed to have unrelated fibre Hilbert spaces $\mathfrak{h}_\lambda$ over an arbitrary measure space $(\Lambda, \mu)$, but we might as well assume $\mu$ to be a locally finite Borel measure on $\Lambda \subset \mathbb{R}$. The definition proceeds with a collection of Hilbert spaces $\{\mathfrak{h}_\lambda\}_{\lambda\in\Lambda}$ exhibiting a $\mu$-measurable dimension function, or *multiplicity function*,

$$N(\lambda) := \dim \mathfrak{h}_\lambda. \tag{2.6}$$

A *base of measurability* is a countable set $\{f_k\}_{k\in\mathbb{N}}$ of $\mathfrak{h}_\lambda$-valued functions (sections) whose values span the fibres:

$$\overline{\operatorname{span}}\{f_k(\lambda)\}_{k\in\mathbb{N}} = \mathfrak{h}_\lambda \quad \text{for } \mu\text{-a.e. } \lambda \in \Lambda,$$

and whose pairwise scalar products $\lambda \mapsto \langle f_j(\lambda), f_k(\lambda)\rangle_{\mathfrak{h}_\lambda}$, $j, k \in \mathbb{N}$, are $\mu$-measurable. In the above example with Lebesgue measure and $\mathfrak{h}_\lambda \subset \mathcal{K}$, a base of measurability is obtained by setting $f_k(\lambda) = P_\lambda \psi_k$, where $\{\psi_k\}_{k\in\mathbb{N}}$ is an orthonormal basis of $\mathcal{K}$. Then an arbitrary $\mathfrak{h}_\lambda$-valued function $f$ is defined to be *measurable* with respect to the base $\{f_k\}$ if the function $\lambda \mapsto \langle f(\lambda), f_k(\lambda)\rangle_{\mathfrak{h}_\lambda}$ is $\mu$-measurable for each $k$. The resulting collection of measurable functions can always be generated by a base of measurability $\{f_k\}$ which is orthonormal in the sense that $\{f_k(\lambda)\}_k$ is an orthonormal basis of $\mathfrak{h}_\lambda$ for $\mu$-a.e. $\lambda$ (see [BS87, Lemma 7.1.1]). A field of fibre Hilbert spaces is called *$\mu$-measurable* once it is equipped with a base of measurability.

Suppose that $\{\mathfrak{h}_\lambda(j)\}_{\lambda\in\Lambda}$, $j = 0, 1$, are two $\mu$-measurable fields of fibre Hilbert spaces over $\Lambda$, with bases of measurability $\{f_k^j\}_{k\in\mathbb{N}}$, and that a function $\lambda \mapsto T(\lambda)$ takes values in the bounded operators $\mathcal{B}(\mathfrak{h}_\lambda(0), \mathfrak{h}_\lambda(1))$

for $\mu$-a.e. $\lambda$. Such a function is called *measurable* provided that the scalar functions

$$\lambda \mapsto \left\langle f_k^1(\lambda), T(\lambda) f_k^0(\lambda) \right\rangle$$

are measurable for $k \in \mathbb{N}$.

Given a $\mu$-measurable field of fibre Hilbert spaces $\{\mathfrak{h}_\lambda\}_{\lambda\in\Lambda}$, a *direct integral* (2.5) is defined to be the set of measurable $\mathfrak{h}_\lambda$-valued functions $f$ (up to equality $\mu$-a.e.) which satisfy

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

and the scalar product on $\mathcal{H}$ is defined by

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

Proof that this defines a Hilbert space can be found in [BS87, §7.1 Sub-§§1-4].

The following theorem is numbered 7.1.4 in [BS87].

THEOREM 2.11. *Suppose* $\{\mathfrak{h}_\lambda(j) : \lambda \in \Lambda\}$, $j = 0, 1$, *are two* $\mu$*-measurable fields of fibre Hilbert spaces whose multiplicity functions coincide for* $\mu$*-a.e.* $\lambda \in \Lambda$*. If* $w$ *is a measurable unitary-valued function* $w(\lambda)\colon \mathfrak{h}_\lambda(0) \to \mathfrak{h}_\lambda(1)$, *then the operator*

$$W = \int_\Lambda^\oplus w(\lambda)\, d\mu(\lambda) : \int_\Lambda^\oplus \mathfrak{h}_\lambda(0)\, d\mu(\lambda) \to \int_\Lambda^\oplus \mathfrak{h}_\lambda(1)\, d\mu(\lambda),$$

*defined by* $W\colon f(\lambda) \mapsto w(\lambda) f(\lambda)$, *is a unitary operator.*

Let $\mathcal{H} =$ (2.5) be a direct integral. Of utmost importance are operators on $\mathcal{H}$ of multiplication by a Borel function $\varphi$, denoted

$$M_\varphi f := \varphi f, \quad f \in \mathcal{H}.$$

In particular, for any indicator function $\chi_\Delta$ of a Borel set $\Delta \subset \Lambda$, the multiplication operator $E(\Delta) := M_{\chi_\Delta}$ is an orthogonal projection onto the subspace consisting of those $\mathfrak{h}_\lambda$-valued functions which are zero for $\mu$-a.e. $\lambda \notin \Delta$. This defines the *spectral measure* $E$ of $\mathcal{H}$. The operator $M_\varphi$ for any Borel function $\varphi$ can then be written as $M_\varphi = \int_\Lambda \varphi(\lambda)\, dE(\lambda)$.

It happens that under the premise of Theorem 2.11, the operators $M_\varphi(j)$, $j = 0, 1$, of multiplication by $\varphi$ in the corresponding direct integrals satisfy the equality $M_\varphi(1) W = W M_\varphi(0)$ ([BS87, Theorem 7.2.2]). This gives a reason why the particular choice of a base of measurability is not so important and goes toward explaining its absence from the notation.

THEOREM 2.12. *Let* (2.5) *be a direct integral. A measurable function* $\lambda \mapsto T(\lambda)$ *which takes values in the bounded operators* $\mathcal{B}(\mathfrak{h}_\lambda)$ *and satisfies*

$$\mu\text{-}\sup_{\lambda\in\Lambda} \|T(\lambda)\|_{\mathfrak{h}_\lambda} < \infty, \tag{2.7}$$

*defines a bounded operator* $T$ *on* $\mathcal{H}$ *by*

$$(Tf)(\lambda) := T(\lambda) f(\lambda), \quad f \in \mathcal{H}. \tag{2.8}$$

*The operator $T$ has norm given by* (2.7) *and commutes with the spectral measure $E$ of $\mathcal{H}$.*

*Conversely, any bounded operator $T$ on $\mathcal{H}$ which commutes with $E$ can be represented by* (2.8) *for some bounded operators $T(\lambda) \in \mathcal{B}(\mathfrak{h}_\lambda)$ defined for $\mu$-a.e. $\lambda \in \Lambda$.*

*Moreover, such a decomposable operator $T$ is self-adjoint, normal, unitary, or a projection, if and only if the same is true of $T(\lambda)$ for $\mu$-a.e. $\lambda$.*

The above theorem is a combination of Theorems 7.2.3 and 7.2.5 in [BS87]. For such a decomposable operator $T$ as it describes, we will use the notation

$$T = \int_\Lambda^\oplus T(\lambda)\, d\mu(\lambda).$$

This section is concluded with a version of the spectral theorem ([BS87, Theorem 7.5.1]).

THEOREM 2.13. *Any self-adjoint operator $H$ on a Hilbert space $\mathcal{H}$ can be diagonalised in a direct integral* (2.5)*, in the sense that there exists a unitary operator $\mathcal{F} \colon \mathcal{H} \to \mathcal{H}$ such that*

$$(\mathcal{F}Hf)(\lambda) = \lambda(\mathcal{F}f)(\lambda),$$

*for any $f \in \operatorname{dom} H$ and $\mu$-a.e. $\lambda \in \Lambda$. Moreover, $\mathcal{F}\varphi(H) = M_\varphi \mathcal{F}$ for any Borel function $\varphi$, in particular $\mathcal{F}$ transforms the spectral measure of $H$ into that of $\mathcal{H}$.*

We note that the direct integral (2.5) which appears in this version of the spectral theorem is determined uniquely only in the sense that the multiplicity function (2.6) and the spectral type of the measure $\mu$ are uniquely determined. In fact, the spectral type and multiplicity are unitary invariants of the self-adjoint operator $H$ which together uniquely determine it up to unitary equivalence ([BS87, Theorem 7.5.2]).

## 2.5. The Helffer-Sjöstrand formula

Let $\varphi$ be a bounded Borel function on the spectrum of a self-adjoint operator $H$. In this section we will consider a useful representation of the bounded operator $\varphi(H)$. Suppose that each function $\varphi$ from some class of functions on the spectrum of $H$ has an integral representation

$$\varphi(\lambda) = \int_S K(\lambda, s)\, d\nu_\varphi(s), \tag{2.9}$$

where $(S, \nu_\varphi)$ is a measure space depending on $\varphi$ and the kernel $K$ is a measurable function on $\mathbb{R} \times S$. Suppose in addition that for whatever reason it is known what is meant by the expression $K(H, s)$ for $s \in S$. Then it is natural to consider the formula

$$\varphi(H) = \int_S K(H, s)\, d\nu_\varphi(s). \tag{2.10}$$

One example of (2.9) is the Cauchy integral formula for holomorphic (analytic) functions, which has the resolvent kernel $K(\lambda, s) = R_s(\lambda)$. Provided that the contour of integration $S$ is within the resolvent set of $H$, the formula (2.10) makes sense and is of course the Riesz-Dunford holomorphic functional calculus. Another example is given by the Fourier transform, where the unitary group $K(H,s) = e^{isH}$ appears. Or assuming $H$ is semibounded, another example is given by the Laplace transform, where $K(H,s) = e^{-sH}$. As an aside, if the class of functions $\varphi$ is large enough (for example if it includes all polynomials, or all test functions), then it is possible to recover the full functional calculus for $H$ by a limiting procedure. For our purposes the resolvent kernel is a practical choice and it happens to be available for a much wider class than the holomorphic functions.

The Helffer-Sjöstrand formula is an instance of (2.10) with the resolvent kernel, which is based on the Cauchy-Green (or Cauchy-Pompeiu) formula. It was initially constructed by E. M. Dyn'kin [Dyn75] and is based on the notion of almost analytic extension introduced by L. Hörmander. For a test function $\varphi \in C_c^\infty(\mathbb{R})$ and a self-adjoint operator $H$, the Helffer-Sjöstrand formula is:

$$\varphi(H) = \frac{1}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z) R_z(H)\, dxdy, \tag{2.11}$$

where $z = x + iy$, $\bar\partial = \frac{1}{2}(\partial_x + i\partial_y)$, and $\tilde\varphi$ is an almost analytic extension of $\varphi$. Although it will not be needed, we note that (2.11) can be shown to hold for any smooth function $\varphi$ which vanishes at infinity sufficiently quickly, such as Schwartz functions (see e.g. [Yaj14; DG97, Section C.2]). One of the main advantages of the Helffer-Sjöstrand formula, quoting [DS99], "is that it allows us to pass easily from resolvent estimates to estimates of other functions of $H$." This section is devoted to its proof.

Theorem 2.14. *Let $\varphi \in C_c^1(\mathbb{C})$, by which we mean $\varphi : \mathbb{C} \to \mathbb{C}$ such that $\varphi(x,y) := \varphi(x+iy) \in C_c^1(\mathbb{R}^2)$. Put $z = x+iy$ and $\bar\partial = (\partial_x + i\partial_y)/2$. Then*

$$\varphi(\zeta) = \frac{1}{\pi}\int_{\mathbb{R}^2} \bar\partial\varphi(z)(\zeta - z)^{-1}\, dxdy. \tag{2.12}$$

This theorem can be concisely restated: The function $f(z) = (\pi z)^{-1}$ is a fundamental solution for the operator $\bar\partial$. In other words, as a generalised function $\bar\partial f$ is equal to the Dirac measure $\delta$.

Proof. This can be seen from the Cauchy-Pompeiu formula:

$$\varphi(\zeta) = \frac{-1}{2\pi i}\int_{\partial D} \varphi(z)(\zeta - z)^{-1}\, dz + \frac{1}{\pi}\int_D \bar\partial\varphi(z)(\zeta - z)^{-1}\, dxdy \tag{2.13}$$

(which holds for example if $\varphi \in C^1(\mathbb{C})$ and $D$ is a disk with $\zeta$ in its interior), by taking $D$ large enough to contain the support of $\varphi$. The Cauchy-Pompeiu formula itself can be derived form Green's theorem as follows. For the complex plane, Green's theorem says

$$\int_{\partial D} \varphi(z)\, dz = 2i \int_D \bar{\partial}\varphi(z)\, dxdy.$$

Then applying Green's theorem to the function $\varphi(z)(\zeta - z)^{-1}$ within the region $D_\epsilon = \{z \in D : |\zeta - z| > \epsilon\}$, and noting that the resolvent function is analytic (i.e. $\bar{\partial}(\zeta - z)^{-1} = 0$) in $D_\epsilon$, we get

$$\int_{\partial D} \varphi(z)(\zeta - z)^{-1}\, dz + i \int_0^{2\pi} \varphi(\zeta + \epsilon e^{i\theta})\, d\theta = 2i \int_{D_\epsilon} \bar{\partial}\varphi(z)(\zeta - z)^{-1}\, dxdy.$$

Since the resolvent function is integrable in $\mathbb{C}$ and $\varphi$ is continuous at $\zeta$, sending $\epsilon \to 0$ gives (2.13).

We now give another proof, simple and direct, and lifted from Rudin's book [Rud87]. Put $\varphi(r,\theta) := \varphi(\zeta + re^{i\theta})$, for $r > 0$ and $\theta \in \mathbb{R}$. If $z = \zeta + re^{i\theta}$, the chain rule gives

$$\bar{\partial}\varphi(z) = \frac{e^{i\theta}}{2}\left(\partial_r + \frac{i}{r}\partial_\theta\right)\varphi(r,\theta).$$

The right hand side of (2.12) is therefore equal to the limit as $\epsilon \to 0$ of

$$-\frac{1}{2\pi}\int_\epsilon^\infty \int_0^{2\pi} \left(\partial_r + \frac{i}{r}\partial_\theta\right)\varphi(r,\theta)\, d\theta dr. \tag{2.14}$$

The integral of $\partial_\theta\, \varphi(r,\theta)$ is zero, since $\varphi(r,\theta)$ is $2\pi$-periodic in $\theta$. So (2.14) becomes

$$-\frac{1}{2\pi}\int_0^{2\pi}\int_\epsilon^\infty \partial_r\, \varphi(r,\theta)\, d\theta dr = \frac{1}{2\pi}\int_0^{2\pi} \varphi(\epsilon,\theta)\, d\theta.$$

As $\epsilon \to 0$, $\varphi(\epsilon,\theta) \to \varphi(\zeta)$ uniformly. This gives (2.12). □

Let $\varphi \in C_c^{p+1}(\mathbb{R})$ for $1 \le p < \infty$. We will say a function $\tilde{\varphi} \in C_c^1(\mathbb{C})$ is an *almost analytic extension* of $\varphi$ if:

- it is almost analytic near the real axis, by which we will mean

$$|\bar{\partial}\tilde{\varphi}(z)| = O(|y|^p) \tag{2.15}$$

  as $|y| \to 0$, and
- it extends $\varphi$, i.e. $\tilde{\varphi}|_{\mathbb{R}} = \varphi$.

Examples of almost analytic extensions of a test function $\varphi$ can be constructed using the formula

$$\tilde{\varphi}(z) = \sum_{n=0}^{\infty} \frac{1}{n!}\varphi^{(n)}(x)(iy)^n \chi(a_n y),$$

where $\chi \in C_c^\infty(\mathbb{R})$ is equal to 1 in a neighbourhood of 0, and $a_n \to \infty$ sufficiently quickly. Another construction is

$$\tilde{\varphi}(z) = \frac{\psi(x)}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{izt}\chi(yt)\hat{\varphi}(t)\, dt,$$

where $\chi$ is as above, $\psi \in C_c^\infty(\mathbb{R})$ is equal to 1 in a neighbourhood of the support of $\varphi$, and $\hat{\varphi}$ is the Fourier transform of $\varphi$. These examples are given in [DS99, Chapter 8] where more information can be found. They rapidly become analytic in the sense that $|\bar{\partial}\tilde{\varphi}(z)| = O(|y|^n)$ as $|y| \to 0$ for all $n \in \mathbb{N}$.

LEMMA 2.15. *For any $\varphi \in C_c^{p+1}(\mathbb{R})$, $1 \le p < \infty$, there exists an almost analytic extension $\tilde{\varphi}$.*

PROOF. Put

$$\tilde{\varphi}(z) = \chi(y) \sum_{k=0}^{p} \frac{1}{k!} (iy)^k \varphi^{(k)}(x), \tag{2.16}$$

where $\chi$ is a test function equal to 1 in a neighbourhood of 0. Clearly, the function $\tilde{\varphi}$ is of class $C_c^1(\mathbb{C})$ and it extends $\varphi$. Further,

$$\bar{\partial}\tilde{\varphi}(z) = \frac{\chi(y)}{2} \frac{1}{p!} (iy)^p \varphi^{(p+1)}(x) + \frac{i\chi'(y)}{2} \sum_{k=0}^{p} \frac{1}{k!} (iy)^k \varphi^{(k)}(x)$$

which implies that $|\bar{\partial}\tilde{\varphi}(z)| \le \text{const.}|y|^p$ for small $|y|$. □

THEOREM 2.16. *Let $H$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $\varphi \in C_c^2(\mathbb{R})$, then* (2.11) *holds for any almost analytic extension $\tilde{\varphi}$.*

PROOF. This proof is taken from [DS99, Chapter 8]. Note that the integrand on the right hand side of (2.11) is compactly supported and is continuous in the open set $y \neq 0$. The condition (2.15) combined with the estimate $\|R_z(H)\| \le |y|^{-1}$ implies that it is also bounded:

$$\|\bar{\partial}\tilde{\varphi}(z) R_z(H)\| \le |\bar{\partial}\tilde{\varphi}(z)||y|^{-1} \le \text{const.} \quad \text{as } |y| \to 0.$$

Denoting the right hand side of (2.11) by $Q$, for any two vectors $f, g \in \mathcal{H}$ we get

$$\begin{aligned} \langle f, Qg \rangle &= \frac{1}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z) \, \langle f, R_z(H) g \rangle \; dxdy \\ &= \frac{1}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z) \int_{\mathbb{R}} (\lambda - z)^{-1} \, d\langle f, E(\lambda) g \rangle \; dxdy, \end{aligned}$$

where $E$ is the spectral measure of $H$. Fubini's theorem gives

$$\langle f, Qg \rangle = \int_{\mathbb{R}} \frac{1}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z) (\lambda - z)^{-1} \, dxdy \, d\langle f, E(\lambda) g \rangle \, .$$

Combining this with (2.12) gives

$$\langle f, Qg \rangle = \int_{\mathbb{R}} \varphi(\lambda) \, d\langle f, E(\lambda) g \rangle = \langle f, \varphi(H) g \rangle$$

and this implies (2.11).

We now give another proof. Using the almost analyticity of $\tilde{\varphi}$, the family of complex-valued functions $z \mapsto \bar{\partial}\tilde{\varphi}(z)(\lambda - z)^{-1}$, for $\lambda \in \mathbb{R}$, can be shown to be uniformly integrable. By this we mean that for any $\epsilon > 0$ and any $\lambda \in \mathbb{R}$,

$$\left| \int_E \bar{\partial}\tilde{\varphi}(z)(\lambda - z)^{-1}\, dxdy \right| < \epsilon$$

whenever $|E|$ is small enough. This follows from the fact that we can find an integrable function which dominates the entire family. Such a dominating function exists because these functions share a compact support and are uniformly bounded:

$$|\bar{\partial}\tilde{\varphi}(z)(\lambda - z)^{-1}| \leq |\bar{\partial}\tilde{\varphi}(z)||y|^{-1} \leq \text{const. as } |y| \to 0,$$

thanks to (2.15). We can therefore conclude that the convergence

$$\frac{1}{\pi}\int_{|y|\geq\epsilon} \bar{\partial}\tilde{\varphi}(z)(\lambda - z)^{-1}\, dxdy \to \varphi(\lambda) \quad \text{ as } \epsilon \to 0$$

is uniform in $\lambda$. Then we can conclude (2.11) using the functional calculus and the absolute continuity of the (operator-valued) integral as a set function. □

With some straightforward changes the same reasoning proves the equality

$$\varphi'(H) = -\frac{1}{\pi}\int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z) R_z^2(H)\, dxdy, \tag{2.17}$$

provided $\varphi$ belongs to the class $C_c^3(\mathbb{R})$. This ensures, by Lemma 2.15 and (2.15), that the mapping $z \mapsto \bar{\partial}\tilde{\varphi}(z)R_z^2(H)$ is bounded. The number version of (2.17) follows easily from (2.12):

$$\begin{aligned}
\varphi'(\lambda) &= \lim_{\mu\to\lambda} \frac{\varphi(\lambda) - \varphi(\mu)}{\lambda - \mu} \\
&= \lim_{\mu\to\lambda} \frac{1}{\pi}\int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z)\frac{(\lambda - z)^{-1} - (\mu - z)^{-1}}{\lambda - \mu}\, dxdy \\
&= \lim_{\mu\to\lambda} \frac{-1}{\pi}\int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z)(\lambda - z)^{-1}(\mu - z)^{-1}\, dxdy \\
&= -\frac{1}{\pi}\int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z)(\lambda - z)^{-2}\, dxdy.
\end{aligned}$$

Other details are omitted.

## 2.6. Schatten ideals of compact operators

A standard reference for this section is I. C. Gohberg and M. G. Krein's famous book [GK69]. We recall that any compact operator $T\colon \mathcal{H} \to \mathcal{K}$ can be written in its Schmidt representation as

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

where $\{f_n\}$ and $\{\varphi_n\}$ are orthonormal sets in $\mathcal{H}$ and $\mathcal{K}$ respectively and $s_n(T)$, the so-called *s-numbers,* are the eigenvalues of $|T|$ written in decreasing order.

For compact operators we will need the analytic Fredholm alternative (see e.g. [RS72, Theorem VI.14]):

THEOREM 2.17. *Let $G$ be an open connected subset of $\mathbb{C}$ and let $T\colon G \to \mathcal{L}_\infty(\mathcal{K})$ be a holomorphic family of compact operators on $\mathcal{K}$. Then $-1 \in \sigma(T(z))$ either for all $z \in G$, or for only those $z$ from the discrete set*

$$R := \{z \in G\colon \exists \varphi \neq 0 \ \ (1 + T(z))\varphi = 0\}.$$

*Further, in the latter case, the operator valued function $z \mapsto (1 + T(z))^{-1}$ is meromorphic in $G$ with finite rank residues and the set of its poles is $R$.*

We also state Weyl's classical theorem on the stability of essential spectrum (see e.g. [RS78, Theorem XIII.14; Sch12, Theorem 8.12]):

THEOREM 2.18. *Let $H_0$ and $H_1$ be self-adjoint operators such that the difference of their resolvents $R_z(H_0) - R_z(H_1)$ is compact for some (and hence all) $z \in \rho(H_0) \cap \rho(H_1)$. Then $\sigma_{ess}(H_0) = \sigma_{ess}(H_1)$.*

Within the Banach space of bounded operators $\mathcal{B}(\mathcal{H}, \mathcal{K})$ are the Schatten ideals $\mathcal{L}_p(\mathcal{H}, \mathcal{K})$, $1 \leq p \leq \infty$, of compact operators $T$ such that

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

When $p = \infty$ this coincides with the norm of $\mathcal{B}(\mathcal{H}, \mathcal{K})$ and we drop the subscript. Each $\mathcal{L}_p$ is a Banach space with the above norm, which for any $T \in \mathcal{L}_p$ satisfies $\|T\|_p \geq \|T\|$, $\|T^*\|_p = \|T\|_p$, and for any bounded operators $A, B$,

$$\|ATB\|_p \leq \|A\| \|T\|_p \|B\|. \tag{2.18}$$

This implies that the multiplication

$$\mathcal{B} \times \mathcal{L}_p \times \mathcal{B} \ni (A, T, B) \mapsto ATB \in \mathcal{L}_p \tag{2.19}$$

is continuous. In fact (2.19) is still continuous with the $so^*$-topology on $\mathcal{B}$, which follows from

LEMMA 2.19. *Let $1 \leq p \leq \infty$. Suppose $A \in \mathcal{L}_p$ and $T_n \to 0$ in the $so^*$-topology as $n \to \infty$. Then $\|T_n A\|_p \to 0$ and $\|AT_n\|_p \to 0$.*

PROOF. Here we follow [Yaf92, Lemma 6.1.3]. For any $\varepsilon > 0$ there exists a finite-rank operator $A_\varepsilon$ such that $\|A - A_\varepsilon\|_p < \varepsilon$. Since $\|T_n\| \leq C$ for some $C > 0$, it follows that

$$\|AT_n\|_p \leq \varepsilon\, C + \|A_\varepsilon T_n\|_p.$$

Hence, it suffices to consider finite-rank or even rank-one operators. For $A = \langle f, \cdot \rangle\, \varphi$,

$$\|AT_n\|_p = \|T_n^* A^*\|_p = |\langle \varphi, T_n^* f \rangle| \leq \|\varphi\| \|T_n^* f\| \to 0,$$

by hypothesis. Similarly, $\|T_n A\|_p \to 0$. □

Of the Schatten ideals, apart from compact operators $\mathcal{L}_\infty$, we are mainly concerned with trace class operators $\mathcal{L}_1$ and Hilbert-Schmidt operators $\mathcal{L}_2$.

If $A$ and $B$ are Hilbert-Schmidt operators, then the product $AB$ is trace class and

$$\|AB\|_1 \le \|A\|_2 \|B\|_2.$$

This is (a special case of) Hölder's inequality.

The square root of a positive trace class operator is Hilbert-Schmidt. Further, if $(A_n)$ is a sequence of positive trace class operators and $A_n \to A$ in $\mathcal{L}_1$, then $\sqrt{A_n} \to \sqrt{A}$ in $\mathcal{L}_2$, which follows from the Birman-Koplienko-Solomyak inequality ([BKS75]):

$$\big\|\sqrt{A} - \sqrt{B}\big\|_2 \le \big\|\sqrt{|A-B|}\big\|_2, \tag{2.20}$$

for nonnegative trace class operators $A$ and $B$.

The following material can be found e.g. in [GK69; BS87; Sim05]. The trace of an operator $T$ from $\mathcal{L}_1(\mathcal{K}) = \mathcal{L}_1(\mathcal{K},\mathcal{K})$ is defined by

$$\operatorname{Tr}(T) = \sum_{n=1}^{\infty} \langle \varphi_n, T\varphi_n \rangle\,, \tag{2.21}$$

where $(\varphi_n)$ is an orthonormal basis in $\mathcal{K}$. Lidskii's theorem asserts that the trace $\operatorname{Tr}(T)$ is equal to the sum of the eigenvalues of $T$ counting multiplicities. The trace is a continuous linear functional on $\mathcal{L}_1(\mathcal{K})$ which satisfies the equality $\operatorname{Tr}(AB) = \operatorname{Tr}(BA)$ whenever both $AB$ and $BA$ are trace class. The proof of this cyclic property is well known at least for bounded $A$ and $B$, in which case it follows from Lidskii's Theorem and the fact that $AB$ and $BA$ have common non-zero eigenvalues with coinciding algebraic multiplicities:

$$\sigma_{AB} \cup \{0\} = \sigma_{BA} \cup \{0\}, \text{ including algebraic multiplicities.} \tag{2.22}$$

If an operator $T$ on $\mathcal{K}$ is trace class, then the infinite-dimensional determinant, or Fredholm determinant, of $1+T$ can be defined as the limit of finite-dimensional determinants

$$\det(1+T) = \lim_{n\to\infty} \det(\delta_{ij} + \langle \varphi_i, T\varphi_j \rangle)_{i,j=1}^n, \tag{2.23}$$

where $\{\varphi_k\}_{k\in\mathbb{N}}$ is any orthonormal basis of $\mathcal{K}$. (On this topic, see e.g. [Sch12, Section 9.4; Sim05, Chapter 3; GK69, Chapter IV; BS87, Chapter IV, §1].)

As a consequence of Lidskii's Theorem, the determinant is also given by the product of eigenvalues

$$\det(1+T) = \prod_{j=1}^{\infty} (1+\lambda_j), \tag{2.24}$$

where $\lambda_j$ are the eigenvalues of $T$ counting multiplicities. The determinant $\det(1+T)$ varies continuously, and also analytically, with $T \in \mathcal{L}_1(\mathcal{K})$.

Moreover, it has the following basic properties for $A, B \in \mathcal{L}_1$

$$|\det(1+A)| \leq e^{\|A\|_1},$$

$$\det e^A = e^{\mathrm{Tr}(A)},$$

$$\det(1+A)^* = \overline{\det(1+A)}, \tag{2.25}$$

$$\det(1+A)(1+B) = \det(1+A)\det(1+B), \tag{2.26}$$

$$\det(1+AB) = \det(1+BA).$$

Further, if $0 \leq A \leq B$ then

$$\mathrm{Tr}(A) \leq \det(1+A), \tag{2.27}$$

$$1 \leq \det(1+A) \leq \det(1+B). \tag{2.28}$$

## 2.7. Ordered exponential

Here for convenience is a reproduction of the appendix to [Aza11a] on ordered (or chronological) exponentials. Let $1 \leq p \leq \infty$, $a < b$ and consider the initial value problem

$$\frac{d}{dr}X(r) = A(r)X(r), \quad X(a) = 1, \tag{2.29}$$

where $A\colon [a,b] \to \mathcal{L}_p(\mathcal{K})$ is a continuous path of $p$-Schatten class operators on a Hilbert space $\mathcal{H}$ and the derivative is taken in $\mathcal{L}_p(\mathcal{K})$.

The *(left) ordered exponential* is by definition (cf. [DG97])

$$\mathrm{Texp}\left(\int_a^r A(s)\,ds\right) := 1 + \sum_{k=1}^{\infty} \int_a^r dr_1 \int_a^{r_1} dr_2 \ldots \int_a^{r_{k-1}} dr_k A(r_1)A(r_2)\ldots A(r_k), \tag{2.30}$$

where $r \geq r_1 \geq \ldots \geq r_k \geq a$. The series converges in $\mathcal{L}_p(\mathcal{K})$, since $\|A\|_{p,\infty} := \sup_{r\in[a,b]} \|A(r)\|_p < \infty$ and so

$$\left\| \int_a^r dr_1 \int_a^{r_1} dr_2 \ldots \int_a^{r_{k-1}} dr_k\, A(r_1)A(r_2)\ldots A(r_k) \right\|_p \leq \frac{(r-a)^k}{k!}\|A\|_{p,\infty}^k.$$

Proposition 2.20. *The initial value problem* (2.29) *has the unique continuous solution*

$$X(r) = \mathrm{Texp}\left(\int_a^r A(s)\,ds\right). \tag{2.31}$$

Proof. Substitution shows that (2.31) is a solution. Supposing $Y(r)$ is another solution, integrating (2.29) gives

$$Y(r) = 1 + \int_a^r A(r_1)Y(r_1)\,dr_1.$$

Iterating this, it can be seen that $Y(r) = X(r)$. □

LEMMA 2.21. *For $r_1 < r_2 < r$, the ordered exponential* (2.30) *satisfies the identity*

$$\operatorname{Texp}\left(\int_{r_1}^{r} A(s)\,ds\right) = \operatorname{Texp}\left(\int_{r_2}^{r} A(s)\,ds\right)\operatorname{Texp}\left(\int_{r_1}^{r_2} A(s)\,ds\right). \tag{2.32}$$

PROOF. A similar argument as in Proposition 2.20 shows that

$$X(r) = \operatorname{Texp}\left(\int_{a}^{r} A(s)\,ds\right) X_a$$

is the unique continuous solution of the initial value problem

$$\frac{d}{dr}X(r) = A(r)X(r), \quad X(a) = X_a \in 1 + \mathcal{L}_p(\mathcal{K}). \tag{2.33}$$

Then the proof is completed by checking the fact that both sides of (2.32) are solutions to (2.33) with $a = r_1$ and $X_{r_1} = \operatorname{Texp}\left(\int_{r_1}^{r_2} A(s)\,ds\right)$. ☐

The above lemma allows Proposition 2.20 to be generalised to any piecewise continuous path $A$. Combined with the multiplicative property of the determinant (2.26), this generalisation can also be made for Proposition 2.22 below.

PROPOSITION 2.22. *If $p = 1$ then the Fredholm determinant of the ordered exponential is given by the formula*

$$\det \operatorname{Texp}\left(\int_{a}^{r} A(s)\,ds\right) = \exp\left(\int_{a}^{r} \operatorname{Tr}(A(s))\,ds\right). \tag{2.34}$$

PROOF. We show that both sides of (2.34) are solutions to the initial value problem

$$x'(r) = \operatorname{Tr}(A(r))\,x(r), \quad x(a) = 1.$$

This is clearly true of the right hand side. Let $x(r)$ be the left hand side. Then from (2.32) and the product property of the determinant (2.26), we have

$$\begin{aligned} x'(r) &= \lim_{h\to 0^+} \frac{1}{h}\left(\det \operatorname{Texp}\left(\int_{r}^{r+h} A(s)\,ds\right) - 1\right) x(r) \\ &= \operatorname{Tr}(A(r))\,x(r), \end{aligned}$$

where the last equality follows from a lengthy but straightforward calculation; in brief, the definition of the determinant (2.23) and an interchange of limits allows the calculation of the derivative to be reduced to the finite-dimensional case, where the definition of the ordered exponential (2.30) and the continuity of $A(s)$ imply that the result is the finite-dimensional trace. ☐

## 2.8. Relative compactness of operators and forms

Let $V$ and $H$ be operators on a Hilbert space $\mathcal{H}$. Suppose $H$ is closed and has nonempty resolvent set $\rho(H)$. The operator $V$ is *relatively bounded* with respect to $H$, or *$H$-bounded*, if $\operatorname{dom} H \subset \operatorname{dom} V$ and the following equivalent conditions hold:

- There exist $a, b \geq 0$ so that

$$\|Vf\| \leq a\|Hf\| + b\|f\|, \tag{2.35}$$

for all $f \in \operatorname{dom} H$.
- The operator $VR_z(H)$ is bounded for some (hence any) complex number $z \in \rho(H)$.
- The operator $V\colon \operatorname{dom} H \to \mathcal{H}$ is bounded.

In the last condition we are considering $\operatorname{dom} H$ as a Hilbert space with the graph scalar product $\langle f, g \rangle_H := \langle Hf, Hg \rangle + \langle f, g \rangle$. These equivalences are not difficult to check, noting that the graph norm $\|f\|_H := (\|Hf\|^2 + \|f\|^2)^{1/2}$ is equivalent to the norm $f \mapsto \|Hf\| + \|f\|$ and the operators $R_z(H)\colon \mathcal{H} \to \operatorname{dom} H$ and $(H - z)\colon \operatorname{dom} H \to \mathcal{H}$ are bounded.

The infimum of constants $a > 0$ for which there exists $b > 0$ such that (2.35) holds is called the *$H$-bound* of $V$. *Relative compactness* is naturally defined by replacing 'bounded' by 'compact' in either of the last two conditions, which remain equivalent. In the case that $V$ is $H$-compact, its $H$-bound is equal to 0 (see e.g. [Sch12, Proposition 8.14]).

LEMMA 2.23. *Suppose $H$ is closed and $V$ is closable. Then the inclusion* $\operatorname{dom} H \subset \operatorname{dom} V$ *already implies that $V$ is $H$-bounded.*

Proof of this lemma can be found e.g. in [Kat84, Remark IV-1.5; Sch12, Lemma 8.4].

Occasionally, we identify a bounded operator $A \in \mathcal{B}(\mathcal{H}, \mathcal{K})$ with its continuous (sesquilinear) form

$$(f, g) \mapsto A[f, g] := \langle f, Ag \rangle \tag{2.36}$$

for $f \in \mathcal{K}$ and $g \in \mathcal{H}$. In the case that $\mathcal{K} = \mathcal{H}$, the notation $A[f] := A[f, f]$ is used.

Below is the representation theorem for semibounded forms (see e.g. [Sch12, Theorem 10.7; RS75; Kat84]). In the context of this theorem we will use the same symbol to denote both a form and its corresponding operator, distinguishing the form by the use of square brackets (as in [Sch12]).

THEOREM 2.24. *There is a one-to-one correspondence between lower-bounded self-adjoint operators and lower-bounded closed forms on a Hilbert space $\mathcal{H}$. Given a self-adjoint operator $H$ on $\mathcal{H}$ which is bounded below by $m$, the corresponding closed form has the domain* $\operatorname{dom}[H] := \operatorname{dom}(H - m)^{1/2}$, *on which it is given by*

$$H[f, g] := \left\langle (H - m)^{1/2} f, (H - m)^{1/2} g \right\rangle + m \langle f, g \rangle . \tag{2.37}$$

*Given a lower-bounded closed form $H[\cdot\,, \cdot]$ on $\mathcal{H}$, the corresponding self-adjoint operator $H$ has a domain consisting of those vectors $g \in \operatorname{dom}[H]$ for which there exists a vector $h$ such that $H[f, g] = \langle f, h \rangle$ for all $f \in \operatorname{dom}[H]$, on which it acts by $Hg = h$.*

Suppose now that $H$ is a lower-bounded self-adjoint operator on $\mathcal{H}$. A symmetric form $V$ is *relatively form-bounded* with respect to $H$ if its domain includes the form domain of $H$, i.e. $\mathrm{dom}[H] \subset \mathrm{dom}[V]$, and the following equivalent conditions hold:

- There exist $a, b \geq 0$, such that

$$|V[f]| \leq a|H[f]| + b\|f\|^2, \tag{2.38}$$

  for all $f \in \mathrm{dom}[H]$.
- The operator $(H-m)^{-1/2}V(H-m)^{-1/2}$ is bounded for some (hence any) real number $m$ such that $H > m$.
- The form $V$ admits a decomposition $V = F^*JF$, where $J \in \mathcal{B}(\mathcal{K})$ and $F\colon \mathcal{H} \to \mathcal{K}$ is $(H-m)^{1/2}$-bounded.

The second and third conditions should be clarified. What is meant by the second condition (cf. [Sim15b, p. 662–663]) is that the form

$$(f, g) \mapsto V[(H-m)^{-1/2}f, (H-m)^{-1/2}g] \tag{2.39}$$

corresponds to a bounded operator, denoted

$$(H-m)^{-1/2}V(H-m)^{-1/2}. \tag{2.40}$$

What is meant by the decomposition $V = F^*JF$ in the third condition is that

$$V[f, g] = \langle Ff, JFg\rangle\,, \tag{2.41}$$

for $f \in \mathrm{dom}[H]$. Note that the operator associated to the form $V$ may have a small domain, which however includes any vector $f \in \mathrm{dom}[H]$ such that $JFf \in \mathrm{dom}\, F^*$, on which it acts as the operator $F^*JF$.

The infimum of constants $a > 0$ for which there exists $b > 0$ such that (2.38) holds is called the *$H$-form-bound* of $V$. The *relative form-compactness* of $V$ with respect to $H$ is defined by replacing 'bounded' by 'compact' in either of the last two conditions, which remain equivalent.

PROPOSITION 2.25. *The defining conditions of relative form-boundedness and form-compactness are equivalent. If $V$ is $H$-form-compact, then its $H$-form-bound is zero.*

Since this information about relative form-boundedness is more difficult to find in the literature than its operator counterpart, here is a proof:

PROOF. Suppose that there are $a, b \geq 0$ so that (2.38) holds. Since $\mathrm{dom}[H] = \mathrm{ran}(H-m)^{-1/2}$, we can use (2.37) to obtain for $f = (H-m)^{-1/2}g$,

$$\begin{aligned} \left|V[(H-m)^{-1/2}g]\right| &\leq a|H[f]| + b\|f\|^2 \\ &\leq a\|g\|^2 + (|m| + b)\|(H-m)^{-1/2}g\|^2 \\ &\leq \text{const.}\,\|g\|^2, \end{aligned}$$

which implies that the form (2.39) is bounded.

The corresponding bounded operator $B :=$ (2.40) we write as the product of bounded operators $B = X^*JX$ and if $B$ is compact, this can be done in such a way that $X$ is compact. Then put $F := X(H-m)^{1/2}$, to obtain a decomposition (2.41) for which $F$ is $(H-m)^{1/2}$-bounded (compact).

Conversely, suppose that $V = F^*JF$ where $F$ is relatively bounded (compact) with respect to $(H-m)^{1/2}$. Then the operator

$$(F(H-m)^{-1/2})^* JF(H-m)^{-1/2},$$

which corresponds to the form (2.39), must be bounded (compact).

Again supposing $V = F^*JF$ with $C := \left\|F(H-m)^{-1/2}\right\| < \infty$, for any $f = (H-m)^{-1/2}g \in \operatorname{dom}[H]$ we have

$$\begin{aligned}|V[f]| &= \left|\left\langle F(H-m)^{-1/2}g, JF(H-m)^{-1/2}g\right\rangle\right| \\ &\le \|J\|C^2\|g\|^2 \\ &= \|J\|C^2\left(\left\|(H-m)^{1/2}f\right\|^2 + m\|f\|^2 - m\|f\|^2\right) \\ &= \|J\|C^2\left(H[f] - m\|f\|^2\right) \\ &\le \|J\|C^2\left(|H[f]| + |m|\|f\|^2\right).\end{aligned}$$

Finally we show that if $V$ is $H$-form-compact, then its $H$-form-bound is zero. Assume the contrary, that is, there exists some $a > 0$ for which there is no $b$ such that (2.38) holds. Then we can find a sequence of vectors $f_n \in \operatorname{dom}[H]$ such that

$$|V[f_n]| > a|H[f_n]| + n\|f_n\|^2 \ge a\|(H-m)^{1/2}f_n\|^2 + (n - a|m|)\|f_n\|^2$$

for any $n \in \mathbb{N}$. Scaling each $f_n$ by $|V[f_n]|^{-1}$, we can assume that $|V[f_n]| = 1$. Then $\|f_n\|^2 < 1/(n - a|m|)$ and $\|(H-m)^{1/2}f_n\|^2 < 1/a$ for any $n$. Thus $f_n$ converges to 0 and the sequence $(H-m)^{1/2}f_n$ is bounded, which must therefore have a weakly convergent subsequence. Passing to such a subsequence, let $g$ be the weak limit of $g_n := (H-m)^{1/2}f_n$. Then for any $h \in \operatorname{dom}[H]$, we have

$$\langle g_n, h\rangle = \left\langle f_n, (H-m)^{1/2}h\right\rangle \to \langle g, h\rangle = \left\langle 0, (H-m)^{1/2}h\right\rangle,$$

hence $g = 0$. Therefore $f_n$ is a weak null sequence in the Hilbert space $\left(\operatorname{dom}[H], \langle\cdot\,,\cdot\rangle_{[H]}\right) := \left(\operatorname{dom}(H-m)^{1/2}, \langle\cdot\,,\cdot\rangle_{(H-m)^{1/2}}\right)$. Yet by assumption $V = F^*JF$ where $J$ is bounded and $F\colon \operatorname{dom}[H] \to \mathcal{H}$ is compact. Thus $F$ maps $f_n$ to a null sequence $Ff_n$ and we arrive at the contradiction

$$1 = |V[f_n]| = \langle Ff_n, JFf_n\rangle \to 0. \qquad \square$$

PROPOSITION 2.26. *Suppose $H$ is a lower-bounded self-adjoint operator and $V$ is a positive self-adjoint operator. Then $V$ is $H$-form-bounded (compact) if and only if $V^{1/2}$ is $|H|^{1/2}$-bounded (compact). Further in the 'bounded' case, the inclusion* $\operatorname{dom}[H] \subset \operatorname{dom}[V]$ *(which is implicit in both statements) is also equivalent.*

PROOF. Since both $V^{1/2}$ and $|H|^{1/2}$ are closed operators, the inclusion of domains $\mathrm{dom}[H] \subset \mathrm{dom}[V]$ already implies that $V^{1/2}$ is $|H|^{1/2}$ bounded by Lemma 2.23. If $V^{1/2}$ is $|H|^{1/2}$-bounded (compact), then it easily follows that $V$ is $H$-form-bounded (compact). As for the converse in the 'compact' case, its premise implies that the form (2.39) corresponds to a compact operator. Using (2.37), this form corresponds to the operator

$$(V^{1/2}(H-m)^{-1/2})^* V^{1/2}(H-m)^{-1/2},$$

whose compactness implies that of $V^{1/2}(H-m)^{-1/2}$ itself and the result follows. □

We note that the correspondence between forms and operators given by Theorem 2.24 extends to sectorial forms (see e.g. [Kat84, Theorem VI-2.1]). Moreover, both notions of relative boundedness can be applied to sectorial operators $H$, $V$, and Kato ([Kat84, VI-§1.7]) writes: "In general it is not clear whether there is any relationship between these two kinds of relative boundedness. If we restrict ourselves to considering only symmetric operators however, form-relative boundedness is weaker than operator-relative boundedness."

LEMMA 2.27. *Let $H$ and $V$ be closed operators. Then the relative boundedness (compactness) of $V$ with respect to $H$ implies the same of $|V|^{1/2}$ with respect to $|H|^{1/2}$.*

For a proof of this lemma see e.g. [Yaj14, Lemma 5.40; RS75, Theorem X.18; Kat84, Theorem VI-1.38].

The following two theorems concern the stability of self-adjointness under relatively bounded perturbations. The first is known as the Kato-Rellich Theorem, see e.g. [RS78, Theorem X.12; Sch12, Theorem 8.5].

THEOREM 2.28. *Let $H$ be a self-adjoint operator and let $V$ be a symmetric operator which is $H$-bounded with $H$-bound less than 1. Then the operator sum $H+V$ is self-adjoint with the same domain as $H$.*

T. Kato famously applied Theorem 2.28 to atomic Hamiltonians. For example the energy of the hydrogen atom is described (in atomic units) by $H = -\Delta - 2/r$, where $-\Delta$ is the Laplacian on $L_2(\mathbb{R}^3, dx)$ and $r = |x|$. Indeed, the Kato-Rellich theorem can be applied to prove the self-adjointness of the Schrödinger operator $H = -\Delta + V$ on $L_2(\mathbb{R}^\nu)$ for any potential $V$ of the form $V(x) = \text{const.}\,|x|^{-\alpha}$, where $0 < \alpha < \min\{\nu/2, 2\}$. The condition $\alpha < \nu/2$ for low-dimensional Schrödinger operators can be removed by instead applying the so-called KLMN theorem below. For a proof see e.g. [RS78, Theorem X.17; Sch12, Theorem 10.21].

THEOREM 2.29. *Let $H$ be a lower-bounded self-adjoint operator and let $V$ be a symmetric form which is $H$-form-bounded with $H$-form-bound less than 1. Then the form sum of $H$ and $V$ corresponds to a lower-bounded self-adjoint operator, denoted $H \dotplus V$, with the same form domain as $H$.*

CHAPTER 3

# The rigging operator and the LAP

By a *rigging operator* we mean a closed operator $F\colon \mathcal{H} \to \mathcal{K}$ between Hilbert spaces, which has trivial kernel and cokernel. In other words, $F$ is injective and $\mathcal{K} = \overline{\operatorname{ran} F}$. We call $\mathcal{H}$ the *main Hilbert space* and $\mathcal{K}$ the *auxiliary Hilbert space*.

As an aside, the partial isometry $U : \mathcal{H} \to \mathcal{K}$ in the polar decomposition $F = U|F|$ is unitary since $\ker(U) = \ker(F) = \{0\}$ and $\operatorname{ran} U = \overline{\operatorname{ran} F} = \mathcal{K}$, so we may naturally identify $\mathcal{H}$ and $\mathcal{K}$. It is for this reason technically unnecessary to allow for $F$ to be other than a positive self-adjoint operator. However, we find the above definition to be convenient.

A rigging operator is closely related to the notion of *rigged Hilbert space*, which usually refers to a triple of embedded spaces:

$$\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-. \tag{3.1}$$

In short, given a Banach space $\mathcal{H}_+$ which is continuously and densely embedded via $j\colon \mathcal{H}_+ \to \mathcal{H}$, the space $\mathcal{H}_-$ is introduced as the space of antilinear functionals on $\mathcal{H}_+$. The adjoint map $j^* : \mathcal{H} \to \mathcal{H}_-$, defined for $f \in \mathcal{H}$ and $g \in \mathcal{H}_+$ by

$$\langle g, j^* f\rangle := \langle jg, f\rangle_{\mathcal{H}} = \langle g, f\rangle_{\mathcal{H}}\,, \tag{3.2}$$

is then also a continuous embedding.

A rigging operator $F\colon \mathcal{H} \to \mathcal{K}$ gives rise to analogous spaces $\mathcal{H}_\pm$, which instantiate the triple (3.1) in the case that $F$ is bounded. We will now discuss this connection, but it will not be logically required elsewhere.

The dense linear subspace $\operatorname{ran} F^*$ of $\mathcal{H}$ can be given the scalar product

$$\langle F^*\varphi, F^*\psi\rangle_+ := \langle \varphi, \psi\rangle_{\mathcal{K}}\,,$$

which makes $F^*$ isometric. If $F$ is bounded, then $\mathcal{H}_+ := (\operatorname{ran} F^*, \langle\cdot\,,\cdot\rangle_+)$ is a Hilbert space and its inclusion $\mathcal{H}_+ \subset \mathcal{H}$ is continuous. Otherwise, let $\mathcal{H}_+$ denote the completion of the inner-product space $(\operatorname{ran} F^*, \langle\cdot\,,\cdot\rangle_+)$. On the other hand, the dense linear subspace $\operatorname{dom} F$ of $\mathcal{H}$ can be given the scalar product

$$\langle f, g\rangle_- = \langle Ff, Fg\rangle_{\mathcal{K}}\,,$$

which makes $F$ isometric. Let $\mathcal{H}_-$ be the completion of $(\operatorname{dom} F, \langle\cdot\,,\cdot\rangle_-)$ which is generally not already complete even when $F$ is bounded. If $F$ is bounded, then $\mathcal{H}$ is continuously included in $\mathcal{H}_-$. The spaces $\mathcal{H}_\pm$ can be succinctly defined as the completions of the dense linear subspace $\operatorname{ran} F^* \cap \operatorname{dom} F$ of $\mathcal{H}$ in the inner products

$$\langle f, g\rangle_{\pm} = \left\langle |F|^{\mp 1} f, |F|^{\mp 1} \right\rangle_{\mathcal{H}}.$$

The operator $F^*$ can be considered as a unitary operator identifying $\mathcal{K}$ and $\mathcal{H}_+$ while $F$ can be considered as a unitary operator identifying $\mathcal{H}_-$ and $\mathcal{K}$.

When $F$ is bounded the spaces $\mathcal{H}_{\pm}$ constitute a particular case of the continuous inclusions (3.1). It has already been noted that $\mathcal{H}_+$ is continuously embedded in $\mathcal{H}$ and we will now check that the anti-dual space $\mathcal{H}_+^{\times}$ is in fact $\mathcal{H}_-$ (cf. [BS91, Proposition S1.2.6]). Since $\mathcal{H}_+$ is dense in $\mathcal{H}$, it follows that $\mathcal{H}$ (identified with $\mathcal{H}^{\times}$) is dense in $\mathcal{H}_+^{\times}$. Therefore it suffices to see that the norms $\|\cdot\|_-$ and $\|\cdot\|_{\mathcal{H}_+^{\times}}$ agree on vectors $f$ in $\mathcal{H}$ :

$$\|f\|_{\mathcal{H}_+^{\times}} = \sup_{\|g\|_+=1} |\langle f, g\rangle_{\mathcal{H}}| = \sup_{\|\varphi\|_{\mathcal{K}}=1} |\langle f, F^*\varphi\rangle_{\mathcal{H}}| = \sup_{\|\varphi\|_{\mathcal{K}}=1} |\langle Ff, \varphi\rangle_{\mathcal{K}}| = \|f\|_-.$$

If a rigged Hilbert space arises from a rigging operator $F$, then statements involving the spaces $\mathcal{H}_{\pm}$ can as a rule be translated to instead involve $F$ and its adjoint $F^*$. The latter language is systematically used from now on.

## 3.1. The sandwiched resolvent

Suppose $H$ is a self-adjoint operator on $\mathcal{H}$ and $F\colon \mathcal{H} \to \mathcal{K}$ is a rigging operator. For any $z$ from the resolvent set $\rho(H)$ of $H$, the *sandwiched resolvent* is the operator

$$T_z(H) := FR_z(H)F^* = F(H-z)^{-1}F^*.$$

The rigging operator doesn't appear in the notation because it is considered to be fixed. The operators $H$ and $F$ will be chosen so that the sandwiched resolvent is a bounded operator on the auxiliary Hilbert space $\mathcal{K}$, or more precisely that it is bounded on a dense domain of definition and hence extends continuously to a bounded operator on $\mathcal{K}$. In such a situation, let it be this bounded extension which is denoted by the symbol $T_z(H)$. We will later assume further that $T_z(H)$ is compact.

THEOREM 3.1. *Let $F\colon \mathcal{H} \to \mathcal{K}$ be a rigging operator and let $H$ be a self-adjoint operator on $\mathcal{H}$. If $F$ is $|H|^{1/2}$-bounded (compact) then the sandwiched resolvent $T_z(H)$ is bounded (compact) for any $z \in \rho(H)$. The converse holds under either of the following additional conditions.*

- *$F$ is bounded.*
- *$H$ is semibounded and* $\operatorname{dom} H \subset \operatorname{dom} F$.

*Also equivalent in the first case is for $F$ to be $H$-bounded (compact). Also equivalent in the second case is for the positive self-adjoint operator $F^*F$ to be $H$-form-bounded (compact).*

We work towards a proof of this theorem with the next few lemmas.

LEMMA 3.2. *Let a self-adjoint operator $H$ and a rigging operator $F$ be such that* $\operatorname{dom} H \subset \operatorname{dom} F$. *Suppose that for some nonreal $z$ the sandwiched resolvent $T_z(H)$ is bounded (compact). Then $F$ is $H$-bounded (compact) and in addition $T_w(H)$ is bounded (compact) for any $w \in \rho(H)$.*

PROOF. Here we follow [Aza11a, Lemma 2.5.1]. The inclusion $\operatorname{dom} H \subset \operatorname{dom} F$ implies that the product $FR_z(H)F^*$ is densely defined on the domain of $F^*$ and it is assumed that this product extends continuously to the bounded (compact) operator $T_z(H)$. The inclusion of domains also implies that $F$ is $H$-bounded by Lemma 2.23. Note that $(T_z(H))^* = (FR_z(H)F^*)^* \supset FR_{\bar{z}}(H)F^*$, from which it follows that $(T_z(H))^* = T_{\bar{z}}(H)$. Supposing that $T_z(H)$ is compact, then so is its adjoint, hence so is the difference

$$\begin{aligned} T_z(H) - T_{\bar{z}}(H) &= F(R_z(H) - R_{\bar{z}}(H))F^* \\ &= 2i \operatorname{Im} z \, FR_z(H)R_{\bar{z}}(H)F^* \\ &= 2i \operatorname{Im} z \, FR_z(H)(FR_z(H))^*. \end{aligned}$$

Strictly speaking, the intermediate equalities hold on $\operatorname{dom} F^*$, but the final equality can be taken literally, as an equality of bounded operators. From this we see that the product of $FR_z(H)$ and its adjoint is compact, which implies that $FR_z(H)$ itself is compact. Indeed, if $A^*A = |A|^2$ is compact, then so is $|A|$, hence so is $A$. So $F$ is $H$-compact.

For the last part let $w \in \rho(H)$. From the equality

$$(z - w)FR_z(H)(FR_w(H))^* = T_z(H) - T_w(H),$$

(which holds a priori on $\operatorname{dom} F^*$) we see that in either case the sandwiched resolvent $T_w(H)$ is bounded, and if $T_z(H)$ is compact, then so is $T_w(H)$. □

LEMMA 3.3. *If $F$ is a closed operator and $B$ is a bounded operator, then $FB$ is closed. Moreover, $(B^*F^*)^* = FB$. If in addition $FB$ is densely defined, then its adjoint $(FB)^*$ is the closure of $B^*F^*$.*

PROOF. We prove these standard facts for completeness. Suppose that $f_n$, $n = 1, 2, \ldots$, is a sequence from the domain of $FB$ which converges to $f$ and also that $FBf_n$ converges to $g$. Then since $B$ is continuous, $Bf_n$ is a sequence from the domain of $F$ which converges to $Bf$. By the closedness of $F$, $Bf$ belongs to $\operatorname{dom} F$, hence $f \in \operatorname{dom} FB$, and $FBf_n$ converges to $g = FBf$. Therefore $FB$ is closed.

To see that $(B^*F^*)^* = FB$ we first consider their domains. From the definition of the adjoint and the boundedness of $B$, the domain of $(B^*F^*)^*$ is the set of those vectors $f$ for which there exists a vector $g$ satisfying the equality

$$\langle f, B^*F^*h \rangle = \langle Bf, F^*h \rangle = \langle g, h \rangle$$

for all vectors $h$ from $\operatorname{dom} B^*F^* = \operatorname{dom} F^*$. This is in other words the set of those $f$ for which $Bf$ belongs to the domain of $(F^*)^*$. And since $F^{**} = F$ by the closedness of $F$, this set coincides with the domain of $FB$. That these operators coincide on their common domain follows from the equality

$$\langle (B^*F^*)^* f, h\rangle = \langle f, B^*F^*h\rangle = \langle Bf, F^*h\rangle = \langle FBf, h\rangle\,,$$

which holds for all $h$ from the dense domain of $F^*$.

What remains to be proved follows from the equality $(B^*F^*)^* = FB$ and the fact that if the adjoint of the operator $B^*F^*$ is densely defined, then its closure coincides with its double adjoint. □

LEMMA 3.4. *Let $H$ be a self-adjoint operator and $F$ a (densely defined) closed operator on a Hilbert space $\mathcal{H}$. Let $\psi$ be a bounded Borel function which is nonzero a.e. with respect to the spectral measure of $H$. Suppose that $F\psi(H)$ is densely defined. Then the following statements are equivalent, in which $(\mathfrak{I}_1, \mathfrak{I}_2)$ stands for one of the pairs of ideals of $\mathcal{B}(\mathcal{H})$ : either $\mathfrak{I}_1 = \mathfrak{I}_2 = \mathcal{B}(\mathcal{H})$, $\mathfrak{I}_1 = \mathfrak{I}_2 = \mathcal{L}_\infty(\mathcal{H})$, or $\mathfrak{I}_1 = \mathcal{L}_1(\mathcal{H})$ and $\mathfrak{I}_2 = \mathcal{L}_2(\mathcal{H})$.*

- (i) *The operator $F\psi(H)$ belongs to $\mathfrak{I}_2$.*
- (ii) *The operator $F\varphi(H)$ belongs to $\mathfrak{I}_2$ for some function $\varphi$ of the same order as $\psi$ in the sense that both $\psi/\varphi$ and $\varphi/\psi$ are bounded Borel functions on $\sigma(H)$.*
- (iii) *The operator $F\varphi(H)$ belongs to $\mathfrak{I}_2$ for any Borel function $\varphi$ which for some $C > 0$ and a.e. $x \in \sigma(H)$ satisfies $|\varphi(x)| \le C|\psi(x)|$.*
- (iv) *For any Borel function $\varphi$ which for some $C > 0$ and $H$-a.e. $x \in \sigma(H)$ satisfies $|\varphi(x)| \le C|\psi(x)|^2$, the operator $F\varphi(H)F^*$ can be continuously extended to an operator which belongs to $\mathfrak{I}_1$.*
- (v) *For some function $\varphi$ of the same order as $\psi$ (in the above sense), the operator $F|\varphi|^2(H)F^*$ can be continuously extended to a positive operator which belongs to $\mathfrak{I}_1$.*
- (vi) *The operator $F|\psi|^2(H)F^*$ can be continuously extended to a positive operator which belongs to $\mathfrak{I}_1$.*

If the equivalent conditions of Lemma 3.4 hold, and if $\varphi$ is as in condition (iv), then the bounded closure of the sandwiched operator $F\varphi(H)F^*$ is equal to

$$\overline{F\varphi(H)F^*} = F\psi_1(H)\left(F\bar{\psi}_2(H)\right)^*, \tag{3.3}$$

for any two Borel functions $\psi_j$, $j = 1, 2$, such that $\varphi(x) = \psi_1(x)\psi_2(x)$ and $|\psi_j(x)| \le C_j|\psi(x)|$ for some $C_j > 0$ and any $x$. Indeed, the operator on the right hand side of (3.3) extends $F\varphi(H)F^*$ by Lemma 3.3 and hence (3.3) holds by the uniqueness of continuous extension. Following from this is the intuitively obvious equality

$$\left(\overline{F\varphi(H)F^*}\right)^* = \overline{F\bar{\varphi}(H)F^*}. \tag{3.4}$$

Also note that if $\varphi_1$ and $\varphi_2$ are as in condition (iv), then so is their sum and by the uniqueness of continuous extension we have

$$\overline{F(\varphi_1+\varphi_2)(H)F^*} = \overline{F\varphi_1(H)F^*} + \overline{F\varphi_2(H)F^*}. \tag{3.5}$$

Proof. Clearly (iii) implies both (i) and (ii).

(i) implies (iii): For any Borel function $\varphi$ which is dominated by $C|\psi|$, the function $\varphi/\psi$ is bounded and hence $(\varphi/\psi)(H)$ is a bounded operator. Then since $F\psi(H)$ belongs to $\mathfrak{I}_2$, so does $F\varphi(H) = F\psi(H)(\varphi/\psi)(H)$.

(ii) implies (iii): This can be seen from the above argument by replacing $\psi$ by the function $\varphi$ appearing in (ii).

(iii) implies (iv): Let $\varphi$ be dominated by $C|\psi|^2$. Then $(\varphi/\psi)$ is dominated by $C|\psi|$ and both $F(\varphi/\psi)(H)$ and $F\overline{\psi}(H)$ belong to $\mathfrak{I}_2$ by (ii). Thus $F(\varphi/\psi)(H)(F\overline{\psi}(H))^*$ belongs to $\mathfrak{I}_1$. Note that $\psi(H)F^* \subset (F\overline{\psi}(H))^*$ and the operator $F\varphi(H)F^* = F(\varphi/\psi)(H)\psi(H)F^*$ is defined on the dense domain of $F^*$, where it is equal to $F(\varphi/\psi)(H)(F\overline{\psi}(H))^*$. (iv) follows by the uniqueness of continuous extension.

Clearly (iv) implies both (v) and (vi).

(vi) implies (i): Since the operator $F\psi(H)$ is densely defined and closed, it follows that the operator $F\psi(H)(F\psi(H))^*$ is self-adjoint (see e.g. [Kat84, Theorem V-3.24]). By Lemma 3.3 $F\psi(H) = (\overline{\psi}(H)F^*)^*$ and we have

$$(F|\psi|^2(H)F^*)^* \supset (\overline{\psi}(H)F^*)^*(F\psi(H))^* = F\psi(H)(F\psi(H))^*.$$

It follows that $F|\psi|^2(H)F^*$ continuously extends to $F\psi(H)(F\psi(H))^*$, which must therefore belong to $\mathfrak{I}_1$. From this it follows that $F\psi(H) \in \mathfrak{I}_2$. Indeed, if $AA^* = |A^*|^2 \in \mathfrak{I}_1$, then $|A^*|$ belongs to $\mathfrak{I}_2$ hence so do $A^*$ and $A$.

(v) implies (ii): This can be seen from the above argument by replacing $\psi$ by the function $\varphi$ appearing in (ii). $\square$

Proof of Theorem 3.1. Consider the following statement: A self-adjoint operator $H$ and a rigging operator $F$ are such that the equivalent conditions of Lemma 3.4 hold with $\psi(x) = (|x|^{1/2} + 1)^{-1}$ and $\mathfrak{I}_1 = \mathfrak{I}_2 = \mathcal{B}$ (or $\mathcal{L}_\infty$). Condition (i) is clearly equivalent to the condition that $F$ is $|H|^{1/2}$-bounded (compact). While condition (iv) implies that the sandwiched resolvent $T_z(H)$ is bounded (or compact).

If $H$ is bounded below then the boundedness (compactness) of the sandwiched resolvent implies condition (v), since in this case the resolvent function $x \mapsto (x+m)^{-1}$ is positive on $\sigma(H)$ for large enough $m$. By Proposition 2.26 also equivalent is for the operator $F^*F$ to be $H$-form-bounded (compact).

In the case that the rigging operator $F$ is bounded, the boundedness (compactness) of the sandwiched resolvent is equivalent to the $H$-boundedness (compactness) of $F$. One direction of this equivalence is obvious, while the other follows from Lemma 3.2. $\square$

Suppose $H$ is a self-adjoint operator on $\mathcal{H}$ and $F\colon \mathcal{H} \to \mathcal{K}$ is a rigging operator such that $\operatorname{dom}|H|^{1/2} \subset \operatorname{dom} F$. Then $F$ is $|H|^{1/2}$-bounded by Lemma 2.23 and it follows from Theorem 3.1 that the sandwiched resolvent $T_z(H)$ is bounded for any $z \in \rho(H)$. A sandwiched version of the so-called first resolvent identity (see (3.17)) holds:

$$T_z(H) - T_w(H) = (z-w)FR_z(H)(FR_{\bar{w}}(H))^* \tag{3.6}$$

and in particular,

$$\operatorname{Im} T_z(H) = \operatorname{Im} z\, FR_z(H)(FR_z(H))^*. \tag{3.7}$$

These equalities follow from (3.3), (3.4), and (3.5). Also note that since $\operatorname{Im} R_z(x) = \operatorname{Im} z\, R_z(x)R_{\bar{z}}(x)$ for any $x$, the operator $\operatorname{Im} T_z(H)$ is the closure of $F \operatorname{Im} R_z(H) F^*$.

The inclusion $\operatorname{Im} T_z(H) \in \mathcal{L}_1(\mathcal{K})$ for $z \in \mathbb{C} \setminus \mathbb{R}$ will be important later. We note that it is equivalent to the inclusion $FR_z(H) \in \mathcal{L}_2(\mathcal{H}, \mathcal{K})$ and holds for any nonreal $z$ as long as it holds for one.

Lemma 3.5. *Suppose $H$, $F$, $\mathfrak{I}_1$, $\mathfrak{I}_2$, and $\psi$ are as in Lemma 3.4 and its equivalent conditions hold. Let $C > 0$. If $\varphi_n$, $n = 1, 2, \ldots$, is a sequence of Borel functions which are dominated by $C|\psi|^2$ and converge pointwise to $\varphi$, then the following convergence holds in $\mathfrak{I}_1$.*

$$\overline{F\varphi_n(H)F^*} \to \overline{F\varphi(H)F^*} \quad \text{as } n \to \infty.$$

Proof. Since $\varphi$ is the pointwise limit of Borel functions which are dominated by $C|\psi|^2$, it is also a Borel function with the same dominating function. By assumption $F\psi(H)$ belongs to $\mathfrak{I}_2$. Also, for any $\chi$ dominated by $C|\psi|^2$, $F(\chi/\psi)(H)$ belongs to $\mathfrak{I}_2$ since $\chi/\psi$ is dominated by $C|\psi|$, and the closure of $F\chi(H)F^*$, equal to $F(\chi/\psi)(H)(F\psi(H))^*$ by (3.3), belongs to $\mathfrak{I}_1$. The proof will be completed if we can ensure that the number

$$\|F(\chi_n/\psi)(H)(F\psi(H))^*\|_{\mathfrak{I}_1},$$

where $\chi_n := \varphi - \varphi_n$, is arbitrarily small for large enough $n$. Note that $\chi_n/\psi^2$ is a sequence of uniformly bounded Borel functions converging pointwise to 0. It follows from the functional calculus that $(\chi_n/\psi^2)(H)$ converges to 0 in the *so*$^*$-topology. By Lemma 2.19, $F(\chi_n/\psi)(H) = (F\psi(H))(\chi_n/\psi^2)(H)$ converges to 0 in $\mathfrak{I}_2$. Therefore, the result follows from the estimate

$$\|F(\chi_n/\psi)(H)(F\psi(H))^*\|_{\mathfrak{I}_1} \le \|F(\chi_n/\psi)(H)\|_{\mathfrak{I}_2} \|F\psi(H)\|_{\mathfrak{I}_2}. \qquad \square$$

Corollary 3.6. *Let $H$ be a self-adjoint operator on $\mathcal{H}$ and let $F \colon \mathcal{H} \to \mathcal{K}$ be a rigging operator which is $|H|^{1/2}$-bounded. Then the sandwiched resolvent $T_z(H)$ is norm-continuous as a function of $z \in \rho(H)$. In fact it is analytic. Moreover, it is continuous at $z = \infty$ where it converges to 0.*

*In addition we note that if the imaginary part $\operatorname{Im} T_z(H)$ belongs to the trace class for some (hence any) nonreal $z$, then it is continuous there and converges to 0 in the trace class norm as $z \to \infty$. Further, for $z \in \mathbb{C}_+$ its square root $\sqrt{\operatorname{Im} T_z(H)}$ is continuous in the Hilbert-Schmidt class where it converges to 0 as $z \to \infty$.*

Proof. The norm-continuity of the sandwiched resolvent $z \to T_z(H)$ and its convergence to 0 as $z \to \infty$ follows easily from Lemma 3.5. So too does the continuity and convergence to 0 as $z \to \infty$ of $z \mapsto \operatorname{Im} T_z(H)$ in the $\mathcal{L}_1$-norm, if $\operatorname{Im} T_z(H) \in \mathcal{L}_1(\mathcal{K})$. Therefore the same can be said of $z \mapsto \sqrt{\operatorname{Im} T_z(H)}$ in the $\mathcal{L}_2$-norm as a result of the Birman-Koplienko-Solomyak inequality (2.20).

The analyticity of $T_z(H)$ can be seen as follows. Let $\psi(x) = (|x|+1)^{-1/2}$. For any $\varphi_1, \varphi_2 \in \mathcal{K}$, consider the function

$$\begin{aligned} z \mapsto \langle \varphi_1, T_z(H)\varphi_2 \rangle &= \langle (F\psi(H))^* \varphi_1, (R_z/\psi)(H)(F\psi(H))^*\varphi_2 \rangle\,, \\ &= \int_{\mathbb{R}} \frac{\sqrt{x+1}}{x-z}\, d\mu(x), \end{aligned}$$

where $\mu$ is a finite measure. This function is analytic on $\mathbb{C} \setminus \mathbb{R}$ and therefore so is $z \mapsto T_z(H)$ by the equivalence of weak and strong analyticity (see e.g. [Yos80, Theorem V.3.1]). □

## 3.2. The abstract limiting absorption principle (LAP)

Let $H$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with spectral measure $E$ and suppose $F\colon \mathcal{H} \to \mathcal{K}$ is a rigging operator such that $\operatorname{dom} F \supset \operatorname{dom} |H|^{1/2}$. Then by Theorem 3.1 the sandwiched resolvent $T_z(H)$ is bounded. One of the main reasons for introducing a rigging operator is that the sandwiched resolvent $T_z(H)$ may have bounded limits as $z$ approaches points of the absolutely continuous spectrum of $H$. Indeed for the right choice of rigging operator these limits exist for a.e. $\lambda \in \mathbb{R}$. This is known as the (abstract) *Limiting Absorption Principle* (LAP).

The LAP is intimately connected to stationary scattering theory and is usually considered within the context of perturbation theory, where the operator $F$ is related to the perturbation: Let $H_0$ and $H_1 = H_0 + V$ be two self-adjoint operators and suppose that the perturbation $V$ is decomposed as $F^*JF$ for bounded $J$. Then the LAP can be used to conclude that for the right choice of $F$ there exists a full set of values $\lambda$ for which the sandwiched resolvents $T_{\lambda+iy}(H_0)$ and $T_{\lambda+iy}(H_1)$ both have limits as $y \to 0^+$. Proofs of the LAP can be divided into two methods: 'smooth' and 'trace class.' The smooth method involves relatively strong conditions on the initial operator $H_0$, which allows a freer choice of the perturbation $V$, or the rigging operator $F$. In contrast the trace class method involves stronger assumptions on the rigging $F$, allowing a virtually arbitrary choice of $H_0$. These methods in their wider context of scattering theory are discussed further in Section 7. The trace class method is the main focus here and because of its importance we provide a proof (see Theorem 3.13), which is lifted from [Yaf92]. A simple case of the LAP which is closer to the spirit of the smooth method is considered at the beginning of Section 5.6.

We will use the notation

$$T_{\lambda\pm i0}(H) := \lim_{y\to 0^+} T_{\lambda\pm iy}(H).$$

Unless otherwise specified these are to be considered as norm limits. Elements of the set

$$\Lambda(H,F) := \left\{ \lambda \in \mathbb{R} \;\middle|\; T_{\lambda+i0}(H) \text{ exists in } \mathcal{B}(\mathcal{K}) \right\}$$

will be called *regular points* of $H$. If $\lambda \in \Lambda(H,F)$ we say that $H$ is *regular* at $\lambda$, whereas if $\lambda \notin \Lambda(H,F)$ then $H$ is said to be *resonant* at $\lambda$.

Note that if $T_{\lambda\pm i0}(H)$ exists, then so does $T_{\lambda\mp i0}(H)$ by continuity of the adjoint operation, and hence

$$\operatorname{Im} T_{\lambda\pm i0}(H) = \lim_{y\to 0^+} \operatorname{Im} T_{\lambda\pm iy}(H).$$

Being the set of points of convergence of a family of continuous functions, $\Lambda(H,F)$ is a Borel set. It obviously contains $\rho(H)\cap\mathbb{R}$. As shown below, it cannot contain any points of the singular spectrum of $H$, so any additional regular points belong to the absolutely continuous spectrum.

THEOREM 3.7. *Let $H$ be a self-adjoint operator on $\mathcal{H}$ with spectral measure $E$ and let $F\colon \mathcal{H}\to\mathcal{K}$ be a rigging operator with* $\operatorname{dom} F \supset \operatorname{dom} |H|^{1/2}$. *Then the operator $E(\Lambda(H,F))$ is an orthogonal projection onto a linear subspace of the absolutely continuous subspace $\mathcal{H}^{(a)}(H)$.*

PROOF. Assume the contrary. Then there exists a null subset $X$ of $\Lambda(H,F)$ such that $E(X)\neq 0$. Since the range of $F^*$ is dense in $\mathcal{H}$, it follows that there exists a vector $F^*\psi$ such that

$$\langle F^*\psi, E(X)F^*\psi\rangle_{\mathcal{H}} \neq 0. \tag{3.8}$$

On the other hand, by definition of the set $\Lambda(H,F)$, for all $\lambda\in X\subset\Lambda(H,F)$ there exists the finite limit

$$\frac{1}{\pi}\lim_{y\to 0^+} \langle \psi, F \operatorname{Im} R_{\lambda+iy}(H)F^*\psi\rangle_{\mathcal{K}}\,.$$

By Theorem 2.4 the set of points $\lambda$ where the above limit exists is a full set whose complement is a support of the singular part of the measure $\mu_{F^*\psi}(\Delta) = \langle F^*\psi, E_\Delta\, F^*\psi\rangle_{\mathcal{H}}$, hence $\langle F^*\psi, E(X)F^*\psi\rangle_{\mathcal{H}} = 0$. This contradicts (3.8) and completes the proof. ☐

COROLLARY 3.8. *If $\Lambda(H,F)$ is a full set, then it supports the absolutely continuous spectral measure of $H$. Moreover, its complement $\mathbb{R}\setminus\Lambda(H,F)$ is a minimal support of the singular spectral measure, i.e. a core of $\sigma_s(H)$.*

In the presence of a rigging operator, if the LAP holds in the sense that $\Lambda(H,F)$ is a full set, then the complement $\mathbb{R}\setminus\Lambda(H,F)$ can be considered as *the* core of $\sigma_s(H)$ since it is unambiguously determined by the rigging operator $F$. Its elements might simply be called *singular points* of $H$ and are at least interpreted in that way. This leads into the topics of [Aza16] surrounding the resonance index, which are discussed further in Section 4.

We will also be concerned with the existence of the limit $\operatorname{Im} T_{\lambda+i0}(H)$ in the stronger topology of the trace class. As well as regular points $\Lambda(H,F)$, we identify a subset of *trace-regular points* of $H$, denoted $\Lambda(H,F;\mathcal{L}_1)$. By definition, a point $\lambda$ belongs to $\Lambda(H,F;\mathcal{L}_1)$ if $\lambda\in\Lambda(H,F)$ and for some bounded neighbourhood $\Delta\subset\mathbb{R}$ of $\lambda$ the convergence

$$FE(\Delta)\operatorname{Im} R_{\lambda+iy}(H)(FE(\Delta))^* \to \operatorname{Im} T_{\lambda+i0}(H) \quad \text{as } y\to 0^+ \tag{3.9}$$

holds in the trace class norm.

Reviewed in detail below are two classical theorems on the abstract LAP, numbered 3.11 and 3.13, which are due to M. Sh. Birman and S. B. Entina [BE67] (they note that a similar result appears in [Bra62]). For the proofs we will follow [Yaf92], where the corresponding theorems are numbered 6.1.5 and 6.1.9, including some supporting lemmas.

LEMMA 3.9. *Any operator $A \in \mathcal{L}_p$ can be represented in the form $A = TB$ (or $A = BT$) where $B \in \mathcal{L}_p$ and $T \in \mathcal{L}_\infty$.*

*On the other hand, if $B$ is a bounded operator such that for some $p < \infty$ and for any $T \in \mathcal{L}_\infty$ the product $TB$ (or $BT$) belongs to $\mathcal{L}_p$, then $B$ necessarily belongs to $\mathcal{L}_p$.*

PROOF. This is a combination of Lemmas 6.1.1–2 from [Yaf92]. Through the Schmidt representation of compact operators the first statement of this lemma can be translated to sequences of $s$-numbers, where it becomes equivalent to the fact that for any positive sequence $(a_n)$ in $\ell_p$ there is always a more slowly convergent positive sequence $(b_n)$ in $\ell_p$ such that $t_n = a_n/b_n \to 0$ as $n \to \infty$.

For the second statement we first note that $B$ must be compact, for which it suffices to see that $|B|$ is compact. If this were not the case then with $E$ denoting the spectral measure of $|B|$, we could find $\lambda > 0$ such that the range $\mathcal{H}_\lambda$ of $E(\lambda, \infty)$ is infinite-dimensional. But then since $|B|$ has a bounded inverse on $\mathcal{H}_\lambda$ the premise implies the contradiction that every compact operator $T$ on $\mathcal{H}_\lambda$ belongs to the class $\mathcal{L}_p$. Now again translating the statement to one about $s$-numbers, it becomes equivalent to the fact that if for any $t_n \to 0$ the sequence $(b_n t_n)$ belongs to $\ell_p$ then so must $(b_n)$. □

LEMMA 3.10. *Let $1 \le p \le \infty$. If $T_n \in \mathcal{L}_p$, $\|T_n\|_p \le C < \infty$, and $T_n$ converges weakly to $T$ as $n \to \infty$, then $T \in \mathcal{L}_p$ and $AT_nB$ converges to $ATB$ in $\mathcal{L}_p$ for any compact operators $A$ and $B$.*

It is not necessary to assume the existence of the weak limit $T$ as a bounded operator in the following sense. Given the uniform boundedness of the norms $\|T_n\| \le C$ and the convergence as $n \to \infty$ for any vectors $f$ and $g$ of the scalar product $\langle f, T_n g\rangle$, say to the number $T[f, g]$, it follows that

$$|T[f, g]| \le C\|f\|\|g\|.$$

Therefore $(f, g) \mapsto T[f, g]$ defines a bounded linear form and hence corresponds to a bounded operator $T$, for which $T_n \to T$ weakly.

PROOF. Here we follow [Yaf92, Lemma 6.1.4] (although we don't find it necessary to appeal to the uniform boundedness principle). For $A \in \mathcal{L}_\infty$, consider the operators $\Gamma_n$ which act from $\mathcal{L}_\infty$ to $\mathcal{L}_p$ and are defined by $\Gamma_n B = AT_nB$. From the estimate

$$\|\Gamma_n B\|_p = \|AT_nB\|_p \le \|A\|\|T_n\|_p\|B\| \le \|A\|C\|B\|, \tag{3.10}$$

it follows that the norms $\|\Gamma_n\|$ are uniformly bounded. We will now show that the sequence $\Gamma_n$, $n = 1, 2, \ldots$, is strongly convergent, which is sufficiently established on the set of finite rank operators $\mathcal{F}$. Indeed, then the required strong convergence can be obtained by a simple $\epsilon/3$ argument using the density of $\mathcal{F}$ in $\mathcal{L}_\infty$ and the uniform boundedness of the norms $\|\Gamma_n\|$. To prove the strong convergence for $B \in \mathcal{F}$, by linearity we can assume $B$ has rank one, say $B = \langle f, \cdot\rangle\, g$, in which case $\Gamma_n B = \langle f, \cdot\rangle\, AT_n g$. Then since $T_n g$ converges weakly to $Tg$ and $A$ is compact, it follows that $AT_n g \to ATg$. Therefore

$$\|\Gamma_n B - ATB\|_p \leq \|f\|\|AT_n g - ATg\| \to 0.$$

So $\Gamma_n$ converges strongly on $\mathcal{F}$ to the operator $\Gamma\colon \mathcal{L}_\infty \to \mathcal{L}_p$ defined by $\Gamma B = ATB$. This operator $\Gamma$ is a priori defined on the dense domain $\mathcal{F}$, but since the strong limit of $\Gamma_n$ is necessarily bounded, as can be inferred from (3.10), it must be that $\Gamma$ is bounded on all of $\mathcal{L}_\infty$ and $\Gamma_n$ converges strongly to $\Gamma$. Therefore $ATB \in \mathcal{L}_p$ and the inclusion $T \in \mathcal{L}_p$ follows from the second part of Lemma 3.9. Since the convergence of $AT_nB$ to $ATB$ in $\mathcal{L}_p$ for any $A, B \in \mathcal{L}_\infty$ is equivalent to the strong convergence for any $A \in \mathcal{L}_\infty$ of $\Gamma_n \to \Gamma$ as $n \to \infty$, the proof is complete. □

THEOREM 3.11. *If $H$ is a self-adjoint operator on a Hilbert space $\mathcal{H}$ and $F\colon \mathcal{H} \to \mathcal{K}$ is Hilbert-Schmidt, then for a.e. $\lambda \in \mathbb{R}$ the operator valued function $F \operatorname{Im} R_{\lambda+iy}(H)F^*$ has a limit in the trace class norm as $y \to 0^+$.*

PROOF. With the intention to use Lemma 3.10, we consider $AF$ in place of $F$ where $A$ is compact and $F$ is Hilbert-Schmidt. This can be done without loss of generality by the first part of Lemma 3.9. By Theorem 2.4, for any $\psi, \varphi \in \mathcal{K}$, the limit

$$\lim_{y\to 0^+} \langle F^*\psi, \operatorname{Im} R_{\lambda+iy}(H)F^*\varphi\rangle \tag{3.11}$$

exists for a.e. $\lambda$. Let $D$, dense in $\mathcal{H}$, be the linear span of some basis. By excluding a countable family of null sets, we can find a common full set $\Lambda$ of values $\lambda$ for which the limit (3.11) exists for any $\psi, \varphi \in D$. Applying Theorem 2.4 to the measure $\operatorname{Tr}(FEF^*)$, where $E$ is the spectral measure of $H$, the limit of

$$\operatorname{Tr}(F \operatorname{Im} R_{\lambda+iy}(H)F^*) = \frac{1}{\pi}\int_{\mathbb{R}} \operatorname{Im} R_{\lambda+iy}(x)\, d\operatorname{Tr}(FE(x)F^*), \tag{3.12}$$

as $y \to 0^+$, also exists for a.e. $\lambda$. Hence the trace class norm of the positive operator $F \operatorname{Im} R_{\lambda+iy}(H)F^*$, equal to (3.12), is bounded with respect to $y$ for a.e. $\lambda$. Deleting from $\Lambda$ the null set of values for which this fails, we obtain a full set of values $\lambda$ for which $\|F \operatorname{Im} R_{\lambda+iy}(H)F^*\|_1$ is bounded and the limit (3.11) exists for any $\psi, \varphi \in D$. Hence for each such $\lambda$, the limit (3.11) exists for any $\psi, \varphi \in \mathcal{H}$. Then Lemma 3.10 implies that $AF \operatorname{Im} R_{\lambda+iy}(H)(AF)^*$ converges in the trace class as $y \to 0^+$. □

LEMMA 3.12. *If $f(z)$ is holomorphic in the upper half-plane and $|f(z)| \geq 1$ for $\operatorname{Im} z > 0$, then $f(z)$ has limit values $f(\lambda + i0)$ at a.e. $\lambda \in \mathbb{R}$.*

PROOF. This is [Yaf92, Lemma 6.1.8] and we reproduce the proof for convenience. We transfer attention to the function $g(z) = 1/f(z)$. It is holomorphic and bounded in $\mathbb{C}_+$, hence its limits $g(\lambda + i0)$ exist at a.e. $\lambda$ by Theorem 2.6(i). Moreover, since it cannot be zero identically by Theorem 2.6(ii), these limits must be nonzero on a full set. On this full set the limits $f(\lambda + i0)$ also exist. □

THEOREM 3.13. *If $H$ is a self-adjoint operator on a Hilbert space $\mathcal{H}$ and $F$ is a Hilbert-Schmidt operator from $\mathcal{H}$ to another Hilbert space $\mathcal{K}$, then for a.e. $\lambda \in \mathbb{R}$ the operator valued function $FR_{\lambda+iy}(H)F^*$ has a limit in the Hilbert-Schmidt norm as $y \to 0$.*

It is shown in [Nab89] that for an arbitrary self-adjoint operator $H$ this result cannot be improved, in the sense that if $F \in \mathcal{L}_{2+\varepsilon}$ with $\varepsilon > 0$, but $F \notin \mathcal{L}_2$, then for some $H$ the LAP fails.

PROOF. As in the proof of Theorem 3.11, we without loss of generality replace $F$ by $AF$ where $A$ is compact and $F$ is Hilbert-Schmidt so that by Lemma 3.10 it suffices to establish weak convergence and a bound on the norm. Denoting $FR_z(H)F^*$ by $T_z$ and using the property (2.27) of the determinant, we have

$$\|T_z\|_2^2 = \mathrm{Tr}(T_{\bar z} T_z) \le \det(1 + T_{\bar z} T_z), \tag{3.13}$$

Then from (2.26), (2.25), and (2.28) by means of the condition $iT_{\bar z} - iT_z \ge 0$ (here we are assuming $\operatorname{Im} z = y > 0$), we obtain

$$1 \le \det(1 + T_{\bar z} T_z) \le \det(1 + iT_{\bar z})(1 - iT_z) = |\det(1 - iT_z)|^2. \tag{3.14}$$

Combining (3.13) and (3.14),

$$\|T_z\| \le |\det(1 - iT_z)|. \tag{3.15}$$

The function $f(z) = \det(1 - iT_z)$ is holomorphic in the upper half-plane and $|f(z)| \ge 1$ by (3.14). Thus the limits $f(\lambda + i0)$ exist for a.e. $\lambda$ by Lemma 3.12. On this set of full measure, call it $\Lambda$, by (3.15) we have

$$\|T_{\lambda+iy}\| \le C(\lambda) \tag{3.16}$$

for any $y > 0$. Applying the same reasoning as in the proof of Theorem 3.11, we find a full set of values $\lambda$ for which the limit $\langle \psi, T_{\lambda+i0}\varphi \rangle$ exists for any $\psi, \varphi \in D$, where $D$ is countable and dense. Then taking the intersection with $\Lambda$, we find a full set for which (3.16) holds and the weak limit $T_{\lambda+i0}$ exists. □

COROLLARY 3.14. *Let $H$ be a self-adjoint operator and let $E$ be its spectral measure. If $F\colon \mathcal{H} \to \mathcal{K}$ is a rigging operator such that $FE(\Delta)$ is Hilbert-Schmidt for any bounded interval $\Delta$, then the LAP holds for $H$.*

PROOF. This is a corollary of Theorem 3.13, which makes the same conclusion – that $\Lambda(H, F)$ is a full set in $\mathbb{R}$, in the case that $F$ is itself Hilbert-Schmidt. Let $\lambda, y \in \mathbb{R}$ with $y > 0$. For a bounded interval $\Delta$, the sandwiched resolvent $T_{\lambda+iy}(H)$ can be split into the sum of two parts using the equality $E(\Delta) + E(\mathbb{R} \setminus \Delta) = 1$. Put $\psi(x) := (|x| + 1)^{-1/2}$. Then the sandwiched resolvent can be written as

$$\begin{aligned} T_{\lambda+iy}(H) &= F(R_{\lambda+iy}/\psi)(H)(F\psi(H))^* \\ &= F(R_{\lambda+iy}/\psi)(H)E(\Delta)(F\psi(H))^* \\ &\qquad + F(R_{\lambda+iy}/\psi)(H)E(\mathbb{R} \setminus \Delta)(F\psi(H))^*. \end{aligned}$$

The first term can be rearranged to read

$$(FE(\Delta))R_{\lambda+iy}(H)(FE(\Delta))^*,$$

which converges as $y \to 0^+$ for a.e. $\lambda$ by Theorem 3.13. The second term is the closure of the operator

$$FR_{\lambda+iy}(E(\mathbb{R} \setminus \Delta)H)E(\mathbb{R} \setminus \Delta)F^*,$$

which converges by Lemma 3.5 for all $\lambda$ in the interior of $\Delta$ since $\lambda \in \rho(E(\mathbb{R} \setminus \Delta)H)$. Therefore $\Delta \setminus \Lambda(H, F)$ is a null set for any bounded interval $\Delta$ and hence $\Lambda(H, F)$ is a full set. □

Corollary 3.15. *Let $H$ be self-adjoint and let $E$ be its spectral measure. If $F$ is a rigging operator such that $FE(\Delta)$ is Hilbert-Schmidt for any bounded interval $\Delta$, then the set of trace-regular points $\Lambda(H, F; \mathcal{L}_1)$ is a full set. Moreover, if $F$ is such that for nonreal $z$ the operator $FR_z(H)$ belongs to the Hilbert-Schmidt class, then for any point $\lambda$ from $\Lambda(H, F; \mathcal{L}_1)$ the limit $\operatorname{Im} T_{\lambda+i0}(H)$ exists in the trace class.*

Proof. Let $\lambda \in \mathbb{R}$, $y > 0$, and let $\Delta$ be a bounded interval. Similarly to the proof of Corollary 3.14, using equality (3.6) we write

$$\begin{aligned} \operatorname{Im} T_{\lambda+iy}(H) &= yFR_{\lambda+iy}(H)E(\Delta)(FR_{\lambda+iy}(H))^* \\ &\qquad + yFR_{\lambda+iy}(H)E(\mathbb{R} \setminus \Delta)(FR_{\lambda+iy}(H))^*. \end{aligned}$$

The first term can be written as $(FE(\Delta)) \operatorname{Im} R_{\lambda+iy}(H)(FE(\Delta))^*$ and converges in the trace class norm as $y \to 0^+$ for a.e. $\lambda$ by Theorem 3.11. The second term is the closure of the operator

$$F \operatorname{Im} R_{\lambda+iy}(E(\mathbb{R} \setminus \Delta))E(\mathbb{R} \setminus \Delta)F^*.$$

For any $\lambda$ from the interior of $\Delta$, it can be concluded from Lemma 3.5 that this term converges to 0 in the usual norm as $y \to 0^+$ and moreover that the same convergence holds in the trace class norm if $FR_z(H)$ is Hilbert-Schmidt. Hence in the latter case $\operatorname{Im} T_{\lambda+iy}(H) \to \operatorname{Im} T_{\lambda+i0}(H)$ in the trace class. Otherwise, it follows that (3.9) holds in the usual norm and therefore, since $(FE(\Delta)) \operatorname{Im} R_{\lambda+iy}(H)(FE(\Delta))^*$ also converges in the trace class norm, the limits must agree so that (3.9) holds in the trace class norm. It follows that the set of points $\lambda$ where the limit (3.9) exists is a full set in (arbitrary) $\Delta$ and thus in $\mathbb{R}$. Hence so is $\Lambda(H, F; \mathcal{L}_1)$ by Corollary 3.14. □

### 3.3. Rigged affine spaces of self-adjoint operators

The first and second resolvent identities:

$$R_z(H) - R_w(H) = (z-w)R_z(H)R_w(H) = (z-w)R_w(H)R_z(H) \tag{3.17}$$

$$R_z(H_0) - R_z(H_1) = R_z(H_1)VR_z(H_0) = R_z(H_0)VR_z(H_1) \tag{3.18}$$

will be used many times in the coming pages. The first one, which is a special case of the second (and has already been used a few times), holds for a closed operator $H$ and any $z$ and $w$ from its resolvent set $\rho(H)$. In the second one, $z \in \rho(H_1) \cap \rho(H_0)$ and the operator $H_1$ is the sum of operators $H_0$ and $V$. It holds for example if $H_0$ and $V$ satisfy the premise of the Kato-Rellich Theorem 2.28 and $H_1$ is the operator sum $H_0 + V$. The proof is a simple algebraic manipulation.

Alternatively, suppose $H_0$ and $V$ satisfy the premise of the KLMN Theorem 2.29 and $H_1$ is the form sum $H_0 \dot{+} V$. In this case, the second resolvent identity can be written as

$$\begin{aligned} \langle f, (R_z(H_0) - R_z(H_1))g\rangle &= V[R_{\bar z}(H_0)f, R_z(H_1)g] \\ &= V[R_{\bar z}(H_1)f, R_z(H_0)g] \end{aligned} \tag{3.19}$$

for any vectors $f$ and $g$. This can be established as follows. Note that $\operatorname{dom}[V]$ contains the form domains of $H_0$ and $H_1$ and hence also contains their operator domains.

$$\begin{aligned} V[R_{\bar z}(H_0)f, R_z(H_1)g] &= (H_1 - z - H_0 + z)[R_{\bar z}(H_0)f, R_z(H_1)g] \\ &= \langle R_{\bar z}(H_0)f, (H_1 - z)R_z(H_1)g\rangle \\ &\qquad - \langle (H_0 - \bar z)R_{\bar z}(H_0)f, R_z(H_1)g\rangle \\ &= \langle f, (R_z(H_0) - R_z(H_1))g\rangle\,. \end{aligned}$$

Given any rigging operator $F\colon \mathcal{H} \to \mathcal{K}$, we consider the space of perturbations

$$\mathcal{A}_0 = \mathcal{A}_0(F) := F^*\mathcal{B}_{sa}(\mathcal{K})F \tag{3.20}$$

with the norm

$$\|F^*JF\|_F := \|J\|,$$

making it isomorphic to the real Banach space of bounded self-adjoint operators on $\mathcal{K}$. If $F$ is bounded, then $\mathcal{A}_0$ consists of bounded self-adjoint operators $V = F^*JF$. But if $F$ isn't bounded, we interpret a perturbation $V = F^*JF \in \mathcal{A}_0$ as the form

$$V[f,g] = \langle Ff, JFg\rangle \quad f, g \in \operatorname{dom} F. \tag{3.21}$$

Now suppose that $H$ is a lower-bounded self-adjoint operator on $\mathcal{H}$, such that $F$ is $|H|^{1/2}$-compact. It follows that each perturbation $V \in \mathcal{A}_0$ is $H$-form-compact. Therefore, by the KLMN Theorem each form sum $H \dot{+} V$ is a lower-bounded self-adjoint operator with the same form domain as $H$. Thus applying Proposition 2.26 and Theorem 3.1, we conclude that the sandwiched resolvent $T_z(H \dot{+} V)$ is bounded for any $z \in \rho(H \dot{+} V)$.

For $H_0 = H$ and $H_1 = H \dotplus V$, where $V = F^*JF$, the second resolvent identity (3.19) holds and can be written as

$$R_z(H_1) - R_z(H_0) = (FR_{\bar{z}}(H_0))^* JFR_z(H_1). \tag{3.22}$$

It is natural to denote the right hand side by $R_z(H_0)VR_z(H_1)$. In this regard also see (3.27).

From (3.22) we also obtain a sandwiched version:

$$T_z(H_0) - T_z(H_1) = T_z(H_0)JT_z(H_1) = T_z(H_1)JT_z(H_0), \tag{3.23}$$

which is justified first on the domain of $F^*$ and then extended to the whole auxiliary Hilbert space.

Recall that we are assuming $F$ to be $|H_0|^{1/2}$-compact. Since the sandwiched resolvent $T_z(H_0)$ is compact by Theorem 3.1, the equality (3.23) implies that $T_z(H_1)$ is also compact. Hence by Theorem 3.1, $F$ is relatively compact with respect to $|H_1|^{1/2}$. Further, any other perturbation from $\mathcal{A}_0$ is relatively form-compact with respect to $H_1$. Note that $(H \dotplus V_1) \dotplus V_2 = H \dotplus (V_1 + V_2)$, since both of these operators correspond to the form $H + V_1 + V_2$. We put

$$\mathcal{A} = \mathcal{A}(H, F) := H \dotplus \mathcal{A}_0, \tag{3.24}$$

which comprises a real affine space of self-adjoint operators over $\mathcal{A}_0$. Although the operator $H$ has been used in the construction of this affine space, it is not a distinguished element; $\mathcal{A}$ can be reconstructed in the same way from any other element.

Such an affine space of self-adjoint operators (3.24), which we will call a *rigged affine space*, will form the basic setting herein. In its definition, we have assumed the semiboundedness of the self-adjoint operator $H$, which is reasonable given that Schrödinger operators are as a rule semibounded and it is a primary aim to accommodate this application. However, restricting to semibounded operators is not necessary in the case that the rigging operator $F$ is itself bounded. In this simpler situation each perturbation $V$ is $H$-compact by Theorem 3.1 and we may use the Kato-Rellich Theorem instead of the KLMN Theorem. As a result the operators of the affine space (3.24) not only share a form domain, but also an operator domain.

To reiterate and summarise:

Definition. Suppose $F \colon \mathcal{H} \to \mathcal{K}$ is a rigging operator. Define a real Banach space of symmetric forms by

$$\mathcal{A}_0 = \{V[f,g] = \langle Ff, JFg\rangle \quad f,g \in \operatorname{dom} F : J \in \mathcal{B}_{sa}(\mathcal{K})\}$$

and equip this space with the norm $\|V\|_F = \|J\|$. For convenience an element of $\mathcal{A}_0$ is written as $V = F^*JF$. Suppose further that $H$ is a lower-bounded self-adjoint operator on $\mathcal{H}$, such that $F$ is $|H|^{1/2}$-compact. Then each form in $\mathcal{A}_0$ is relatively form-compact with respect to $H$ and we define a *rigged affine space* of self-adjoint operators by (3.24). In the case that the rigging operator $F$ is bounded, the operator $H$ need not be assumed to be semibounded and the form sum in (3.24) can be replaced by an operator sum. As usual we often leave the rigging operator implicit in our notation.

Some basic properties of a rigged affine space $\mathcal{A}$:

- Any $V \in \mathcal{A}_0$ is relatively form-compact with respect to any $H \in \mathcal{A}$.
- All operators $H \in \mathcal{A}$ share a common form domain $\operatorname{dom}[\mathcal{A}]$. In the case that $F$ is bounded we can say further that each $V \in \mathcal{A}_0$ is relatively compact with respect to any $H \in \mathcal{A}$ and all operators $H \in \mathcal{A}$ share a common operator domain $\operatorname{dom} \mathcal{A}$.
- The sandwiched resolvent $T_z(H)$ is compact for any $H \in \mathcal{A}$.
- For any two operators $H_0$ and $H_1$ from $\mathcal{A}(F)$ there is a perturbation $V = F^*JF \in \mathcal{A}_0$ such that $H_1 = H_0 \dotplus V$. For these two operators, we have the second resolvent identity (3.18), which is interpreted as (3.22), as well as its sandwiched version (3.23).

Continuing the last item above, from (3.23) and the density of the range of the operator $F^*$, we obtain the equalities

$$FR_z(H_0) - FR_z(H_1) = T_z(H_0)JFR_z(H_1) = T_z(H_1)JFR_z(H_0). \tag{3.25}$$

The difference of resolvents of any two operators from $\mathcal{A}(F)$ is compact by (3.22). Thus it follows from Weyl's Theorem 2.18 that all operators in $\mathcal{A}$ share a common essential spectrum, which we will denote by $\sigma_{ess}$.

In the case of a rigged affine space $\mathcal{A}(F)$ which consists of semibounded self-adjoint operators, it will be assumed that the shared form domain $\mathcal{D} = \operatorname{dom}[\mathcal{A}]$ is mapped to a dense set in the auxiliary Hilbert space $\mathcal{K}$ by the rigging operator $F$, i.e.

$$\overline{F\mathcal{D}} = \mathcal{K}. \tag{3.26}$$

This is already true in the case that $F$ is bounded, since with $\psi(x) = (|x|+1)^{-1/2}$ we have $\mathcal{D} = \operatorname{ran} \psi(H)$ and $\operatorname{ran}(F\psi(H))^{\perp} = \ker(\psi(H)F^*) = \{0\}$. In general, it is not restrictive to assume (3.26); if it were not true we could simply redefine $\mathcal{K}$ by (3.26).

In defining a rigged affine space we have included only symmetric perturbations, but this is not necessary. If $\mathcal{A}(F)$ is a rigged affine space of self-adjoint operators, then any perturbation $F^*JF$, where $J$ is bounded but not necessarily self-adjoint, is relatively form-compact with respect to any $H \in \mathcal{A}$ and

$$\mathcal{A} \dotplus F^*\mathcal{B}(\mathcal{K})F$$

defines a larger complex affine space of sectorial operators. However, we are primarily interested in the real subspace $\mathcal{A}$ of self-adjoint operators.

Let $\mathcal{A}$ be a rigged affine space and let $H_0, H_1 \in \mathcal{A}$ and $V \in \mathcal{A}_0$. Suppose $\varphi$ and $\psi$ are Borel functions satisfying $|\varphi(x)|, |\psi(x)| \leq \text{const.}(|x|+1)^{-1/2}$. Then we will use the notation

$$\varphi(H_0)V\psi(H_1) \tag{3.27}$$

to refer to the compact operator corresponding to the form

$$(f,g) \mapsto V[\bar{\varphi}(H_0)f, \psi(H_1)g].$$

Note that this operator doesn't depend on the rigging operator, in the sense that if $\mathcal{A}(F_1)$ and $\mathcal{A}(F_2)$ are two rigged affine spaces such that $H_0, H_1 \in \mathcal{A}(F_1) \cap \mathcal{A}(F_2)$ and $V \in \mathcal{A}_0(F_1) \cap \mathcal{A}_0(F_2)$, then the result is the same. However, if $F$ is the rigging operator and $V = F^* JF$ then it can be practical to write

$$\varphi(H_0) V \psi(H_1) = (F\bar{\varphi}(H_0))^* JF\psi(H_1).$$

The following proposition shows a typical instance in which a rigged affine space can arise – by perturbing a self-adjoint operator in a relatively compact direction.

Proposition 3.16. *Suppose we are a given an initial self-adjoint operator $H_0$ and relatively compact self-adjoint perturbation $V$. If either $V$ is bounded or $H_0$ is bounded below, then there exists a rigged affine space $\mathcal{A}$, with $H_0 \in \mathcal{A}$ and $V \in \mathcal{A}_0$.*

Proof. An essential requirement is to find a closed injective operator $F$ and a bounded operator $J$ so that $V = F^* JF$ (understood in the sense of (3.21)). One possibility is $F = \sqrt{|V|}$ and $J = \operatorname{sgn} V$. In order to ensure that $F$ is injective, let $F_0$ be a positive injective operator on the kernel of $V$ which we chose to be Hilbert-Schmidt. Set $F = \sqrt{|V|} + F_0$ and let $\mathcal{K} = \overline{\operatorname{ran} F}$. The real Banach space $\mathcal{A}_0(F)$ contains $V$ by construction. In fact it contains any operator $\psi(V)$, where $\psi$ is a real-valued Borel function which is zero at zero and satisfies $|\psi(x)| \leq C|x|$, for some $C > 0$ and a.e. $x$ with respect to the spectral measure of $V$, e.g. the positive and negative parts $V_\pm$ of $V$. Lemma 2.27 implies that $F$ is $|H_0|^{1/2}$-compact and the rigged affine space $\mathcal{A} = H_0 \dotplus \mathcal{A}_0(F)$ satisfies the requisite conditions. □

CHAPTER 4

# The resonance index

The resonance index appeared in print in the paper [Aza16], where it is studied in detail. It is a tangible realisation of the idea of (infinitesimal) spectral flow, which unlike other definitions also makes sense within the essential spectrum. Outside of the essential spectrum, spectral flow has been variously studied in terms of concepts such as the intersection number and the total Fredholm index. An axiomatic description is given by J. Robbin and D. Salamon in [RS95]. Proof that the total resonance index satisfies these axioms, as well as direct proofs of its coincidence with the intersection number and total Fredholm index, can be found in the detailed study of resonance index outside of the essential spectrum [Aza17].

In this chapter the resonance index will be considered on a rigged affine space $\mathcal{A}(F)$. While its spirit is the same, this is not exactly the setting which appears in [Aza16]. One difference is that in [Aza16] the perturbations $V = F^*JF$ are chosen so that

$$JF \operatorname{dom}[\mathcal{A}] \subset \operatorname{dom} F^*,$$

which implies that they can be considered as operators, relatively bounded with respect any self-adjoint operator in $\mathcal{A}$. The situation is complicated by the fact that in [Aza16] it is not assumed that the operators from $\mathcal{A}$ are semibounded and instead the perturbations are assumed to be relatively compact. However, there is no difference whatsoever in the case that the rigging operator $F$ is bounded. We claim that all of the important results translate virtually unchanged and for the most part this is immediately clear, mainly because the roles of the resolvent $R_z(H)$ and the perturbation $V = F^*JF$ are overshadowed by those of the sandwiched resolvent $T_z(H)$ and the bounded operator $J$. Some things less clear are confirmed to hold at the end of Section 4.2.

## 4.1. Resonance points

Suppose that $\mathcal{A}(F)$ is a rigged affine space of self-adjoint operators, which will be fixed throughout this chapter. This section addresses questions about the dependence of the regularity condition $\lambda \in \Lambda(H, F)$ on the operator $H \in \mathcal{A}$. Along the way some equalities are established which play a significant role here as well as in later chapters.

The following convenient notation also appears in [Yaf92, p. 115]. For any self-adjoint operator $H \in \mathcal{A}$, attach one copy of $\Lambda(H, F)$ to each complex half-plane forming the sets

$$\Pi_\pm(H,F) := \mathbb{C}_\pm \cup \Lambda(H,F) \tag{4.1}$$

and then define

$$\Pi(H,F) := \Pi_+(H,F) \sqcup \Pi_-(H,F). \tag{4.2}$$

Elements of $\Pi_\pm(H,F)$ in the disjoint union $\Pi(H,F)$ can be distinguished by their imaginary parts. That is, $z \in \Pi(H,F)$ can be written as $\lambda \pm iy$, where $\lambda = \operatorname{Re} z$ and $y = |\operatorname{Im} z|$, so that $\lambda \pm i0$ distinguishes between the two copies of $\Lambda(H,F)$ when $\lambda$ is a regular point of $H$. The set $\Pi(H,F;\mathcal{L}_1)$ is similarly defined: just replace $\Lambda(H,F)$ by $\Lambda(H,F;\mathcal{L}_1)$ in the definition of $\Pi(H,F)$.

One reason for introducing the set $\Pi(H,F)$ is to index the operators $T_z(H)$ and there will be little need to distinguish $\lambda + i0$ from $\lambda - i0$ if the limits $T_{\lambda+i0}(H)$ and $T_{\lambda-i0}(H)$ are equal. In this regard, since $z \mapsto T_z(H)$ is continuous on the resolvent set $\rho(H)$, we can identify $\lambda + i0$ and $\lambda - i0$ if $\lambda \in \Lambda(H,F) \cap \rho(H) = \Lambda(H,F) \setminus \sigma_{ess}$. What is important is that for a regular point $\lambda \in \sigma_{ess}$ the operators $T_{\lambda\pm i0}(H)$ may differ.

For any $H \in \mathcal{A}$, the sandwiched resolvent $T_z(H)$ is compact for any nonreal $z$ and for $\lambda \in \Lambda(H,F)$ the operators $T_{\lambda\pm i0}(H)$ are compact as the norm limits of compact operators. In other words, $T_z(H)$ is compact for any $z \in \Pi(H,F)$.

For any two operators $H_0$ and $H_1 = H_0 \dotplus V$, $V = F^*JF$, from the affine space $\mathcal{A}$, the sandwiched version of the second resolvent identity (3.23) holds for any $z$ from the intersection $\Pi(H_1,F) \cap \Pi(H_0,F)$. Indeed since it holds for any nonreal $z = \lambda \pm iy$, if $\lambda$ belongs to the intersection $\Lambda(H_1,F) \cap \Lambda(H_0,F)$ then taking the limit as $y \to 0$ shows that it holds for $z = \lambda \pm i0$ as well.

LEMMA 4.1. *Consider a straight line $H_r = H_0 \dotplus rV$, $V = F^*JF$, $r \in \mathbb{R}$, in the affine space $\mathcal{A}(F)$. For any $z \in \Pi(H_0,F) \cap \Pi(H_r,F)$, the spectra of the compact operators $JT_z(H_0)$ and $T_z(H_0)J$ cannot contain the number $-r^{-1}$.*

Note that if $z$ is nonreal, then the inclusion $z \in \Pi(H_0,F) \cap \Pi(H_r,F)$ is automatic, so that this lemma implies that the operators $JT_z(H_0)$ and $T_z(H_0)J$ do not have nonzero real eigenvalues.

PROOF. We can immediately dispense with the case $r = 0$. Since the compact operators $T_z(H_0)J$ and $JT_z(H_0)$ share the same nonzero eigenvalues by (2.22), it suffices to consider one. Assume contrary to the claim, that $-r^{-1}$ is an eigenvalue of $JT_z(H_0)$. Letting $\psi \neq 0$ be a corresponding eigenvector, we have

$$(1 + rJT_z(H_0))\psi = 0.$$

But since $z \in \Pi(H_0,F) \cap \Pi(H_r,F)$, the sandwiched second resolvent identity

$$T_z(H_0) = T_z(H_r)(1 + rJT_z(H_0))$$

holds and implies the contradiction

$$0 \neq -r^{-1}\psi = JT_z(H_0)\psi = JT_z(H_r)(1 + rJT_z(H_0))\psi = 0. \qquad \square$$

Corollary 4.2. *Let $V = F^*JF$ be a perturbation from the real Banach space $\mathcal{A}_0(F)$ and suppose that*

$$JF\,\mathrm{dom}[\mathcal{A}] \subset \mathrm{dom}\,F^*. \tag{4.3}$$

*Then as an operator $V = F^*JF$ is $H$-bounded for any self-adjoint operator $H \in \mathcal{A}$ and for any nonreal $z$, the operators $JT_z(H)$, $T_z(H)J$, $VR_z(H)$, and the closure of $R_z(H)V$, all share the same nonzero eigenvalues (counting multiplicities) none of which can be real.*

Proof. The inclusion (4.3) implies that $V$ is $H$-bounded by Lemma 2.23. From Lemma 4.1 and (2.22) we know that $T_z(H)J$ and $JT_z(H)$ share the same nonzero eigenvalues and none are real. With $\varphi(x) = (|x|+1)^{-1/2}$ and $\varphi_z(x) = (|x|+1)^{1/2}(x-z)^{-1}$, from (3.3) we have

$$T_z(H)J = F\varphi_z(H)(F\varphi(H))^*J.$$

By (2.22), this operator therefore has the same nonzero eigenvalues as the operators

$$(F\varphi(H))^*JF\varphi_z(H) = \varphi(H)V\varphi_z(H),$$
$$V\varphi_z(H)\varphi(H) = VR_z(H).$$

Lemma 3.3 implies that $\overline{R_z(H)V} = (VR_{\bar z}(H))^*$. The nonzero eigenvalues of this operator are the conjugates of those for $VR_{\bar z}(H)$, which are shared with $T_{\bar z}(H)J$ and hence are the conjugates of those for $JT_z(H)$. □

We can now establish some important equalities. Let $H_0$ and $H_1 = H_0 \dotplus V$ be any two operators from $\mathcal{A}(F)$, where $V = F^*JF$. Suppose $z \in \Pi(H_0,F) \cap \Pi(H_1,F)$. Following from Lemma 4.1 and the sandwiched second resolvent identity (3.23), we get

$$T_z(H_1) = (1+T_z(H_0)J)^{-1}T_z(H_0) = T_z(H_0)(1+JT_z(H_0))^{-1}. \tag{4.4}$$

From the first of these equalities and the density of the range of $F^*$, we also obtain the equality

$$FR_z(H_1) = (1+T_z(H_0)J)^{-1}FR_z(H_0) \tag{4.5}$$

and by taking its adjoint

$$(FR_z(H_1))^* = (FR_z(H_0))^*(1+JT_{\bar z}(H_0))^{-1}. \tag{4.6}$$

One more equality worth noting (cf. [KK71, p. 144; RS79, (99); Aza16, (2.7.11)]):

$$\mathrm{Im}\,T_z(H_1) = (1+T_{\bar z}(H_0)J)^{-1}\,\mathrm{Im}\,T_z(H_0)(1+JT_z(H_0))^{-1}. \tag{4.7}$$

This is implied for $z = \lambda \pm iy$, $y > 0$, by (3.7), (4.5), and (4.6). Then the case $z = \lambda \pm i0$, $\lambda \in \Lambda(H_0,F) \cap \Lambda(H_1,F)$, follows by taking the limit $y \to 0^+$.

By the continuity of the inverse and Lemma 4.1, the factor $(1+T_z(H_0)J)^{-1}$ is norm-continuous as a function of $J$. Therefore it follows from the above equalities that the operators $T_z(H)$ and $FR_z(H)$ vary norm-continuously with $H \in \mathcal{A}$. Moreover, these operator valued functions are continuous in the norm the Schatten ideal $\mathcal{L}_p$ if it is assumed that their value at some $H_0$ belongs to $\mathcal{L}_p$. This is one reason that these equalities will be important later.

PROPOSITION 4.3. *Let $H_0$ and $H_1 = H_0 \dotplus V$, $V = F^*JF$, be two operators from the affine space $\mathcal{A}(F)$. Suppose $H_0$ is regular at $\lambda$. Then $H_1$ is resonant at $\lambda$ if and only if the compact operator $T_{\lambda+i0}(H_0)J$ has $-1$ as an eigenvalue.*

This proposition holds if the operator $T_{\lambda+i0}(H)J$ is replaced by any one of the operators $JT_{\lambda\pm i0}(H)$ or $T_{\lambda-i0}(H)J$, as is evident from its proof.

PROOF. By the Fredholm alternative, $-1$ is an eigenvalue of $T_{\lambda+i0}(H_0)J$ if and only if the operator $1 + T_{\lambda+i0}(H_0)J$ is not invertible. Put $z = \lambda + iy$ with $y > 0$ and consider the equality (4.4). By letting $y \to 0$, it can be inferred that if $(1 + T_{\lambda+i0}(H_0)J)^{-1}$ exists then so does $T_{\lambda+i0}(H_1)$. And by Lemma 4.1, existence of the operator $T_{\lambda+i0}(H_1)$ implies invertibility of the operator $1 + T_{\lambda+i0}(H_0)J$. □

The union of the sets $\Lambda(H, F)$ over a collection of operators $\{H_r\}_{r\in\mathcal{I}} \subset \mathcal{A}$ will be denoted $\Lambda(\{H_r\}, F)$. Its elements will be called *essentially regular* points of the collection. Elements of $\Lambda(\mathcal{A}, F)$ are just called essentially regular. Similarly, we define

$$\Lambda(\{H_r\}, F; \mathcal{L}_1) := \bigcup_{r\in\mathcal{I}} \Lambda(H_r, F; \mathcal{L}_1)$$

and call the elements *essentially trace-regular* points of $\{H_r\}$.

Let $\lambda$ be essentially regular. The set of operators from the rigged affine space $\mathcal{A}$ which are resonant at $\lambda$ is called the *resonance set* at $\lambda$. It is denoted by $R(\lambda; \mathcal{A})$. In particular we will consider one-dimensional sections of the resonance set. If $H_r$, $r \in \mathbb{R}$, is a path in $\mathcal{A}$, then its intersection with the resonance set can be identified with those values of the coupling parameter $r$ at which the intersection occurs. This set of values $r \in \mathbb{R}$ such that $H_r \in R(\lambda; \mathcal{A})$ is denoted $R(\lambda; \{H_r\})$ and is called the *resonance set of the path.*

Suppose that a path $H_r$ in $\mathcal{A}(F)$ depends on $r$ analytically. By the definition of the norm on $\mathcal{A}_0(F)$, this means that for any $s \in \mathbb{R}$, $H_r = H_s \dotplus V_{r-s}$, where $V_{r-s} = F^*J_{r-s}F$ and $r \mapsto J_{r-s}$ is an analytic path in $\mathcal{B}(\mathcal{K})$. We consider the path $J_{r-s}$ to be analytically extended to a neighbourhood of the real axis. In this way $H_r$ can be considered as an analytic function with values in the larger affine space $\mathcal{A} \dotplus F^*\mathcal{B}(\mathcal{K})F$. Let $s \in \mathbb{R}$ and $z \in \Pi(H_s, F)$. Then the function $r \mapsto T_z(H_s)J_{r-s}$ (defined on a neighbourhood of $\mathbb{R}$) is an analytic compact operator valued function. It follows from the analytic Fredholm alternative (Theorem 2.17), that the operator valued function

$$r \mapsto (1 + T_z(H_s)J_{r-s})^{-1} \tag{4.8}$$

is meromorphic and its pole-set is the discrete set of points $r$ for which $-1$ is an eigenvalue of the compact operator $T_z(H_s)J_{r-s}$. These poles are called *resonance points* of the path $H_r$ corresponding to $z$. A resonance point at $z$ is usually denoted by $r_z$. Note that $\overline{r_z} = r_{\bar z}$. Points which are resonant at $\bar z$ are called *anti-resonance points* at $z$.

The definition of resonance points doesn't depend on the choice of regular point $s$. Indeed, if $s_1$ and $s_2$ are two regular points at $z$, i.e. $z \in \Pi(H_{s_1}, F) \cap \Pi(H_{s_2}, F)$, then the equality (4.4) applies and

$$\begin{aligned} 1 + T_z(H_{s_1})J_{r-s_1} &= 1 + (1 + T_z(H_{s_2})J_{s_1-s_2})^{-1}T_z(H_{s_2})J_{r-s_1} \\ &= 1 + T_z(H_{s_2})J_{s_1-s_2} + T_z(H_{s_2})J_{r-s_1} \\ &= 1 + T_z(H_{s_2})J_{r-s_2}. \end{aligned}$$

And of course this notion of resonance points agrees with the previous one, in the sense that if $\lambda \in \Lambda(H_s, F)$, then by Proposition 4.3, the discrete set of real resonance points corresponding to $\lambda$ coincides with the resonance set $R(\lambda; \{H_r\})$ defined above.

In the present context equality (4.4) reads

$$T_z(H_r) = (1 + T_z(H_s)J_{r-s})^{-1}T_z(H_s)$$

and due to the meromorphicity of the factor (4.8), the left hand side can be considered as a meromorphic compact operator valued function of the coupling parameter $r$. With $z = \lambda \pm iy$, $y \geq 0$, resonance points $r_z$ of the path $H_r$ are thus poles of $r \mapsto T_z(H_r)$ and the resonance set $R(\lambda; \{H_r\})$ is the intersection of the pole set of $r \mapsto T_{\lambda+i0}(H_r)$ with the real line.

THEOREM 4.4. *Let $H_r$ be an analytic path in $\mathcal{A}(F)$ and suppose $\lambda$ is essentially regular. Then either the resonance set $R(\lambda; \{H_r\})$ is the whole real line, or it is discrete in which case it consists of the real poles of the function $r \mapsto T_{\lambda+i0}(H_r)$.*

## 4.2. Resonance index

Suppose a triple $(\lambda, H_{r_\lambda}, V)$ is chosen as follows: the real number $\lambda$ is an essentially regular point; the operator $H_{r_\lambda} \in \mathcal{A}$ is resonant at $\lambda$; and the direction $V = F^*JF \in \mathcal{A}_0$ is regularising, in the sense that $\lambda$ is an essentially regular point of the straight line $H_r = H_{r_\lambda} \dotplus (r - r_\lambda)V$. Or in other words suppose that $\lambda$ is an essentially regular point of a straight line $H_r$ in the direction $V$ and $r_\lambda$ is a resonance point of this path.

Let $s \in \mathbb{R}$ be any regular point of the path $H_r$, i.e. $s \notin R(\lambda; \{H_r\})$, and put $z = \lambda \pm iy$, $y \geq 0$. Then from the previous section $r_z$ is a resonance point if and only if one of the following equivalent conditions holds:

- $r_z$ is a pole of the compact operator valued function

  $$r \mapsto T_z(H_r) = (1 + (r - s)T_z(H_s)J)^{-1}T_z(H_s),$$

  which is meromorphic in $\mathbb{C}$.
- the compact operator $T_z(H_s)J$ has an eigenvalue at

$$\sigma_z(s) := (s - r_z)^{-1}. \tag{4.9}$$

Consider shifting the point $\lambda$ slightly to $\lambda + iy$ for small positive (or negative) $y$. Note that the compact operator $T_{\lambda+iy}(H_s)J$ is continuous as a function of $y \geq 0$ and depends analytically on $y > 0$. By a well known result on the perturbation of isolated eigenvalues (see e.g. [Kat84]) the eigenvalue $\sigma_\lambda(s)$ of $T_{\lambda+i0}(H_s)J$ may in general split into finitely many eigenvalues $\sigma^1_{\lambda+iy}(s), \ldots, \sigma^N_{\lambda+iy}(s)$ of $T_{\lambda+iy}(H_s)J$. These $N$ eigenvalues are stable for small $y$ and are collectively known as the $\sigma_\lambda(s)$-group. Via the correspondence (4.9), we may alternatively consider the $r_\lambda$-group of resonance points $r^j_{\lambda+iy}$, $j = 1, \ldots, N$, which split from $r_\lambda$ (see Figure 4.1 below). Note that for each $j$, the resonance point $r^j_{\lambda+iy}$ and the eigenvalue $\sigma^j_{\lambda+iy}$ lie in the same complex half-plane. By Lemma 4.1, none of the resonance points of the $r_\lambda$-group are real. The number of resonance points counting multiplicities which lie in the upper complex half-plane $\mathbb{C}_+$ is denoted $N_+$. The number lying in the lower half-plane $\mathbb{C}_-$ is denoted $N_-$. The difference $N_+ - N_-$ is the *resonance index*

$$\operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V) := N_+ - N_-.$$

Note that the resonance index doesn't depend on the rigging operator, in the sense that if $\lambda$ is an essentially regular point of the path $H_r$ with respect to two different rigging operators, the resulting real resonance points and corresponding resonance indices are equal. This is because both notions are characterised in terms of the eigenvalues (4.9) for $y > 0$ which converge to the real axis when $y \to 0^+$ and by (2.22) these eigenvalues are common to the following compact operators, the second of which doesn't depend on $F$ (see (3.27)).

$$T_{\lambda+iy}(H_s)J = F\varphi_{\lambda+iy}(H_s)(F\varphi(H_s))^*J,$$
$$\varphi(H_s)V\varphi_{\lambda+iy}(H_s) = (F\varphi(H_s))^*JF\varphi_{\lambda+iy}(H_s),$$

where $\varphi(x) = (|x|+1)^{-1/2}$ and $\varphi_z(x) = (|x|+1)^{1/2}(x-z)^{-1}$.

Again suppose $\lambda$ is an essentially regular point of a straight line $H_r$ in the direction $V = F^*JF$. Let $z = \lambda \pm iy$, $y \geq 0$, and let $r_z$ be a resonance point corresponding to $z$. By $P_z(r_z)$ we denote the Riesz idempotent

$$P_z(r_z) = \frac{1}{2\pi i}\oint_{C(\sigma_z(s))} (\sigma - T_z(H_s)J)^{-1}\, d\sigma, \tag{4.10}$$

where $C(\sigma_z(s))$ is a small positively oriented circle enclosing the eigenvalue $\sigma_z(s) = (r_z - s)^{-1}$. Then $P_z(r_z)$ is a finite-rank (not necessarily orthogonal) projection onto the generalised eigenspace of the compact operator $T_z(H_s)J$ at the isolated eigenvalue $\sigma_z(s)$. The rank of $P_z(r_z)$ is called the *multiplicity* of the resonance point $r_z$, usually denoted by $N$.

The projection $P_z(r_z)$ is also the residue of the meromorphic function $r \mapsto T_z(H_r)J$ at the pole $r_z$. Hence it does not depend on the choice of regular point $s$ in (4.10).

PROPOSITION 4.5. *The finite-rank projection $P_z(r_z)$ defined by* (4.10) *satisfies the equality*

$$P_z(r_z) = \frac{1}{2\pi i} \oint_{C(r_z)} T_z(H_r) J \, dr, \tag{4.11}$$

*where $C(r_z)$ is a small circle enclosing the resonance point $r_z$.*

This appears as Proposition 3.2.3 in [Aza16]. The proof is reproduced here for convenience.

PROOF. Put $A_z(r) = T_z(H_r)J$. Let $s$ be a non-resonant complex number outside the circle $C(r_z)$. Using the sandwiched second resolvent identity (4.4),

$$\begin{aligned} \oint_{C(r_z)} A_z(r)\, dr &= \oint_{C(r_z)} (1 + (r-s)A_z(s))^{-1} A_z(s)\, dr \\ &= \oint_{C(r_z)} \frac{1}{r-s} \left(1 - (1 + (r-s)A_z(s))^{-1}\right) dr \\ &= \oint_{C(r_z)} \frac{1}{s-r} (1 + (r-s)A_z(s))^{-1}\, dr, \end{aligned}$$

where in the last line we have used Cauchy's theorem and the analyticity of $(r-s)^{-1}$ within $C(r_z)$. Let $C(\sigma_z(s))$ be the image of the contour $C(r_z)$ under the mapping $r \mapsto \sigma(r) = (s-r)^{-1}$. Then $C(\sigma_z(s))$ winds once around $\sigma_z(s) = (s-r_z)^{-1}$ and by making the change of variables $r \leftrightarrow \sigma(r)$, we obtain

$$\begin{aligned} \oint_{C(r_z)} A_z(r)\, dr &= \oint_{C(\sigma_z(s))} \sigma(1 - \sigma^{-1}A_z(s))^{-1}\sigma^{-2}\, d\sigma \\ &= \oint_{C(\sigma_z(s))} (\sigma - A_z(s))^{-1}\, d\sigma \\ &= 2\pi i P_z(r_z). \end{aligned}$$

□

For small positive or negative $y$, we define

$$P^{\uparrow}_{\lambda+iy}(r_\lambda) = \sum_{r^j_{\lambda+iy} \in\, \mathbb{C}_+} P_{\lambda+iy}(r^j_{\lambda+iy}),$$

where the sum is taken over those resonance points $r^j_{\lambda+iy}$ of the $r_\lambda$-group which belong to the upper complex half-plane $\mathbb{C}_+$. Similarly, the idempotent $P^{\downarrow}_{\lambda+iy}(r_\lambda)$ is defined as the sum of idempotents $P_{\lambda+iy}(r^j_{\lambda+iy})$ for resonance points $r^j_{\lambda+iy}$ of the $r_\lambda$-group in the lower half-plane $\mathbb{C}_-$.

Since the trace of $P_z(r_z)$ is equal to the multiplicity of $r_z$, for small positive $y$ the resonance index at $r_\lambda$ is given by

$$\operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V) = \operatorname{Tr}\left(P^{\uparrow}_{\lambda+iy}(r_\lambda)\right) - \operatorname{Tr}\left(P^{\uparrow}_{\lambda-iy}(r_\lambda)\right). \tag{4.12}$$

If $C(r_\lambda)$ is a small circle enclosing the resonance point $r_\lambda$, then for small positive $y$, it also encloses all resonance and anti-resonance points $r^j_{\lambda+iy}$

of the $r_\lambda$-group. Let $C_+(r_\lambda)$ denote the positively oriented upper closed semicircle formed by cutting $C(r_\lambda)$ at the real axis (see Figure 4.1). Then from (4.11), we get

$$\oint_{C_+(r_z)} \frac{1}{\pi} \operatorname{Im} T_{\lambda+iy}(H_r) J \, dr = P^{\uparrow}_{\lambda+iy}(r_\lambda) - P^{\uparrow}_{\lambda-iy}(r_\lambda).$$

Combining this with (4.12) proves the proposition below, which is Proposition 5.3.2 in [Aza16].

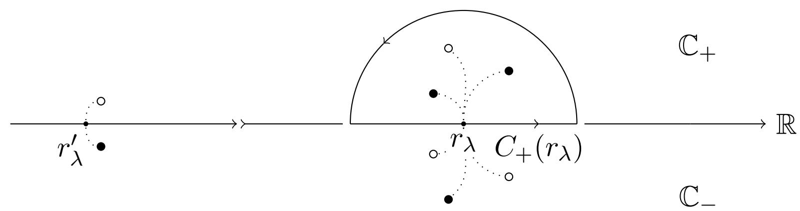


FIGURE 4.1. This picture shows a region of the complex plane in the vicinity of two real resonance points $r_\lambda$ and $r'_\lambda$. The dotted trails show the splitting of these resonance points into the $r_\lambda$- and $r'_\lambda$-groups. Solid dots stand for resonance points corresponding to $z = \lambda + iy$, $y > 0$, whereas circles stand for anti-resonance points of $z$ (i.e. resonance points of $\bar{z}$). The positively oriented semicircle $C_+(r_\lambda)$ encloses all resonance and anti-resonance points of the $r_\lambda$-group in the upper half-plane. The distance between $r_\lambda$ and $r'_\lambda$ is likely much larger than the diameter of $C_+(r_\lambda)$. The multiplicity of $r_\lambda$ is 3, the multiplicity of $r'_\lambda$ is 1, and their resonance indices are respectively 1 and $-1$.

PROPOSITION 4.6. *Let $\lambda$ be an essentially regular point of a straight line $H_r$ in a rigged affine space $\mathcal{A}(F)$ in the direction $V = F^*JF$. Suppose $r_\lambda$ belongs to the resonance set $R(\lambda; \{H_r\})$. Let $C(r_\lambda)$ be a small positively oriented circle enclosing $r_\lambda$ and no other resonance points and let $C_+(r_\lambda)$ be the positively oriented closed semicircle forming the boundary of the region of $\mathbb{C}_+$ enclosed by $C(r_\lambda)$ (as in Figure 4.1). Then for any small enough positive number $y$,*

$$\operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V) = \operatorname{Tr}\left( \int_{C_+(r_\lambda)} \frac{1}{\pi} \operatorname{Im} T_{\lambda+iy}(H_r) J \, dr \right). \tag{4.13}$$

The characterisation of the resonance index given in Proposition 4.6 is all that will be required in order to connect it to the singular SSF. The information in the remainder of this section has more relevance to the considerations of the paper [Aza16] than it does to the rest of this document. It is included here because it supports the interpretation of the resonance index as the infinitesimal flow of singular spectrum and because the given proofs have required some adjustment to the setting of a rigged affine space.

As above, suppose $\lambda$ is an essentially regular point of the straight line $H_r$ in the direction $V$. Let $r_z$ be a resonance point corresponding to $z = \lambda \pm iy$ for $y \geq 0$. The range of the projection $P_z(r_z)$ is denoted by $\Upsilon_z(r_z)$ and its elements are known as *resonance vectors*. Moreover, the vector spaces of resonance vectors of order $\leq k$ are defined by

$$\Upsilon_z^k(r_z) := \ker(1 + (r_z - s)T_z(H_s)J)^k. \tag{4.14}$$

The increasing sequence of vector spaces

$$\{0\} = \Upsilon_z^0(r_z) \subset \Upsilon_z^1(r_z) \subset \Upsilon_z^2(r_z) \subset \dots$$

stabilises and the union is $\Upsilon_z(r_z)$. It can be shown ([Aza16, Proposition 3.1.2]) that the vector spaces (4.14) do not depend on the choice of regular point $s$. The integer

$$d = \min\{k \in \mathbb{N} : \Upsilon_z^k(r_z) = \Upsilon_z(r_z)\} \tag{4.15}$$

is called the *order* of the resonance point $r_z$. Also, $m = \dim \Upsilon_z^1(r_z)$ is called the *geometric multiplicity* of $r_z$.

The operator $\mathbf{A}_z(r_z)$ is defined by the formula

$$\mathbf{A}_z(r_z) = \frac{1}{2\pi i} \int_{C_{r_z}} (r - r_z)T_z(H_r)J\,dr,$$

where $C(r_z)$ is a circle enclosing $r_z$ and no other resonance points. This operator satisfies

$$\mathbf{A}_z(r_z) = \mathbf{A}_z(r_z)P_z(r_z) = P_z(r_z)\mathbf{A}_z(r_z).$$

Moreover, while $P_z(r_z)$ is the residue of the meromorphic function $r \mapsto A_z(r) := T_z(H_r)J$ at the pole $r_z$, the powers of $\mathbf{A}_z(r_z)$ constitute the rest of the principal part of the Laurent series of $A_z(r)$ at $r_z$ ([Aza16, Proposition 3.3.1]), that is, in a neighbourhood of $r_z$,

$$A_z(r) = \tilde{A}_z(r) + (r - r_z)^{-1}P_z(r_z) + (r - r_z)^{-2}\mathbf{A}_z(r_z) + \ldots + (r - r_z)^{-d}\mathbf{A}_z^{d-1}(r_z),$$

where $\tilde{A}_z(r)$ is the holomorphic part and the positive integer $d$ happens to be the order of $r_z$ defined by (4.15). Further ([Aza16, Theorem 3.4.3]), $\mathbf{A}_z(r_z)$ is nilpotent with $\mathbf{A}_z^d(r_z) = 0$ and it lowers the order of a resonance vector in the sense that

$$\mathbf{A}_z(r_z)\Upsilon_z^k(r_z) = \Upsilon_z^{k-1}(r_z),$$

for any $k = 1, \ldots, d$.

PROPOSITION 4.7. *Let $z$ be nonreal and let $r_z$ be a resonance point corresponding to $z$. Then $\Upsilon_z(r_z) \subset F\mathcal{D}$, where $\mathcal{D} = \operatorname{dom}[\mathcal{A}]$.*

PROOF. This is clear if $F$ is bounded, so suppose otherwise. Since a resonance vector $u \in \Upsilon_z(r_z)$ is a solution of the resonance equation

$$(1 + (r_z - s)T_z(H_s)J)u = 0, \tag{4.16}$$

for regular $s$, it belongs to the range of the operator $T_z(H_s)J$. Since $z$ is nonreal and thus belongs to the resolvent set of $H_s$,

$$T_z(H_s)J = F\psi(H_s)(F\psi_{\bar z}(H_s))^* J,$$

where $\psi(x) = (|x|+1)^{-1/2}$ and $\psi_z(x) = (|x|+1)^{1/2}(x-z)^{-1}$. Since $\mathcal{D} = \operatorname{ran}\psi(H_s)$, we see that $\Upsilon_z(r_z) \subset F\mathcal{D}$. □

LEMMA 4.8. *Suppose $F\colon \mathcal{H} \to \mathcal{K}$ is an unbounded rigging operator and $\mathcal{A}(F)$ is a rigged affine space. Let $H_s$ be semibounded operator from $\mathcal{A}$ and let $z$ be an element of its resolvent set $\rho(H)$. Suppose $H_s$ is bounded below by $m \in \mathbb{R}$ and put*

$$\begin{aligned} \psi_z(x) &= (x-m)^{1/2}(x-z)^{-1}, \quad \psi(x) = (x-m)^{-1/2}, \\ f &= \psi_{\bar z}(H_s) f_0, \quad \chi = \psi(H_s)\chi_0, \end{aligned} \tag{4.17}$$

*for some $f_0, \chi_0 \in \mathcal{H}$. Then there is the equality*

$$(H_s - z)[f,\chi] = \langle f_0, \chi_0\rangle .$$

Note that $f$ and $\chi$ in this lemma belong to the form domain $\mathcal{D} = \operatorname{dom}[\mathcal{A}]$ and the set of all such vectors exhausts $\mathcal{D}$.

PROOF. Using the representation theorem for semibounded operators (Theorem 2.24),

$$(H_s - z)[f,\chi] = \left\langle (H_s - m)^{1/2} f, (H_s - m)^{1/2}\chi \right\rangle + (m-z)\langle f,\chi\rangle$$

Then since $(x-m)^{1/2}\psi_z(x) = 1+(z-m)(x-z)^{-1}$ and $\psi(x)\psi_z(x) = (x-z)^{-1}$, by the definitions of $f$ and $\chi$, we get

$$\begin{aligned} (H_s - z)[f,\chi] &= \langle f_0, (1+(z-m)R_z(H_s))\,\chi_0\rangle + (m-z)\langle f_0, R_z(H_s)\chi_0\rangle \\ &= \langle f_0, \chi_0\rangle . \end{aligned}$$

□

PROPOSITION 4.9. *Let $z$ be nonreal and let $r_z$ be a resonance point corresponding to $z$. If $F\chi^{(k)}$ is a resonance vectors of order $k$, then for any $f \in \mathcal{D} = \operatorname{dom}[\mathcal{A}]$,*

$$\begin{aligned} (H_{r_z} - z)\big[f, \chi^{(1)}\big] &= 0, \\ (H_{r_z} - z)\big[f, \chi^{(2)}\big] &= -V\big[f, \chi^{(1)}\big], \\ &\ldots \\ (H_{r_z} - z)\big[f, \chi^{(k)}\big] &= -V\big[f, \chi^{(k-1)}\big], \end{aligned}$$

*where the vectors $\chi^{(j)}$ satisfy $F\chi^{(k-j)} = \mathbf{A}_z^j(r_z)F\chi^{(k)}$.*

PROOF. This is a consequence of the equality

$$(1+(r_z - s)A_z(s))P_z(r_z) = -A_z(s)\mathbf{A}_z(r_z),$$

which can be proved as in [Aza16, Proposition 3.4.6]. It implies that for any $j = 1, \dots, k$,

$$(1 + (r_z - s)A_z(s))F\chi^{(j)} = -A_z(s)F\chi^{(j-1)}. \tag{4.18}$$

To complete the proof, if $F$ is bounded then the proof of [Aza16, Corollary 3.4.7] applies. In the case $F$ is unbounded and $\mathcal{A}(F)$ consists of semibounded operators, the same argument can be adjusted as follows.

Let $s$ be a regular point and put $A_z(s) := T_z(H_s)J$. Supposing $m < H_s$, since $\chi^{(j)} \in \mathcal{D}$ we may use the notation (4.17) and write $\chi^{(j)} = \psi(H_s)\chi_0^{(j)}$ for some $\chi_0^{(j)} \in \mathcal{H}$. Then using the fact that $F\psi(H_s)$ has trivial kernel, we obtain

$$\chi_0^{(j)} + (r_z - s)(F\psi_{\bar{z}}(H_s))^* JF\chi^{(j)} = -(F\psi_{\bar{z}}(H_s))^* JF\chi^{(j-1)},$$

where $\psi_z$ is as in (4.17). For any other $f = \psi_{\bar{z}}(H_s)f_0 \in \mathcal{D}$, making use of Lemma 4.8,

$$\begin{aligned}
(H_{r_z} - z)\big[f, \chi^{(j)}\big] &= (H_s - z)\big[f, \chi^{(j)}\big] + (r_z - s)V\big[f, \chi^{(j)}\big] \\
&= \left\langle f_0, \chi_0^{(j)} \right\rangle + (r_z - s)\left\langle f_0, (F\psi(H_s))^* JF\chi^{(j)} \right\rangle \\
&= -\left\langle f_0, (F\psi(H_s))^* JF\chi^{(j-1)} \right\rangle \\
&= -V\big[f, \chi^{(j-1)}\big].
\end{aligned}$$

□

THEOREM 4.10. *Let $\lambda$ be an essentially regular point of a straight line $H_r$ in the direction $V = F^*JF$ within a rigged affine space $\mathcal{A}(F)$. Put $z = \lambda \pm iy$, $y \geq 0$. If $z$ is an eigenvalue of the operator $H_{r_z} = H_r \dot{+} (r_z - r)V$, then the complex number $r_z$ is a resonant point of the path $H_r$ corresponding to $z$. If $z$ is outside of $\sigma_{ess}$, then the converse holds. Moreover, the rigging operator $F$ is an injection of the eigenspace of $H_{r_z}$ at $z$ into $\Upsilon_z^1(r_z)$ and a linear isomorphism if $z \notin \sigma_{ess}$.*

This theorem is a combination of Theorems 4.1.1 and 4.3.2 in [Aza16].

PROOF. In the case that $F$ is bounded, the proofs in [Aza16] apply. If on the other hand $F$ is not bounded and $\mathcal{A}$ consists of semibounded operators, we can modify the arguments as follows.

Suppose $z$ is an eigenvalue of $H_{r_z}$ and let $\chi$ be a corresponding eigenvector. Let $s \in \mathbb{R}$ be any regular point of the path. It follows that $z$ can not be an eigenvalue of $H_s$. We first consider the case that $z$ is outside of $\sigma_{ess}$ and hence belongs to the resolvent set $\rho(H_s)$. For any $f \in \mathcal{D} = \operatorname{dom}[\mathcal{A}]$ there holds the equality

$$(H_s - z)[f, \chi] = (s - r_z)V[f, \chi], \tag{4.19}$$

which is obtained by adding $(s - r_z)V$ to the eigenvalue equation for $H_{r_z}$. Supposing $H_s > m$, there exist $f_0, \chi_0 \in \mathcal{H}$ so that we may again use the notation (4.17) and by the lemma

$$(H_s - z)[f, \chi] = \langle f_0, \chi_0 \rangle .$$

Combining this with (4.19) and factorising the perturbation $V$ gives

$$\begin{aligned}\langle f_0, \chi_0\rangle &= (s - r_z)\langle Ff, JF\chi\rangle \\ &= (s - r_z)\langle f_0, (F\psi_z(H_s))^* JF\chi\rangle,\end{aligned}$$

which holds for any $f_0 \in \mathcal{H}$ and hence implies the equality of vectors

$$\chi_0 = (s - r_z)(F\psi_z(H_s))^* JF\chi. \tag{4.20}$$

Therefore,

$$\begin{aligned}F\chi &= F\psi(H_s)\chi_0 \\ &= (s - r_z)F\psi(H_s)(F\psi_z(H_s))^* JF\chi \\ &= (s - r_z)T_z(H_s)JF\chi,\end{aligned}$$

showing that $F\chi$ is a first order resonance vector.

For the case that $z = \lambda$ is within $\sigma_{ess}$, we will write $\lambda$ instead of $z$ and allow $z$ to refer to $\lambda \pm iy$ for small positive $y$. Then we consider the modified version of (4.19)

$$(H_s - z)[f, \chi] + iy\langle f, \chi\rangle = (s - r_\lambda)V[f, \chi].$$

By applying the above argument we obtain the equality

$$F\chi + iyFR_z(H_s)\chi = (s - r_\lambda)T_z(H_s)JF\chi.$$

Since the right hand side converges as $y \to 0^+$, so does the left hand side. It remains to show that the limit $g := \lim_{y\to 0^+} iyFR_z(H_s)\chi$ is zero. Since $\lambda$ is not an eigenvalue of $H_s$, the operator $yR_z(H_s)$ converges weakly to zero. Hence $\langle \varphi, g\rangle = 0$ for any $\varphi \in \operatorname{dom} F^*$, from which it follows that $g = 0$.

Now suppose $r_z$ is a resonance point of $H_r$ corresponding to $z = \lambda \pm iy$, $y \geq 0$, with $\lambda \notin \sigma_{ess}$. Let $u \in \Upsilon_z(r_z)$. From Proposition 4.7 it must be that $u \in F\mathcal{D}$, say $u = F\chi$. With $s \in \mathbb{R}$ again denoting a regular point and for any $f \in \operatorname{dom}[\mathcal{A}]$, we may again write (4.17). Since $F\psi(H_s)$ has trivial kernel, from the resonance equation (4.16) we obtain (4.20). Then combining this with Lemma 4.8,

$$\begin{aligned}(H_s - z)[f, \chi] &= \langle f_0, \chi_0\rangle \\ &= \langle f_0, (r_z - s)(F\psi_z(H_s))^* JF\chi\rangle \\ &= (r_z - s)V[f, \chi].\end{aligned}$$

Thus $H_{r_z}[f, \chi] = z\langle f, \chi\rangle$ for any $f \in \operatorname{dom}[H_{r_z}]$ from which it follows that $\chi \in \operatorname{dom} H_{r_z}$ and $H_{r_z}\chi = z\chi$ as required. $\square$

CHAPTER 5

# The spectral shift function (SSF)

The majority of this chapter consists in an exposition of the SSF for relatively trace class perturbations. This material is well-known. Indeed M. G. Kreĭn himself, having established the existence of the SSF assuming a trace class difference $V := H_1 - H_0$ in [Kre53], later extended this to resolvent comparable pairs by transformation from the case of unitary pairs with trace class difference in [Kre62]. However, the point of view taken here seems to be new. As discussed in the introduction, the approach is as follows. The primitive object is considered to be the *infinitesimal spectral shift measure* which takes the form

$$\Phi_H(V)(\varphi) = \mathrm{Tr}(V\varphi(H)), \quad \varphi \in C_c(\mathbb{R}).$$

To define this object on a rigged affine space of self-adjoint operators $\mathcal{A}$, it is necessary to impose a condition of trace class type, which is the subject of Section 5.2.

We will consider only 'relatively trace class' perturbations. More precisely we assume that a rigged affine space $\mathcal{A}(F)$ has a relatively Hilbert-Schmidt rigging operator $F$, in the sense that $FR_z(H) \in \mathcal{L}_2(\mathcal{H}, \mathcal{K})$, for $z \in \mathbb{C} \setminus \mathbb{R}$ and $H \in \mathcal{A}$. This implies that any pair of self adjoint operators $H_0, H_1 \in \mathcal{A}$ satisfies the condition

$$R_z(H_1) - R_z(H_0) \in \mathcal{L}_1(\mathcal{H}), \quad z \in \mathbb{C} \setminus \mathbb{R}. \tag{5.1}$$

Adopting terminology which appears in [Yaf92], a pair $H_0, H_1$ of self-adjoint operators satisfying (5.1) will be called *resolvent comparable.*

Assuming it is well defined, the infinitesimal spectral shift measure $\Phi$ can be viewed as a generalised 1-form on the affine space $\mathcal{A}$. Moreover, by using double operator integral techniques it can be proved to be exact. Therefore its integral along any path $H_r$ in $\mathcal{A}$ depends only on the pair of endpoints $H_0$, $H_1$. This defines the *spectral shift measure* in keeping with the Birman-Solomyak formula:

$$\xi(\varphi; H_1, H_0) = \int_0^1 \Phi_{H_r}\big(\dot{H}_r\big)(\varphi)\, dr, \quad \varphi \in C_c(\mathbb{R}).$$

By reduction to the case of a trace class perturbation, the spectral shift measure can be shown to be absolutely continuous. Hence it can be identified with a locally integrable function, namely the SSF.

This material takes us to Section 5.4. In Section 5.5, the decomposition of the SSF into absolutely continuous and singular parts is discussed. Finally in Section 5.6, a counterexample taken from [Aza11a] is reviewed, which shows the path-dependence of the singular SSF.

## 5.1. SSF for trace class perturbations

This section consists of a review of Kreĭn's famous theorem on the existence of the SSF for trace class perturbations. Other expositions can be found e.g. in [Sch12, Chapter 9; BY93, §3; Yaf92, Chapter 8].

THEOREM 5.1. *Let $H_0$ and $H_1$ be self-adjoint operators on a Hilbert space $\mathcal{H}$ with a trace class difference $V := H_1 - H_0$. Then there is a unique integrable function $\xi \in L_1(\mathbb{R})$ which satisfies the trace formula*

$$\operatorname{Tr}(\varphi(H_1) - \varphi(H_0)) = \int_{\mathbb{R}} \varphi'(\lambda)\xi(\lambda)\, d\lambda \tag{5.2}$$

*for all test functions $\varphi \in C_c^\infty(\mathbb{R})$.*

As an aside, the premise of Theorem 5.1 is equivalent to the assumption that $H_0$ and $H_1$ belong to a rigged affine space $\mathcal{A}(F)$ with a Hilbert-Schmidt rigging operator $F$.

PROOF. It suffices to show that (5.2) holds when $\varphi$ is the resolvent function $\varphi = R_z$, $z \in \mathbb{C} \setminus \mathbb{R}$. This can be seen using the Helffer-Sjöstrand formula, which for any test function $\varphi$ implies the equality

$$\varphi(H_1) - \varphi(H_0) = \frac{1}{\pi} \int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z) \left(R_z(H_1) - R_z(H_0)\right)\, dxdy, \tag{5.3}$$

where $z = x + iy$, $\bar\partial = \frac{1}{2}\partial_x + \frac{i}{2}\partial_y$, and $\tilde\varphi$ is an almost analytic extension of $\varphi$ (see Section 2.5). Since $\|R_z(H_1) - R_z(H_0)\|_1 \le |y|^{-2}\|V\|_1$, which follows from the second resolvent identity and the estimate $\|R_z(H)\| \le |y|^{-1}$, and since (2.15) holds with $p = 2$, the integrand on the right hand side of (5.3) is a bounded and compactly supported $\mathcal{L}_1$-valued function. It follows that the left hand side belongs to the trace class and

$$\operatorname{Tr}\left(\varphi(H_1) - \varphi(H_0)\right) = \frac{1}{\pi} \int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z) \operatorname{Tr}\left(R_z(H_1) - R_z(H_0)\right)\, dxdy.$$

Then after substituting the trace formula for $R_z$, an application of Fubini's theorem shows that the right hand side is equal to

$$\frac{1}{\pi} \int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z) \left( - \int_{\mathbb{R}} R_z^2(\lambda)\xi(\lambda)\, d\lambda \right) dxdy \\ = \int_{\mathbb{R}} \left( -\frac{1}{\pi} \int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z) R_z^2(\lambda)\, dxdy \right) \xi(\lambda)\, d\lambda$$

and the trace formula for the test function $\varphi$ now follows from (2.17).

Suppose first that the perturbation $V$ has rank one, in which case it must be that $V = \alpha \langle v, \cdot\rangle\, v$ for some $\alpha \in \mathbb{R}$ and $\|v\| = 1$. For convenience suppose $\alpha > 0$. (The case $\alpha < 0$ can be reduced to an exchange of the roles of $H_0$ and $H_1$.) Then put

$$\Delta(z) = \Delta_{H_1/H_0}(z) := 1 + \alpha \langle v, R_z(H_0)v \rangle \,. \tag{5.4}$$

This is a Nevanlinna function – it is holomorphic in the upper half-plane $\mathbb{C}_+$ where its imaginary part $\operatorname{Im} \Delta(z) = \alpha \langle v, \operatorname{Im} R_z(H_0)v \rangle$ is positive.

Hence the function $f(z) := \log \Delta(z)$ (the principal branch) is also a Nevanlinna function with $\operatorname{Im} f(z) = \arg \Delta(z) \in (0, \pi]$. Moreover, $|yf(iy)|$ is bounded for large $y > 0$. To check this, we use the approximation $\log(1+ w) \approx w$ for small $w$ to calculate

$$\begin{aligned} \lim_{y\to\infty} -iyf(iy) &= \lim_{y\to\infty} -iy(\Delta(iy) - 1) \\ &= \lim_{y\to\infty} \alpha \int_{\mathbb{R}} \frac{-i\lambda y + y^2}{\lambda^2 + y^2}\, d\langle v, E_0(\lambda)v\rangle \\ &= \alpha \int_{\mathbb{R}} d\langle v, E_0(\lambda)v\rangle = \alpha, \end{aligned} \tag{5.5}$$

where the dominated convergence theorem was used in the last line.

It can therefore be concluded from Theorem 2.9 that $f(z)$ is the Cauchy-Stieltjes transform

$$f(z) = \log \Delta(z) = \int_{\mathbb{R}} \frac{\xi(\lambda)}{\lambda - z}\, d\lambda \tag{5.6}$$

of the function $\xi \in L_1(\mathbb{R})$ given by

$$\xi(\lambda) := \pi^{-1} \lim_{y\to 0} \arg \Delta(\lambda + iy) \in [0, 1]. \tag{5.7}$$

Combining (5.6) and (5.5) shows that this function satisfies

$$\alpha = \lim_{y\to\infty} -iyf(iy) = \lim_{y\to\infty} \int_{\mathbb{R}} \frac{-iy\,\xi(\lambda)}{\lambda - iy}\, d\lambda = \int_{\mathbb{R}} \xi(\lambda)\, d\lambda, \tag{5.8}$$

where dominated convergence was again used to calculate the limit.

To show that the function $\xi$ defined by (5.7) satisfies the trace formula, we differentiate the formula (5.6) for nonreal $z$ :

$$(\Delta(z))^{-1} \alpha \left\langle v, R_z^2(H_0)v \right\rangle = -\int_{\mathbb{R}} \frac{\xi(\lambda)}{(\lambda - z)^2}\, d\lambda. \tag{5.9}$$

Since $V = \alpha \langle v, \cdot \rangle\, v$, the second resolvent identity takes the form

$$R_z(H_0) - R_z(H_1) = \alpha \langle R_{\bar z}(H_0)v, \cdot\rangle\, R_z(H_1)v. \tag{5.10}$$

It follows that $R_z(H_1)v = (\Delta(z))^{-1} R_z(H_0)v$, which upon insertion back into (5.10) results in the equality

$$R_z(H_0) - R_z(H_1) = (\Delta(z))^{-1} \alpha \langle R_{\bar z}(H_0)v, \cdot\rangle\, R_z(H_0)v. \tag{5.11}$$

The trace of this rank one operator is given by the left hand side of (5.9). Thus we have established the trace formula (5.2) in the case $\varphi = R_z$, for a rank-one perturbation.

For a pair $H_0, H_1$, of self-adjoint operators with trace class difference $V = H_1 - H_0$, the perturbation determinant is defined for $z \in \rho(H_0)$ by

$$\Delta(z) = \Delta_{H_1/H_0}(z) := \det(1 + VR_z(H_0)) = \det((H_1 - z)R_z(H_0)),$$

which clearly generalises (5.4). Some of its relevant properties are collected below, whose proofs can be found e.g. in [Sch12, Section 9.6; Yaf92, Part 1 of §8.1].

*Let $H_0, H_1$ and $H_2$ be self-adjoint operators such that their pairwise differences are trace class. The perturbation determinant $\Delta(z)$ is a holomorphic function, which for any nonreal $z$ satisfies the equalities*

$$\Delta_{H_2/H_0}(z) = \Delta_{H_2/H_1}(z)\Delta_{H_1/H_0}(z), \tag{5.12}$$

$$(\Delta_{H_1/H_0}(z))^{-1}\Delta'_{H_1/H_0}(z) = \operatorname{Tr}(R_z(H_0) - R_z(H_1)). \tag{5.13}$$

Let $H_0$ be self-adjoint. For an arbitrary self-adjoint and trace class perturbation $V$, there is an orthonormal basis $\{v_k\}$ and summable sequence $\{\alpha_k\} \subset \mathbb{R}$ so that $V$ is the $\mathcal{L}_1$-limit of the following finite rank operators

$$V_n := \sum_{k=1}^{n} \alpha_k \langle v_k, \cdot\rangle v_k.$$

Moreover, we have $\|V\|_1 = \sum_{k=1}^{\infty} |\alpha_k|$ and $\operatorname{Tr}(V) = \sum_{k=1}^{\infty} \alpha_k$. Let $H_n = H_0 + V_n$ and let $\xi_n$ be the SSF for the pair $H_{n-1}, H_n$, which differ by the rank one perturbation $\alpha_n \langle v_n, \cdot\rangle v_n$. Then it can be shown using (5.8) that the series $\sum_{k=1}^{n} \xi_n$ converges in $L_1(\mathbb{R})$. Let $\xi$ denote its limit, which therefore satisfies the equalities

$$\int_{\mathbb{R}} |\xi(\lambda)|\, d\lambda = \|V\|_1, \quad \int_{\mathbb{R}} \xi(\lambda)\, d\lambda = \operatorname{Tr}(V).$$

Moreover, the multiplicative property (5.12) and the identity (5.6) imply

$$\Delta_{H_n/H_0}(z) = \prod_{k=1}^{n} \Delta_{H_n/H_{n-1}}(z) = \exp\left(\int_{\mathbb{R}} \frac{\sum_{k=1}^{n} \xi_k(\lambda)}{\lambda - z}\, d\lambda\right),$$

which in the limit $n \to \infty$ generalises (5.6):

$$\log \Delta_{H_0+V/H_0}(z) = \int_{\mathbb{R}} \frac{\xi(\lambda)}{\lambda - z}\, d\lambda.$$

Finally, differentiating this equality using (5.13) establishes the trace formula in the case $\varphi = R_z$.

Finally to prove the uniqueness, it suffices to check that the trace formula (5.2) defines a locally integrable function $\xi$ up to an additive constant, since only one such function can be integrable. We claim that the left hand side of (5.2) defines a generalised function, which according to the right hand side is equal to the (negative of the) generalised derivative of $\xi$. So the difference of two locally integrable functions $\xi_1$ and $\xi_2$ which satisfy (5.2) has generalised derivative zero and is therefore constant (see e.g. [GS64, Section 2.6]).

To check that the formula

$$\xi'(\varphi) := \mathrm{Tr}(\varphi(H_0) - \varphi(H_1)) \tag{5.14}$$

defines a generalised function, suppose that $\varphi_n$, $n = 1, 2, \ldots$, is a sequence of test functions supported in a common compact set such that $\|\varphi_n^{(m)}\|_\infty \to 0$ as $n \to \infty$ for $m = 0, 1, \ldots$. It follows from the Helffer-Sjöstrand that

$$\xi'(\varphi_n) = \frac{1}{\pi} \int_{\mathbb{R}} \bar{\partial}\tilde{\varphi}_n(z)\, \mathrm{Tr}(R_z(H_0) - R_z(H_1))\, dxdy$$

and it can be seen from (2.16) that the almost analytic extensions can be chosen so that the integrand converges uniformly to zero as $n \to \infty$. Dominated convergence then implies that $|\xi'(\varphi_n)| \to 0$. It follows that $\xi'$ (which is obviously linear) is continuous on $C_c^\infty(\mathbb{R})$ and hence a generalised function. □

## 5.2. A trace condition

Following M. Sh. Birman and M. Z. Solomyak, the SSF corresponding to a pair of self-adjoint operators $H_0$ and $H_1 = H_0 + V$ can be viewed as the density of the measure

$$\Delta \mapsto \int_0^1 \mathrm{Tr}(VE_r(\Delta))\, dr,$$

where $E_r$ is the spectral measure of $H_r = H_0 + rV$. To give this proper sense in the setting of a rigged affine space $\mathcal{A}(F)$ we require a condition of trace class type. If $H_r \in \mathcal{A}$, with $V = F^*JF \in \mathcal{A}_0$, then for any bounded Borel set $\Delta$, the expression $\mathrm{Tr}(VE_r(\Delta))$ can be interpreted as $\mathrm{Tr}((FE_r(\Delta))^*JFE_r(\Delta))$ provided the inclusion

$$FE_r(\Delta) \in \mathcal{L}_2(\mathcal{H}, \mathcal{K}) \tag{5.15}$$

holds. A trace condition should at least imply (5.15), which already implies the LAP by Corollary 3.14. We will make a significantly stronger assumption than (5.15):

Definition 5.2. Let $\mathcal{A}(F)$ be a rigged affine space. We will say that $\mathcal{A}$ is *resolvent comparable* if

$$FR_z(H) \in \mathcal{L}_2(\mathcal{H}, \mathcal{K}) \tag{5.16}$$

for any $H \in \mathcal{A}$ and any nonreal $z$.

For a rigged affine space to be resolvent comparable, it is enough for the inclusion (5.16) to hold for some $H_0 \in \mathcal{A}$ and some nonreal $z$. That it then holds for any other nonreal $w$ follows from the boundedness of the function $R_w/R_z$ and hence of the operator $(H_0 - z)R_w(H_0)$. It holds for any other $H_1 \in \mathcal{A}$ due to the equality (4.5).

This resolvent comparable assumption is well-known to hold for low-dimensional Schrödinger operators. Proof can be derived from results which address the following kind of questions. Let $H$ be a Schrödinger operator and let $f$ and $g$ be two functions. When is the operator

$$g(x)f(H) \tag{5.17}$$

Hilbert-Schmidt? These kind of questions are discussed in B. Simon's book [Sim05] in the case of the free Hamiltonian $H = -\Delta$. For many other Schrödinger operators $H = -\Delta + V$, Schatten ideal properties of the operator (5.17) can be reduced to the case of the free Hamiltonian with the aid of the second resolvent identity; this is a well known method which is also used in the proof of the LAP for Schrödinger operators with short range potentials, see e.g. [Agm75]. For more general Schrödinger operators of the form $H = -\Delta + V$, Schatten ideal properties of the product (5.17) are surveyed in [Sim82] (see in particular [Sim82, Theorem B.9.1]).

For now, we use the method involving the second resolvent identity, beginning with the basic result:

Proposition 5.3. *If $f, g \in L_2(\mathbb{R}^\nu)$, then the operator $g(x)f(-i\nabla)$ is Hilbert-Schmidt.*

Proof. This is a simple case of the more general result [Sim05, Theorem 4.1]. With $\wedge$ and $\vee$ referring respectively to the Fourier transform and its inverse, the operator $g(x)f(-i\nabla)$ is interpreted $L_2(\mathbb{R}^\nu) \ni \varphi(x) \mapsto g\big(f\hat{\varphi}\big)^\vee$. Since this is an integral operator

$$\big(g\big(f\hat{\varphi}\big)^\vee\big)(x) = \frac{1}{(2\pi)^{\nu/2}} \int_{\mathbb{R}} g(x)\check{f}(x-y)\varphi(y)\, dy,$$

whose kernel $K(x,y) = (2\pi)^{-\nu/2} g(x)\check{f}(x-y)$ satisfies the inequality $\|K\|_2 \leq (2\pi)^{-\nu/2}\|g\|_2\|f\|_2$, it is therefore Hilbert-Schmidt (see e.g. [Sim05, Theorem 2.11; RS72, Theorem VI.23]). □

Applying Proposition 5.3 to the function $f(x) = (x^2 - z)^{-1}$, a function which is square-integrable only when $\nu \leq 3$ (the same restriction on the dimension appears in [Sim82, Theorem B.9.1]), gives

Corollary 5.4. *If $g \in L_2(\mathbb{R}^\nu)$, where $\nu = 1, 2,$ or 3, then the operator $g(x)R_z(-\Delta)$ is Hilbert-Schmidt.*

Corollary 5.5. *Let $H_0 = -\Delta + V_0$ be a Schrödinger operator on $L_2(\mathbb{R}^\nu)$, $\nu = 1, 2,$ or 3, where $V_0 \in L_\infty(\mathbb{R}^\nu)$, and let $V \in L_1(\mathbb{R}^\nu)$. Then there exists a resolvent comparable rigged affine space $\mathcal{A}$ such that $H_0 \in \mathcal{A}$ and $V \in \mathcal{A}_0$.*

Proof. Since $V \in L_1(\mathbb{R}^\nu)$, we have $F := \sqrt{|V|} \in L_2(\mathbb{R}^\nu)$. From Corollary 5.4, it follows that the operator $FR_z(-\Delta)$ is Hilbert-Schmidt. Then using the second resolvent identity (3.18), the operator

$$FR_z(H_0) = FR_z(-\Delta)(1 - V_0 R_z(H_0))$$

is also Hilbert-Schmidt. Now Proposition 3.16 completes the proof. □

The remainder of this section collects some properties of resolvent comparable rigged affine space which will be useful later. Firstly, for an analytic path in such an affine space the property of regular points expressed in Theorem 4.4 holds for trace-regular points as well:

THEOREM 5.6. *Let $\mathcal{A}(F)$ be a resolvent comparable rigged affine space and let $H_r$ be an analytic path in $\mathcal{A}(F)$. Suppose $\lambda$ is an essentially regular point of the path $H_r$. Then $\lambda$ belongs to $\Lambda(H_r, F; \mathcal{L}_1)$ if and only if $r$ does not belong to the discrete resonance set $R(\lambda; \{H_r\})$.*

PROOF. By Theorem 4.4, the inclusion $\lambda \in \Lambda(H_r, F; \mathcal{L}_1) \subset \Lambda(H_r, F)$ means that $r \notin R(\lambda; \{H_r\})$. It remains to show that if $\lambda$ belongs to $\Lambda(H_r, F)$ then it also belongs to $\Lambda(H_r, F; \mathcal{L}_1)$. Given that $\lambda \in \Lambda(H_0, F; \mathcal{L}_1)$, this follows from the equality (3.7). □

PROPOSITION 5.7. *Let $\mathcal{A}$ be a rigged affine space and let $H$ be an arbitrary fixed operator from $\mathcal{A}$. Put $p = 1$ if $\mathcal{A}$ is resolvent comparable and $p = \infty$ otherwise. Then for $z \in \mathbb{C} \setminus \mathbb{R}$, the function*

$$\mathcal{A}_0 \ni V \mapsto R_z(H \dotplus V) - R_z(H) \in \mathcal{L}_p(\mathcal{H})$$

*is continuously Fréchet differentiable with derivative at $V_0$ given by*

$$V \mapsto -R_z(H \dotplus V_0) V R_z(H \dotplus V_0). \tag{5.18}$$

PROOF. Suppose $F$ is the rigging operator. Let $H_0 = H \dotplus V_0$ and $H_1 = H_0 \dotplus V$, where $V = F^* J F$. By the second resolvent identity (3.22) and equality (4.5),

$$\begin{aligned} R_z(H_1) - R_z(H_0) &= -(F R_{\bar{z}}(H_0))^* J F R_z(H_1) \\ &= -(F R_{\bar{z}}(H_0))^* J (1 + T_z(H_0) J)^{-1} F R_z(H_0). \end{aligned}$$

Therefore when $\|J\|$ is small, so that $(1 + T_z(H_0)J)^{-1} = \sum_{k=0}^{\infty} (-T_z(H_0)J)^k$, we have

$$\|R_z(H_1) - R_z(H_0) + (F R_{\bar{z}}(H_0))^* J F R_z(H_0)\|_1 = O(\|J\|^2).$$

The continuity of the derivative (5.18) as a function of $H_0$ follows from the $\mathcal{L}_2$-continuity of $F R_z(H_0)$, which itself follows from (4.5). □

COROLLARY 5.8. *The convergence $H_n \to H$ of a sequence $\{H_n\}_{n \in \mathbb{N}}$ of operators in a rigged affine space $\mathcal{A}$ implies its norm-resolvent convergence, i.e. $\|R_z(H_n) - R_z(H)\| \to 0$. Moreover, for any continuous function $f$ which vanishes at infinity, we have $f(H_n) \to f(H)$ in $\mathcal{B}(\mathcal{H})$.*

PROOF. The norm-resolvent convergence follows directly from Proposition 5.7 and implies the convergence $f(H_n) \to f(H)$. For proof we refer to [RS72, Theorem VIII.20(a)]. We will later prove a stronger result, Theorem 5.17, for test functions $f$ using the Helffer-Sjöstrand formula. □

Proposition 5.9. *Let $\mathcal{A}(F)$ be a rigged affine space and let $H$ be an arbitrary fixed operator from $\mathcal{A}$. Put $q = 2$ if $\mathcal{A}$ is resolvent comparable and $q = \infty$ otherwise. Then for $z \in \mathbb{C} \setminus \mathbb{R}$, the function*

$$\mathcal{A}_0 \ni V \mapsto FR_z(H \dotplus V) - FR_z(H) \in \mathcal{L}_q(\mathcal{H}, \mathcal{K})$$

*is continuously Fréchet differentiable with derivative at $V_0$ given by*

$$V \mapsto -FR_z(H \dotplus V_0)VR_z(H \dotplus V_0). \tag{5.19}$$

The proof is very similar to that of Proposition 5.7 and has been omitted.

## 5.3. Double operator integrals

For the basic theory of the SSF in resolvent comparable rigged affine spaces we will need double operator integrals (DOI's). The notion of a multiple operator integral (MOI) was introduced by Y. L. Daletskiĭ and S. G. Kreĭn ([DK56]) and further developed by M. Sh. Birman and M. Z. Solomyak (see e.g. [BS03]) and many others (e.g. [Pav71; Ste77]). MOI's take the form

$$\begin{aligned} &T_f^{H_0,\dots,H_n}(V_1,\dots,V_n) \\ &\quad = \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} f(\lambda_0,\dots,\lambda_n)\, dE_{H_0}(\lambda_0) V_1 dE_{H_1}(\lambda_1) \dots V_n dE_{H_n}(\lambda_n), \end{aligned} \tag{5.20}$$

where $f\colon \mathbb{R}^{n+1} \to \mathbb{C}$ is a Borel function, $H_0, H_1, \dots, H_n$ are self-adjoint operators with spectral measures $E_0, E_1, \dots, E_n$, and $V_1, \dots, V_n$, are some perturbations. Such objects are ubiquitous, appearing for example in the Taylor expansions of operator valued functions such as $V \mapsto e^{i(H+V)}$.

MOI's were naturally defined by those mathematicians already mentioned via operator valued measures. However we will take a convenient alternative approach which appears in [ACDS09; Pel06]. In this approach an MOI is defined as the integral of an operator valued function with respect to a scalar valued measure. This is achieved through an integral representation of the multi-variate function $f\colon \mathbb{R}^{n+1} \to \mathbb{C}$ in which the integrand separates its variables. This integral representation of $f$ is otherwise quite arbitrary and the resulting MOI is shown not to depend on the choice. In the context of a resolvent comparable affine space we can get away with just one such representation (see (5.27) below), but further generalisation no doubt requires a different choice. We will follow the definition of MOI's given in [ACDS09], adapting it slightly for rigged affine spaces. Strictly speaking we only need DOI's, but we might as well include higher order operator integrals when it doesn't involve much additional work.

The following notation is used throughout this section. As usual $\mathcal{A}$ denotes a rigged affine space. If it is resolvent comparable, then $p = 1$ and $q = 2$. Otherwise $p = q = \infty$.

DEFINITION 5.10. For $n \in \mathbb{N}$, suppose a complex valued function $f$ of $n+1$ real variables has a representation of the form

$$f(\lambda_0, \dots, \lambda_n) = \int_S \alpha_0(\lambda_0, s) \dots \alpha_n(\lambda_n, s)\, d\nu(s), \tag{5.21}$$

called a *Birman-Solomyak (BS) representation.* For our purposes we can assume $S$ to be a subset of a Euclidean space, $\nu$ to be a finite measure, and the functions $\alpha_j$, $j = 0, \dots, n$ to be measurable functions on $\mathbb{R} \times S$, which for $\nu$-a.e. $s \in S$ satisfy the estimate

$$|\alpha_j(x, s)| \le C(|x| + 1)^{-1}, \tag{5.22}$$

for some $C > 0$ and a.e. $x \in \mathbb{R}$.

Then for $H_0, \dots H_n \in \mathcal{A}$ and $V_1, \dots, V_n \in \mathcal{A}_0$, an $(n+1)$*-tuple operator integral* is defined by the formula

$$T_f^{H_0,\dots,H_n}(V_1, \dots, V_n) := \int_S \alpha_0(H_0, s) V_1 \alpha_1(H_1, s) V_2 \dots V_n \alpha_n(H_n, s)\, d\nu(s). \tag{5.23}$$

The requirement (5.22) does not appear in [ACDS09], since there the perturbations $V_j$, $j = 1, \dots, n$, are bounded operators. It is included here so that we may interpret the integrand of (5.23) as a compact operator valued function using the notation (3.27) (a product of such operators). The integral (5.23) can then be understood as a Bochner integral (see e.g. [HP57, Section 3.7; Yos80, Section V.5]):

LEMMA 5.11. *In the context of Definition 5.10, the function*

$$S \ni s \mapsto \alpha_0(H_0, s) V_1 \alpha_1(H_1, s) V_2 \dots V_n \alpha_n(H_n, s) \in \mathcal{L}_p(\mathcal{H}) \tag{5.24}$$

*is Bochner-integrable (where $p = 1$ or $p = \infty$ accordingly if $\mathcal{A}$ is resolvent comparable or not).*

PROOF. Let $\beta$ be a bounded measurable function on $\mathbb{R} \times S$. Then it follows that for $H \in \mathcal{A}$ the function $S \ni s \mapsto \beta(H, \cdot) \in \mathcal{B}(\mathcal{H})$ is bounded and weakly measurable. Let $F$ be the rigging operator and let $V_n = F^* J_n F$. Since the functions $\alpha_j$ satisfy (5.22), the integrand (5.24) can be written as the product

$$\beta_0(H_0, s)(F\psi^2(H_0))^* J_1 F \psi(H_1) \beta_1(H_1, s)(F\psi(H_1))^* J_2 \dots \dots (F\psi(H_{n-1}))^* J_n F \psi^2(H_n) \beta_n(H_n, s) \tag{5.25}$$

where $\psi(x) := (|x| + 1)^{-1/2}$ and $\beta_j(x, s) = (|x| + 1)\alpha_j(x, s)$. Since each function $\beta_j(H_j, \cdot)$ is bounded and weakly measurable, so is the function (5.24). Since the weakly measurable function (5.24) takes values in the separable space $\mathcal{L}_p(\mathcal{H})$, it follows from the Dunford-Pettis theorem on the equivalence of weak and strong measurability (see e.g. [HP57, Theorem 3.5.5]) that it is Bochner measurable. Since $(S, \nu)$ is assumed to be a finite measure space, the boundedness of this function implies its integrability (using Bochner's criterion for integrability e.g. [HP57, Theorem 3.7.4]). □

Lemma 5.12. *The MOI* $T_f^{H_0,\dots,H_n}(V_1,\dots,V_n)$ *does not depend on the BS representation* (5.21) *of the function* $f$.

Proof. Here we follow [ACDS09, Lemma 4.3]. First suppose that $V_j = F^* J_j F$, $j = 1,\dots,n$ where $J_j$ are the rank-one operators $J_j = \langle \varphi_j, \cdot\rangle\, \psi_j$ for some some vectors $\varphi_j$ and $\psi_j$ from the domain of the operator $F^*$. In this case $V_j$ is the rank-one operator $V_j = \langle F^*\varphi_j, \cdot\rangle\, F^*\psi_j$.

Note that $V_j$ does not belong to $\mathcal{A}_0$ unless $J_j$ is self-adjoint, but this is not important here; the expression (5.23) makes sense when $V_j = F^* J_j F$ are the forms defined by any bounded operators $J_j \in \mathcal{B}(\mathcal{K})$.

Also let $V_0 = \langle v, \cdot\rangle\, w$ be an arbitrary rank-one operator on the main Hilbert space $\mathcal{H}$. Then

$$\begin{aligned}
E &:= \operatorname{Tr}\left(V_0 \int_S \alpha_0(H_0,s)V_1\dots V_n\alpha_n(H_n,s)\,d\nu(s)\right)\\
&= \operatorname{Tr}\left(\int_S V_0\alpha_0(H_0,s)V_1\dots V_n\alpha_n(H_n,s)\,d\nu(s)\right)\\
&= \int_S \operatorname{Tr}\left(V_0\alpha_0(H_0,s)V_1\dots V_n\alpha_n(H_n,s)\right)d\nu(s)\\
&= \int_S \operatorname{Tr}\left(\alpha_0(H_0,s)V_1\dots V_n\alpha_n(H_n,s)V_0\right)d\nu(s).
\end{aligned}$$

For rank-one operators $\theta_{\zeta,\xi} := \langle \zeta, \cdot\rangle\, \xi$, we have the properties: $\operatorname{Tr}(\theta_{\zeta,\xi}) = \langle \zeta,\xi\rangle$, $A\theta_{\zeta,\xi} = \theta_{\zeta,A\xi}$ for any bounded operator $A$, and $\theta_{\zeta_1,\xi_1}\dots\theta_{\zeta_n,\xi_n} = \langle\zeta_1,\xi_2\rangle\dots\langle\zeta_{n-1},\xi_n\rangle\,\theta_{\zeta_n,\xi_1}$. Hence the above expression becomes

$$\int_S \langle F^*\varphi_1, \alpha_1(H_1,s)F^*\psi_2\rangle \dots \langle F^*\varphi_n, \alpha_n(H_n,s)w\rangle\, \langle v, \alpha_0(H_0,s)F^*\psi_1\rangle\, d\nu(s).$$

If $\mu^j_{f,g} := \langle f, E_j g\rangle$, where $E_j$ is the spectral measure of $H_j$, the same expression can be written as

$$\int_S \left(\int_{\mathbb{R}} \alpha_1(\lambda_1,s)\,d\mu^1_{F^*\varphi_1,F^*\psi_2}(\lambda_1)\right)\dots\left(\int_{\mathbb{R}} \alpha_0(\lambda_0,s)\,d\mu^0_{v,F^*\psi_1}(\lambda_0)\right)d\nu(s).$$

All of the measures appearing here have finite variation and Fubini's theorem implies

$$\begin{aligned}
E &= \int_{\mathbb{R}^{n+1}} \left(\int_S \alpha_0(\lambda_0,s)\dots\alpha_n(\lambda_n,s)\,d\nu(s)\right) d\mu^0_{v,F^*\psi_1}(\lambda_0)\dots d\mu^n_{F^*\varphi_n,w}(\lambda_n)\\
&= \int_{\mathbb{R}^{n+1}} f(\lambda_0,\dots,\lambda_n)\,d\mu^0_{v,F^*\psi_1}(\lambda_0)\dots d\mu^n_{F^*\varphi_n,w}(\lambda_n).
\end{aligned}$$

If $A$ and $B$ are bounded operators, then $A = B$ if and only if $\operatorname{Tr}(VA) = \operatorname{Tr}(VB)$ for all rank-one operators $V$. Using this fact, the above argument shows that the multiple operator integral (5.23) does not depend on the

BS representation (5.21) in the case that the operators $J_j$ are the rank-one operators $J_j = \langle \varphi_j, \cdot \rangle\, \psi_j$.

For the general case we consider the bounded self-adjoint operators $J_j$ as the strong-limits of the finite rank operators

$$J_{j,l} := \sum_{k=1}^{l} \langle \varphi_k, \cdot \rangle\, \psi_{j,k,l},$$

where $\{\varphi_k\}_{k\in\mathbb{N}}$ is an orthonormal basis consisting of vectors from the dense domain of the operator $F^*$ and $\{\psi_{j,k,l}\}_{l\in\mathbb{N}}$ is a sequence of vectors from $\operatorname{dom} F^*$ which converges to $J_j\varphi_k$. By linearity, it follows that the definition (5.23) does not depend on the representation (5.21) in the case that $J_j$ are the finite-rank operators $J_{j,l}$ for any $l \in \mathbb{N}$. Then the general case follows by a continuity argument. Specifically, since for any $g \in \mathcal{H}$,

$$\alpha_0(H_0, s)V_{1,l} \dots V_{n,l}\alpha_n(H_n, s)g \to \alpha_0(H_0, s)V_1 \dots V_n\alpha_n(H_n, s)g$$

as $l \to \infty$, an application of the dominated convergence theorem for the Bochner integral shows that the expression $T_f^{H_0,\dots,H_n}(V_1, \dots, V_n)g$ doesn't depend on the BS representation for any $g \in \mathcal{H}$, completing the proof. □

The focus will herein be on double operator integrals. A simple example of a DOI is a product such as

$$T_f^{H_0,H_1}(V) = \varphi(H_0)V\psi(H_1),$$

where $f(\lambda_0, \lambda_1) = \varphi(\lambda_0)\psi(\lambda_1)$, plus we require that $\varphi$ and $\psi$ have the same dominating function as (5.22). A familiar particular case is the operator $R_z(H_0)V R_z(H_1)$. Supposing $H_1 = H_0 \dot{+} V$, the following important equality generalises the second resolvent identity.

$$T_{\varphi^{[1]}}^{H_1,H_0}(V) = \varphi(H_1) - \varphi(H_0). \tag{5.26}$$

Here, the function of two variables $\varphi^{[1]}$ is the first divided difference of $\varphi$ defined by

$$\varphi^{[1]}(\lambda_0, \lambda_1) := \frac{\varphi(\lambda_0) - \varphi(\lambda_1)}{\lambda_0 - \lambda_1},$$

which if $\varphi$ is smooth is naturally interpreted on the diagonal as the derivative $\varphi^{[1]}(\lambda, \lambda) := \varphi'(\lambda)$. Higher divided differences are defined recursively by

$$\varphi^{[n]}(\lambda_0, \dots, \lambda_n) = \frac{\varphi^{[n-1]}(\lambda_0, \dots, \lambda_{n-1}) - \varphi^{[n-1]}(\lambda_1, \dots, \lambda_n)}{\lambda_0 - \lambda_n}.$$

Other than the resolvent $\varphi = R_z$, the equality (5.26) holds for many functions $\varphi$ which fall off at infinity, for example test functions (see Proposition 5.14). An excellent tool for proving this is the Helffer-Sjöstrand formula, since it expresses $\varphi(H)$ in terms of $R_z(H)$.

Considering first the scalar version (2.12) of the Helffer-Sjöstrand formula, for any $\varphi \in C_c^3(\mathbb{R})$ we obtain from it a BS representation of the first divided difference:

$$\varphi^{[1]}(\lambda_0, \lambda_1) = -\frac{1}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z)(\lambda_0 - z)^{-1}(\lambda_1 - z)^{-1}\, dxdy, \tag{5.27}$$

where $\tilde{\varphi}$ is an almost analytic extension of $\varphi$ and $z = x + iy$. That this is a BS representation of the form (5.21) is confirmed by taking the measure space $(S, \nu)$ to be the compact set $S = \operatorname{supp} \tilde{\varphi} \subset \mathbb{C}$ with the absolutely continuous measure $d\nu(z) = -\pi^{-1}\bar{\partial}\tilde{\psi}(z)\, dxdy$ and defining the functions $\alpha_j(\lambda_j, z) = (\lambda_j - z)^{-1}$, $j = 0, 1$.

Although we will not technically require $n$-tuple operator integrals for $n \geq 3$, it seems natural to consider them in the next few propositions, which also allows a slight shortening of the proofs of Theorem 5.17 and Lemma 5.20.

PROPOSITION 5.13. *For any $\varphi \in C_c^{n+2}(\mathbb{R})$, its $n$-th divided difference has the BS-representation*

$$\varphi^{[n]}(\lambda_0, \dots, \lambda_n) = \frac{(-1)^n}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z)(\lambda_0 - z)^{-1} \dots (\lambda_n - z)^{-1}\, dxdy,$$

*where $\tilde{\varphi}$ is an almost analytic extension of $\varphi$ and $z = x + iy$.*

PROOF. The case when $n = 1$ is of course (5.27). The BS-representations of higher divided differences are easily established by induction. Note that requiring the function $\varphi$ to belong to $C_c^{n+2}(\mathbb{R})$ ensures (by (2.15) and Lemma 2.15) that an almost analytic extension $\tilde{\varphi}$ satisfies $|\bar{\partial}\tilde{\varphi}(z)| = O(|y|^{n+1})$ as $y \to 0$, which counteracts the growth of $n + 1$ resolvents. □

Suppose $\varphi$ is as in Proposition 5.13. Then for any $n + 1$ self-adjoint operators $H_0, \dots, H_n$ from the affine space $\mathcal{A}$ and any $n$ perturbations $V_1, \dots, V_n$ from $\mathcal{A}_0$, we can write the $(n + 1)$-tuple operator integral

$$\begin{aligned} T_{\varphi^{[n]}}^{H_0,\dots,H_n}&(V_1, \dots, V_n) \\ &= \frac{(-1)^n}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\varphi}(z) R_z(H_0) V_1 R_z(H_1) \dots V_n R_z(H_n)\, dxdy. \end{aligned} \tag{5.28}$$

For a positive function $\varphi$ with square root $\psi = \sqrt{\varphi} \in C_c^3(\mathbb{R})$, the following alteration of (5.27) will be also prove useful later on.

$$\begin{aligned} \varphi^{[1]}(\lambda_0, \lambda_1) &= \psi^{[1]}(\lambda_0, \lambda_1)(\psi(\lambda_0) + \psi(\lambda_1)) \\ &= -\frac{1}{\pi} \int_{\mathbb{R}^2} \bar{\partial}\tilde{\psi}(z)(\lambda_0 - z)^{-1}(\psi(\lambda_0) + \psi(\lambda_1))(\lambda_1 - z)^{-1}\, dxdy. \end{aligned} \tag{5.29}$$

Note that the finite sum of BS representations can again be written as a BS representation in which the integral is taken over a disjoint union of measure spaces. For example (5.29) can be written in the form (5.21), by taking $(S, \nu)$ to be the disjoint union $S = (\operatorname{supp} \varphi, k)$, $k = 0, 1$, with in this case the same measure on each copy of $\operatorname{supp} \varphi$, namely $d\nu(z, k) = -\pi^{-1}\bar{\partial}\tilde{\psi}(z)\, dxdy$, and defining the functions $\alpha_j(\lambda_j, z, k) = (\lambda_j - z)^{-1}(\psi(\lambda_j))^{\delta_{j,k}}$.

PROPOSITION 5.14. *For any $\varphi \in C_c^3(\mathbb{R})$ and for any two self-adjoint operators $H_0$ and $H_1 = H_0 \dotplus V$ from the affine space $\mathcal{A}$, there holds the equality* (5.26)*. More generally, for any $\varphi \in C_c^{n+2}(\mathbb{R})$, any $n+1$ self-adjoint operators $H_0, H_1, \dots H_n \in \mathcal{A}$, and any $n+1$ perturbations $V_1, \dots, V_n$ and $V$ from $\mathcal{A}_0$, there is the equality*

$$(5.30)\quad T_{\varphi^{[n]}}^{H_0,\dots,H_k\dotplus V,\dots,H_n}(V_1,\dots,V_n) - T_{\varphi^{[n]}}^{H_0,\dots,H_k,\dots,H_n}(V_1,\dots,V_n) = T_{\varphi^{[n+1]}}^{H_0,\dots,H_k\dotplus V,H_k,\dots,H_n}(V_1,\dots,V_k,V,V_{k+1},\dots,V_n).$$

PROOF. The equality (5.26), which can be considered as (5.30) in the case that $n = 0$ by writing $\varphi^{[0]} := \varphi$ and $T_\varphi^{H_0} := \varphi(H_0)$, follows easily from the Helffer-Sjöstrand formula (2.11), the second resolvent identity, and the BS representation (5.27):

$$\begin{aligned}\varphi(H_1) - \varphi(H_0) &= \frac{1}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z)(R_z(H_1) - R_z(H_0))\,dxdy \\ &= -\frac{1}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z)R_z(H_1)VR_z(H_0)\,dxdy \\ &= T_{\varphi^{[1]}}^{H_1,H_0}(V).\end{aligned}$$

The general case is established in much the same way. Supposing $F$ is the rigging operator and using (5.28), the difference on the left hand side of (5.30) can be rewritten as

$$(E) := \frac{(-1)^n}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z)A(T_z(H_k\dotplus V) - T_z(H_k))B\,dxdy,$$

in which $A$ and $B$ are the bounded operators defined by

$$\begin{aligned}A &= (FR_{\bar z}(H_0))^* J_1 T_z(H_1)\dots T_z(H_{k-1})J_k, \\ B &= J_{k+1}T_z(H_{k+1})\dots J_n F R_z(H_n),\end{aligned}$$

where $V_j = F^*J_jF$, $j = 1,\dots,n$. With $V = F^*JF$, we now apply the second resolvent identity in the form

$$T_z(H_k\dotplus V) - T_z(H_k) = -T_z(H_k\dotplus V)JT_z(H_k)$$

(unless $k = n$ or $k = 0$, in which case we instead use (3.25) or its adjoint respectively), to obtain

$$\begin{aligned}(E) &= \frac{(-1)^{n+1}}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z)AT_z(H_k\dotplus V)JT_z(H_k)B\,dxdy \\ &= \frac{(-1)^{n+1}}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z)R_z(H_0)V_1\dots \\ &\qquad \dots V_kR_z(H_k\dotplus V)VR_z(H_k)V_{k+1}\dots V_nR_z(H_n)\,dxdy,\end{aligned}$$

which according to (5.28) is equal to the right hand side of (5.30). $\square$

LEMMA 5.15. *Let $H$ be an operator from the affine space $\mathcal{A}$ and let $w \in \mathbb{C} \setminus \mathbb{R}$. Then for any $z \in K \setminus \mathbb{R}$, where $K$ is a compact subset of $\mathbb{C}$, there exist positive constants which do not depend on $H$ so that the following estimates hold, in which $y = \operatorname{Im} z$.*

$$\|FR_z(H)\|_q \leq \text{const.}\, |y|^{-1} \|FR_w(H)\|_q, \tag{5.31}$$

$$\|T_z(H)\| \leq \|T_w(H)\| + \text{const.}\, |y|^{-1} \|FR_w(H)\|^2. \tag{5.32}$$

PROOF. Using the first resolvent identity (3.17) we have

$$FR_z(H) = FR_w(H)(1 + (z - w)R_z(H)).$$

Then the estimate $\|R_z(H)\| \leq |y|^{-1}$ gives

$$\begin{aligned} \|FR_z(H)\|_q &\leq \|1 + (z-w)R_z(H)\| \|FR_w(H_0)\|_q \\ &\leq \left(1 + \frac{|z-w|}{|y|}\right) \|FR_w(H_0)\|_q. \end{aligned}$$

Since $z$ belongs to the compact set $K$, there is a constant $C_1 > 0$ such that $|z - w| < C_1$. There is also a constant $C_2 > 0$ large enough so that $|y| + C_1 < C_2$. Then $1 + C_1/|y| < C_2/|y|$ and we obtain (5.31). The estimate (5.32) now easily follows from (5.31) and the equality 3.6. □

PROPOSITION 5.16. *For any $\varphi \in C_c^{n+2}(\mathbb{R})$, any $n+1$ self-adjoint operators $H_0, H_1, \ldots H_n \in \mathcal{A}$, and any $n$ perturbations $V_1, \ldots, V_n \in \mathcal{A}_0$, there is the estimate*

$$\begin{aligned} &\left\| T_{\varphi^{[n]}}^{H_0,\ldots,H_n}(V_1, \ldots, V_n) \right\|_p \\ &\qquad \leq \text{const.}\, \|FR_w(H_0)\|_q \|FR_w(H_n)\|_q \|V_1\|_F \ldots \|V_n\|_F \\ &\qquad\qquad \times \prod_{k=1}^{n-1} \left( \text{const.}\, \|T_w(H_k)\| + \|FR_w(H_k)\|^2 \right), \end{aligned}$$

*where $w$ is a fixed nonreal number and the unspecified constants depend only on $w$ and $\varphi$.*

PROOF. It follows from (5.28) that

$$\begin{aligned} &\left\| T_{\varphi^{[n]}}^{H_0,\ldots,H_n}(V_1, \ldots, V_n) \right\|_p \leq \\ &\frac{1}{\pi} \int_{\mathbb{R}^2} |\bar{\partial}\tilde{\varphi}(z)| \|FR_z(H_0)\|_q \left( \prod_{k=1}^{n-1} \|V_k\|_F \|T_z(H_k)\| \right) \|V_n\|_F \|FR_z(H_n)\|_q \, dxdy. \end{aligned}$$

Then the proof is completed by applying Lemma 5.15 and using the fact that $\bar{\partial}\tilde{\varphi}(z)$ is compactly supported and satisfies $|\bar{\partial}\tilde{\varphi}(z)| = O(|y|^{n+1})$. □

THEOREM 5.17. *For any $\varphi \in C_c^4(\mathbb{R})$ and for any self-adjoint operator $H_0$ from the affine space $\mathcal{A}$, the function*

$$\mathcal{A}_0 \ni V \mapsto \varphi(H_0 \dotplus V) - \varphi(H_0) \in \mathcal{L}_p(\mathcal{H})$$

*is continuously Fréchet differentiable. Its derivative at $V$ is the double operator integral $T^{H_1,H_1}_{\varphi^{[1]}}$ in which $H_1 := H_0 \dotplus V$.*

PROOF. For convenience we will calculate the derivative (and show it to be continuous) at 0, which is not restrictive if we allow a conflict of notation between the theorem's statement and proof. Using Proposition 5.14 we obtain the equalities

$$\begin{aligned}\varphi(H_1) - \varphi(H_0) &= T^{H_1,H_0}_{\varphi^{[1]}}(V)\\ &= T^{H_0,H_0}_{\varphi^{[1]}}(V) + T^{H_1,H_0}_{\varphi^{[1]}}(V) - T^{H_0,H_0}_{\varphi^{[1]}}(V)\\ &= T^{H_0,H_0}_{\varphi^{[1]}}(V) + T^{H_1,H_0,H_0}_{\varphi^{[2]}}(V,V).\end{aligned}$$

It is required to show that when the norm of $V$ is small, the $p$-norm of the last triple operator integral is negligible in comparison. Suppose $V = F^*JF$ in which case $\|V\|_F = \|J\|$. Proposition 5.16 with $n = 3$ implies the following estimate in which $w \in \mathbb{C} \setminus \mathbb{R}$ is fixed and the constant doesn't depend on $V$.

$$\begin{aligned}\left\|T^{H_0,H_0,H_1}_{\varphi^{[2]}}(V,V)\right\|_p &\le \text{const.}\,\|J\|^2\|FR_w(H_1)\|_q\\ &\le \text{const.}\,\|J\|^2\sum_{k=0}^{\infty}\|J\|^k,\end{aligned}$$

where the last inequality has an adjusted constant and holds if $\|J\|$ is small enough; in obtaining it we have used equality (4.5) and expressed the inverse $(1 + JT_w(H_0))^{-1}$ as a geometric series. Therefore, for small $\|V\|_F = \|J\|$ we conclude that

$$\left\|\varphi(H_1) - \varphi(H_0) - T^{H_0,H_0}_{\varphi^{[1]}}(V)\right\|_p = O(\|V\|_F^2).$$

The continuity of the derivative employs a similar kind of argument. With $H_0$ and $V$ as above, and for any other $W \in \mathcal{A}_0$, we get

$$\begin{aligned}&\left\|T^{H_1,H_1}_{\varphi^{[1]}}(W) - T^{H_0,H_0}_{\varphi^{[1]}}(W)\right\|_p\\ &\qquad\le \left\|T^{H_1,H_1}_{\varphi^{[1]}}(W) - T^{H_1,H_0}_{\varphi^{[1]}}(W)\right\|_p + \left\|T^{H_1,H_0}_{\varphi^{[1]}}(W) - T^{H_0,H_0}_{\varphi^{[1]}}(W)\right\|_p\\ &\qquad\le \left\|T^{H_1,H_1,H_0}_{\varphi^{[2]}}(W,V)\right\|_p + \left\|T^{H_1,H_0,H_0}_{\varphi^{[1]}}(V,W)\right\|_p\\ &\qquad\le \text{const.}\,\|W\|_F f(\|V\|_F),\end{aligned}$$

where the unspecified constant doesn't depend on $V$ or $W$ and the function $f$ on $\mathbb{R}$ is such that $f(\|V\|_F) = O(\|V\|_F)$ as $\|V\|_F \to 0$. Considering $T^{H_0,H_0}_{\varphi^{[1]}}$ as an operator from $\mathcal{A}_0$ to $\mathcal{L}_p(\mathcal{H})$ this implies that

$$\left\|T^{H_1,H_1}_{\varphi^{[1]}} - T^{H_0,H_0}_{\varphi^{[1]}}\right\| = O(\|V\|_F) \text{ as } \|V\|_f \to 0,$$

completing the proof. $\square$

LEMMA 5.18. *Let* $(S,\nu)$ *be a measure space and let* $\alpha\colon S\to\mathcal{B}(\mathcal{H})$ *be a Bochner integrable, bounded operator valued function. Suppose* $F\colon\mathcal{H}\to\mathcal{K}$ *is a closed operator such that* $F\alpha(s)\in\mathcal{B}(\mathcal{H},\mathcal{K})$ *for a.e.* $s\in S$ *and the bounded operator valued function* $F\alpha\colon S\to\mathcal{B}(\mathcal{H},\mathcal{K})$ *is also Bochner integrable. Then*

$$F\int_S \alpha(s)\,d\nu(s)=\int_S F\alpha(s)\,d\nu(s), \tag{5.33}$$

*as an equality of bounded operators.*

PROOF. If a bounded operator valued function such as $\alpha$ is Bochner integrable, then so is $\alpha f\colon s\mapsto\alpha(s)f$ for any $f\in\mathcal{H}$ as is easily checked. Hence for any $f\in\mathcal{H}$, the vector valued functions $\alpha f\colon S\to\mathcal{H}$ and $F\alpha f\colon S\to\mathcal{K}$ are Bochner integrable. Since $F\colon\mathcal{H}\to\mathcal{K}$ is closed, we can apply [HP57, Theorem 3.7.12] to obtain

$$F\int_S \alpha(s)f\,d\nu(s)=\int_S F\alpha(s)f\,d\nu(s). \tag{5.34}$$

In particular, for any $f\in\mathcal{H}$ the vector $\int_S\alpha(s)f\,d\nu(s)$ belongs to the domain of $F$. It follows that the range of the bounded operator $\int_S\alpha(s)\,d\nu(s)$ is contained in $\operatorname{dom}F$. The operator on the left hand side of (5.33) is thus a closed operator defined on all of $\mathcal{H}$, hence a bounded operator by the closed graph theorem. Therefore the equality (5.33) holds, since these operators act in the same way by (5.34). □

Lemma 5.18 allows the interchange the rigging operator and the integral of an MOI. Indeed, if $\alpha=$ (5.24) is the integrand of an MOI (5.23), then $F\alpha$ is also integrable by the argument of Lemma 5.11. Note that in the case that the affine space $\mathcal{A}$ is resolvent comparable, $F\alpha$ is integrable in $\mathcal{L}_2$ whereas $\alpha$ is integrable in $\mathcal{L}_1$. In fact it is not necessary to use Lemma 5.18 to justify this particular kind of interchange as shown by the next more specific lemma.

LEMMA 5.19. *The range of the MOI* $T_f^{H_0,\dots,H_n}(V_1,\dots,V_n)$ *belongs to the domain of the rigging operator* $F$ *and*

$$FT_f^{H_0,\dots,H_n}(V_1,\dots,V_n)=\int_S F\alpha_0(H_0,s)V_1\alpha_1(H_1,s)V_2\dots V_n\alpha_n(H_n,s)\,d\nu(s),$$

*where the integral on the right is taken in the topology of* $\mathcal{L}_q(\mathcal{H},\mathcal{K})$.

PROOF. Let the integrand of the MOI be denoted $\alpha=$ (5.24). Its representation $\alpha(s)=$ (5.25) can be written as $\alpha(s)=\psi(H_0)\beta(s)$, where $\psi(x)=(|x|+1)^{-1/2}$ and the function $\beta$ is integrable in $\mathcal{L}_q$ by the argument of Lemma 5.11. Therefore

$$\int_S\alpha(s)\,d\nu(s)=\psi(H_0)\int_S\beta(s)\,d\nu(s).$$

Since $\operatorname{ran}\psi(H_0)$ belongs to the domain of $F$ it follows that so does the range of the MOI. Then since $F\psi(H_0)$ is bounded,

$$F\int_S \alpha(s)\,d\nu(s) = F\psi(H_0)\int_S \beta(s)\,d\nu(s) = \int_S F\psi(H_0)\beta(s)\,d\nu(s),$$

which completes the proof. □

As a particular example which will be used later, let $H_0$ and $H_1$ be self-adjoint operators from a rigged affine space $\mathcal{A}(F)$, let $V = F^*JF \in \mathcal{A}_0(F)$, and let $\varphi \in C_c^3(\mathbb{R})$. Then we have

$$FT^{H_0,H_1}_{\varphi^{[1]}}(V) = -\frac{1}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde\varphi(z)T_z(H_0)JFR_z(H_1)\,dxdy. \tag{5.35}$$

Since it will also be used later, we consider the adjoint of (5.35):

$$\left(FT^{H_0,H_1}_{\varphi^{[1]}}(V)\right)^* = -\frac{1}{\pi}\int_{\mathbb{R}^2} \bar\partial\tilde{\bar\varphi}(z)(FR_{\bar z}(H_1))^*JT_z(H_0)\,dxdy. \tag{5.36}$$

The right hand side needs some justification. As can be seen from (2.16), we can choose almost analytic extensions $\tilde\varphi$, $\tilde{\bar\varphi}$, of $\varphi$ and its conjugate $\bar\varphi$ so that $\overline{\tilde\varphi(z)} = \tilde{\bar\varphi}(\bar z)$. In this way we have

$$\begin{aligned}\bar\partial\tilde{\bar\varphi}(\bar z) &= \frac{1}{2}\left(\partial_x\tilde{\bar\varphi}\right)(\bar z) + \frac{i}{2}\left(\partial_y\tilde{\bar\varphi}\right)(\bar z)\\ &= \frac{1}{2}\partial_x\left(\overline{\tilde\varphi(z)}\right) - \frac{i}{2}\partial_y\left(\overline{\tilde\varphi(z)}\right)\\ &= \overline{\bar\partial\tilde\varphi(z)}.\end{aligned}$$

Therefore, (5.36) can be obtained from (5.35) by interchanging the adjoint and integral and making the change of variables $z \leftrightarrow \bar z$.

Lemma 5.20. *Let $H_0$ be any self-adjoint operator from the rigged affine space $\mathcal{A}(F)$. For any $\varphi \in C_c^4(\mathbb{R})$, the function*

$$\mathcal{A}_0 \ni V \mapsto F\varphi(H_0 \dot{+} V) - F\varphi(H_0) \in \mathcal{L}_q(\mathcal{H},\mathcal{K})$$

*is continuously Fréchet differentiable and with $H_1 := H_0 \dot{+} V$ its derivative at $V$ is equal to $FT^{H_1,H_1}_{\varphi^{[1]}}$.*

Proof. The proof follows similar lines to that of Theorem 5.17 and some details are omitted. From Lemma 5.19 and Proposition 5.14 it follows that

$$\begin{aligned}(E) &:= \left\|F\varphi(H_1) - F\varphi(H_0) - FT^{H_0,H_0}_{\varphi^{[1]}}(V)\right\|_q\\ &= \left\|FT^{H_1,H_0}_{\varphi^{[1]}}(V) - FT^{H_0,H_0}_{\varphi^{[1]}}(V)\right\|_q\\ &= \left\|FT^{H_1,H_0,H_0}_{\varphi^{[2]}}(V,V)\right\|_q\\ &\le \frac{1}{\pi}\int_{\mathbb{R}^2} |\bar\partial\tilde\varphi(z)|\|T_z(H_1)\|\|V\|_F\|T_z(H_0)\|\|V\|_F\|FR_z(H_0)\|_q\,dxdy.\end{aligned}$$

Using Lemma 5.15 in an obvious modification of Proposition 5.16 then shows that $(E) \leq \text{const.}\,\|V\|_F^2$.

The continuity of the derivative is proved by making the appropriate changes to the corresponding argument in the proof Theorem 5.17. □

## 5.4. Spectral averaging and the SSF

This section closely mimics the paper [AS08]. The infinitesimal spectral shift measure is defined and proved to be exact, and then the SSF is defined and proved to be absolutely continuous. The proofs of Theorem 5.23 and Proposition 5.24 have undergone some adjustment due to the different setting, but those of Corollaries 5.25 and 5.26 and Proposition 5.27 are virtually unchanged. Throughout the remainder of this chapter, $\mathcal{A}(F)$ will denote a resolvent comparable rigged affine space.

For any $H \in \mathcal{A}$, $V \in \mathcal{A}_0$, and Borel functions $\varphi$, $\psi$ satisfying the estimate $|\varphi(x)|, |\psi(x)| \leq \text{const.}(|x|+1)^{-1}$, the inclusion

$$\varphi(H)V\psi(H) \in \mathcal{L}_1(\mathcal{H}) \tag{5.37}$$

holds by the resolvent comparability of $\mathcal{A}$.

PROPOSITION 5.21. *For any test functions $\varphi$ and $\psi$ and any self-adjoint operator $H$ from the affine space $\mathcal{A}$, the map*

$$(V_1, V_2, V_3) \mapsto \varphi(H \dotplus V_1)V_2\psi(H \dotplus V_3) \in \mathcal{L}_1(\mathcal{H})$$

*is continuously Fréchet differentiable.*

PROOF. By Lemma 5.20, both $(F\bar{\varphi}(H \dotplus V_1))^*$ and $F1_\psi(H \dotplus V_3)$ are smooth in the Hilbert-Schmidt norm. And obviously $\mathcal{A}_0 \ni V_2 = F^*J_2F \mapsto J_2 \in \mathcal{B}(\mathcal{K})$ is smooth. Therefore,

$$\varphi(H \dotplus V_1)V_2\psi(H \dotplus V_3) = (F\bar{\varphi}(H \dotplus V_1))^*J_2F\psi(H \dotplus V_3)$$

is smooth in the trace class norm. □

Consider the trace of the operator (5.37) in the case that $\varphi$ is a test function and $\psi$ is equal to 1 on the support of $\varphi$. By the cyclic property of the trace, it is equal to $\mathrm{Tr}(V\varphi(H))$ if $V$ is trace class (i.e. the rigging operator $F$ is Hilbert Schmidt). Whether or not $V$ is trace class, it is unaffected by the values of $\psi$ outside of the support of $\varphi$ and offers a natural interpretation of the expression $\mathrm{Tr}(V\varphi(H))$ in the setting of a resolvent comparable rigged affine space. Supposing $V = F^*JF$, it is also equal to

$$\mathrm{Tr}(\varphi(H)V\psi(H)) = \mathrm{Tr}\left((F\bar{\varphi}(H)))^*JF\psi(H)\right) = \mathrm{Tr}\left(JF\psi(H)(F\bar{\varphi}(H)))^*\right).$$

Note that the operator appearing alongside $J$ on the far right is the closure of the operator $F(\varphi{\cdot}\psi)(H)F^* = F\varphi(H)F^*$

The *infinitesimal spectral shift measure* is defined by the formula (which is another way to write the trace discussed above)

$$\Phi_H(V)(\varphi) := \mathrm{Tr}\left(E(\operatorname{supp}\varphi)V\varphi(H)\right), \quad \varphi \in C_c(\mathbb{R}), \tag{5.38}$$

for $H \in \mathcal{H}$ with spectral measure $E$, and $V \in \mathcal{A}_0$.

The notation $\Phi_H(V)(\varphi)$ is intended to suggest a generalised 1-form on the affine space $\mathcal{A}$. Indeed, for any test function $\varphi$, $\Phi(\varphi)$ is a 1-form on $\mathcal{A}$, while for any point $H \in \mathcal{A}$ and direction $V \in \mathcal{A}_0$, $\Phi_H(V)$ is a generalised function, in particular a real measure. No deep theory of such objects is required.

The fact that $\Phi(\varphi)$ is indeed a 1-form on the affine space $\mathcal{A}$ for any $\varphi \in C_c^\infty(\mathbb{R})$ is not difficult to check. Its linearity is obvious and its smoothness ($C^1$ is enough here) follows from Proposition 5.21.

Before proving the exactness of the infinitesimal spectral shift measure as a 1-form, let's consider its most basic properties as a measure, beginning with the fact that $\Phi_H(V)$ for fixed $H$ and $V$ is indeed a measure. If $(\varphi_n) \subset C_c(\mathbb{R})$ is a sequence of functions supported in a compact interval $K$ such that $\|\varphi_n\|_\infty \to 0$, i.e. $\varphi_n \to 0$ in the inductive limit topology of $C_c(\mathbb{R})$, then

$$|\Phi_H(V)(\varphi_n)| \leq \|1_K(H)V1_K(H)\|_1 \, \|\varphi_n\|_\infty \to 0, \tag{5.39}$$

where $1_K \in C_c(\mathbb{R})$ is equal to 1 on $K$. This implies that $\Phi_H(V)$ is a continuous linear functional on $C_c(\mathbb{R})$, hence a (possibly unbounded) measure. It is real valued, since for real valued $\varphi = \varphi_+ - \varphi_-$, it is the difference of the traces of self-adjoint operators

$$\mathrm{Tr}(1_\varphi(H)V\varphi(H)) = \mathrm{Tr}\left(\sqrt{\varphi_+}(H)V\sqrt{\varphi_+}(H)\right) - \mathrm{Tr}\left(\sqrt{\varphi_-}(H)V\sqrt{\varphi_-}(H)\right).$$

From this we also see that $\Phi_H(V)$ is positive if $V$ is.

To prove the exactness of the infinitesimal spectral shift measure, we will use the following

LEMMA 5.22. *Let $V$ and $W$ be directions in $\mathcal{A}_0$ and put $H_r = H_0 \dotplus rW$. Then for any test function $\varphi$, there holds the equality*

$$\frac{d}{ds}\Phi_{H_r \dotplus rsV}(W)(\varphi)\Big|_{s=0} = r\frac{d}{dr}\Phi_{H_r}(V)(\varphi). \tag{5.40}$$

PROOF. Suppose that $F$ is the rigging operator, $V = F^*JF$, and $W = F^*KF$. Let $1_\varphi$ be a test function equal to 1 on $\operatorname{supp}\varphi$. Then the left hand side of (5.40) can be written as

$$(E) := \frac{d}{ds}\,\mathrm{Tr}\left((F1_\varphi(H_r \dotplus rsV))^* KF\varphi(H_r \dotplus rsV)\right)\Big|_{s=0}.$$

It follows from Lemma 5.20 that the operator valued function of $s$ within the trace is $\mathcal{L}_1$-differentiable. We get,

$$\begin{aligned}(E) &= \mathrm{Tr}\left(\frac{d}{ds}(F1_\varphi(H_r \dotplus rsV))^*\Big|_{s=0} KF\varphi(H_r)\right) \\ &\qquad\qquad + \mathrm{Tr}\left((F1_\varphi(H_r))^* K\frac{d}{ds}F\varphi(H_r \dotplus rsV)\Big|_{s=0}\right) \\ &=: (I) + (II).\end{aligned}$$

Consider the first term $(I)$ on the right. Using Lemma 5.20 and the equality (5.36), it is equal to

$$\begin{aligned}(I) &= \operatorname{Tr}\left(\left(FT^{H_r,H_r}_{1_\varphi^{[1]}}(V)\right)^* KF\varphi(H_r)\right)\\ &= \operatorname{Tr}\left(\left(-\frac{r}{\pi}\int_{\mathbb{R}^2}\bar\partial\tilde{1}_\varphi(z)(FR_{\bar z}(H_r))^* JT_z(H_r)\,dxdy\right) KF\varphi(H_r)\right).\end{aligned}$$

By bringing the bounded operator $KF\varphi(H_r)$ within the integral, the integrand becomes $\mathcal{L}_1$-valued and moreover the trace and integral can then be interchanged. The result is

$$\begin{aligned}(I) &= -\frac{r}{\pi}\int_{\mathbb{R}^2}\bar\partial\tilde{1}_\varphi(z)\operatorname{Tr}\left((FR_{\bar z}(H_r))^* JT_z(H_r)KF\varphi(H_r)\right)dxdy\\ &= -\frac{r}{\pi}\int_{\mathbb{R}^2}\bar\partial\tilde{1}_\varphi(z)\operatorname{Tr}\left((F\bar\varphi(H_r))^* JT_z(H_r)KFR_z(H_r)\right)dxdy,\end{aligned}$$

where the second line follows from the cyclic property of the trace and the equality $F\varphi(H_r)(FR_{\bar z}(H_r))^* = FR_z(H_r)(F\bar\varphi(H_r))^*$. Now again interchanging the trace and integral and unwinding through the previous steps,

$$\begin{aligned}(I) &= r\operatorname{Tr}\left((F\bar\varphi(H_r))^* J\left(-\frac{1}{\pi}\int_{\mathbb{R}^2}\bar\partial\tilde{1}_\varphi(z)T_z(H_r)KFR_z(H_r)\,dxdy\right)\right)\\ &= r\operatorname{Tr}\left((F\bar\varphi(H_r))^* J\left(\frac{d}{dr}F1_\varphi(H_r)\right)\right).\end{aligned}$$

Similarly, it can be shown that

$$(II) = r\operatorname{Tr}\left(\left(\frac{d}{dr}(F\bar\varphi(H_r))^*\right) JF1_\varphi(H_r)\right),$$

so by combining these expressions for $(I)$ and $(II)$, we see that

$$\begin{aligned}(E) &= r\operatorname{Tr}\left(\frac{d}{dr}(F\bar\varphi(H_r))^* JF1_\varphi(H_r)\right)\\ &= r\frac{d}{dr}\operatorname{Tr}(1_\varphi(H_r)V\varphi(H_r)),\end{aligned}$$

which is the right hand side of (5.40). □

THEOREM 5.23. *The 1-form $\Phi(\varphi)$ is exact for any test function $\varphi$.*

PROOF. For any $H \in \mathcal{A}$ and test function $\varphi$, we let $\theta_H^\varphi$ denote the integral of $\Phi(\varphi)$ along the line from some fixed $H_0$ to $H$, with the aim to show $d\theta_H^\varphi(V) = \Phi_H(V)(\varphi)$. That is, let $H_r = H_0 \dotplus rW$ where $H_1 = H$ and put

$$\theta_H^\varphi = \int_0^1 \Phi_{H_r}(W)\,dr.$$

The derivative of this 0-form is by definition

$$\begin{aligned}
d\theta_H^\varphi(V) &= \frac{d}{ds}\theta_{H+sV}^\varphi\Big|_{s=0} \\
&= \lim_{s\to 0}\int_0^1 \frac{1}{s}\big(\Phi_{H_r\dot+ rsV}(W+sV)(\varphi) - \Phi_{H_r}(W)(\varphi)\big)\,dr \\
&= \lim_{s\to 0}\int_0^1 \bigg(\Phi_{H_r\dot+ rsV}(V)(\varphi) + \frac{1}{s}\big(\Phi_{H_r\dot+ rsV}(W)(\varphi) - \Phi_{H_r}(W)(\varphi)\big)\bigg)dr.
\end{aligned}$$

By the smoothness of $H \mapsto \Phi_H(V)(\varphi)$ (Proposition 5.21) and Lemma 5.22, upon interchanging the limit and integral we get

$$\begin{aligned}
d\theta_H^\varphi(V) &= \int_0^1 \Phi_{H_r}(V)(\varphi)\,dr + \int_0^1 \frac{d}{ds}\Phi_{H_r\dot+ rsV}(W)(\varphi)\Big|_{s=0}\,dr \\
&= \int_0^1 \Phi_{H_r}(V)(\varphi)\,dr + \int_0^1 r\frac{d}{dr}\Phi_{H_r}(V)(\varphi)\,dr.
\end{aligned}$$

Integrating the last term by parts gives the result. □

The *spectral shift measure* $\xi(\varphi) = \xi(\varphi; H_1, H_0)$ is defined, in keeping with the Birman-Solomyak formula, as the integral of $\Phi(\varphi)$ along a piecewise $C^1$ path $H_r$ from $H_0$ to $H_1$ in $\mathcal{A}$. That is,

$$\begin{aligned}
\xi(\varphi; H_1, H_0) &:= \int_{H_r} \Phi(\varphi) \\
&= \int_0^1 \operatorname{Tr}\Big(E_r(\operatorname{supp}\varphi)\dot H_r \varphi(H_r)\Big)\,dr,
\end{aligned} \tag{5.41}$$

where here and below, $E_r$ denotes the spectral measure of $H_r$ and $\dot H_r$ denotes its derivative. Theorem 5.23 implies that this definition does not depend on the piecewise $C^1$ path $H_r$.

Some basic properties of the spectral shift measure: First it is clearly additive in the sense that $\xi(H_2, H_0) = \xi(H_2, H_1) + \xi(H_1, H_0)$. To check that $\xi(\varphi)$ is a (possibly unbounded) measure, the same argument as for the infinitesimal spectral shift measure applies, except this time we use the fact that the convergence (5.39) is locally uniform on the affine space $\mathcal{A}$, which follows from Proposition 5.21. Also by the same reasoning as for the infinitesimal spectral shift measure, it is a real measure, which is positive if $H_1 = H_0 \dot+ V$ with $V \geq 0$.

The *spectral shift function (SSF)* is defined to be the locally integrable density of the spectral shift measure. It is shown below (Proposition 5.27) that the spectral shift measure is absolutely continuous and hence can be identified with the SSF.

We need the following version of the chain rule (cf. [BS75; Sim98]).

PROPOSITION 5.24. *Let $H_r$ be a $C^1$ path in $\mathcal{A}$ and let $\varphi$ be a test function. Then, for the path $r \mapsto \varphi(H_r)$, the chain rule holds under the trace in the* *following sense. For any bounded Borel function $f$,*

$$\operatorname{Tr}\left(\frac{d\varphi(H_r)}{dr} f(H_r)\right) = \operatorname{Tr}\left(E_r(\operatorname{supp}\varphi)\dot{H}_r\varphi'(H_r)f(H_r)\right). \tag{5.42}$$

PROOF. By choosing a positive test function $\varphi_1$ which dominates $\varphi$ and is such that $\sqrt{\varphi_1}$ is smooth, $\varphi = \varphi_1 - (\varphi_1 - \varphi)$ is the difference of positive test functions with smooth square roots. It follows that we may assume without loss of generality that $\varphi \geq 0$ such that $\psi := \sqrt{\varphi} \in C_c^\infty(\mathbb{R})$. In this case by making use of the BS representation (5.29), Theorem 5.17 implies

$$\begin{aligned}\frac{d\varphi(H_r)}{dr} &= T^{H_r,H_r}_{\varphi^{[1]}}(\dot{H}_r)\\ &= -\frac{1}{\pi}\int_{\mathbb{R}^2} \bar{\partial}\tilde{\psi}(z)R_z(H_r)\psi(H_r)\dot{H}_r R_z(H_r)\,dxdy\\ &\qquad\qquad - \frac{1}{\pi}\int_{\mathbb{R}^2}\bar{\partial}\tilde{\psi}(z)R_z(H_r)\dot{H}_r\psi(H_r)R_z(H_r)\,dxdy.\end{aligned}$$

Therefore after substituting this into the left hand side of (5.42) and then interchanging the integral and trace, we obtain

$$(E) := \operatorname{Tr}\left(\frac{d\varphi(H_r)}{dr}f(H_r)\right) = -\frac{1}{\pi}\int_{\mathbb{R}^2}\bar{\partial}\tilde{\psi}(z)\operatorname{Tr}(\dots)\,dxdy,$$

where the trace in the integrand on the right is equal to

$$\begin{aligned}\operatorname{Tr}(\dots) &= \operatorname{Tr}\left(R_z(H_r)\psi(H_r)\dot{H}_r R_z(H_r)f(H_r)\right)\\ &\qquad + \operatorname{Tr}\left(R_z(H_r)\dot{H}_r\psi(H_r)R_z(H_r)f(H_r)\right)\\ &= 2\operatorname{Tr}\left(\psi(H_r)\dot{H}_r R_z^2(H_r)f(H_r)\right).\end{aligned}$$

Supposing $F$ is the rigging operator and $\dot{H}_r = F^*\dot{J}_r F$, it follows that

$$\begin{aligned}(E) &= -\frac{2}{\pi}\int_{\mathbb{R}^2}\bar{\partial}\tilde{\psi}(z)\operatorname{Tr}\left(\left(F\bar{\psi}(H_r)\right)^*\dot{J}_r F R_z^2(H_r)f(H_r)\right)dxdy\\ &= 2\operatorname{Tr}\left(\left(F\bar{\psi}(H_r)\right)^*\dot{J}_r\left(-\frac{1}{\pi}\int_{\mathbb{R}^2}\bar{\partial}\tilde{\psi}(z)FR_z^2(H_r)\,dxdy\right)f(H_r)\right).\end{aligned}$$

Consider the integral now isolated in brackets. Lemma 5.18 and the equality (2.17) imply that it is equal to the operator $F\psi'(H_r)$. Therefore

$$\begin{aligned}(E) &= 2\operatorname{Tr}\left(\left(F\bar{\psi}(H_r)\right)^*\dot{J}_r F\psi'(H_r)f(H_r)\right)\\ &= 2\operatorname{Tr}\left(\psi(H_r)\dot{H}_r\psi'(H_r)f(H_r)\right).\end{aligned}$$

By cycling under the trace and using the fact that $2\psi'\psi = \varphi'$, this can be written as the right hand side of (5.42). □

Proposition 5.24 has two important corollaries below, namely the trace formula and the invariance principle.

COROLLARY 5.25. *The spectral shift measure satisfies the trace formula*

$$\operatorname{Tr}(\varphi(H_1) - \varphi(H_0)) = \xi(\varphi'; H_1, H_0), \tag{5.43}$$

*for any $H_0, H_1 \in \mathcal{A}$ and test function $\varphi$.*

PROOF. Integrating (5.42) with $f = 1$ results in the equality

$$\int_0^1 \operatorname{Tr}\left(\frac{d(\varphi(H_r) - \varphi(H_0))}{dr}\right) dr = \xi(\varphi'; H_1, H_0)$$

and (5.43) follows by interchanging the trace and derivative, which is justified by Theorem 5.17. □

Combining (5.43) with Kreĭn's classical result (Theorem 5.1) implies that in the case of trace class perturbations, the spectral shift measure is absolutely continuous and its density coincides with the SSF as defined by the trace formula.

COROLLARY 5.26. *Let $H_0, H_1 \in \mathcal{A}$, let $\varphi$ be a real-valued test function, and let $\xi$ and $\xi_\varphi$ be the spectral shift measures of the pairs $H_1, H_0$ and $\varphi(H_1), \varphi(H_0)$ respectively. Then for any bounded Borel function $f$,*

$$\xi_\varphi(f) = \xi(f \circ \varphi \cdot \varphi'). \tag{5.44}$$

PROOF. Integrating (5.42) with $f = f \circ \varphi$ gives

$$\int_0^1 \operatorname{Tr}\left(\frac{d\varphi(H_r)}{dr} f(\varphi(H_r))\right) dr = \xi(f \circ \varphi \cdot \varphi').$$

The left hand side is equal to $\xi_\varphi(f)$ by the path independence of the spectral shift measure (Theorem 5.23). □

PROPOSITION 5.27. *On a resolvent comparable rigged affine space, the spectral shift measure defined by* (5.41) *is absolutely continuous.*

PROOF. This neat proof essentially consists in the reduction to the case of a trace class perturbation using the invariance principle (5.44).

Let $\mu$ be the singular part of the spectral shift measure. We will show that $\mu$ is translation invariant. It therefore must be a multiple of Lebesgue measure, leaving $\mu = 0$ as the only possibility.

Fix $0 < \varepsilon << 1$ and let $E$ be a Borel subset of $[\varepsilon, 1-\varepsilon]$ with zero Lebesgue measure. To demonstrate translation invariance it is enough to show that $\mu(E) = \mu(a + E)$ for any real $a$. For any $a, b \in \mathbb{R}$ with $b - a > 2$, consider a test function $\varphi_{a,b}$ whose graph looks like a smoothed isosceles trapezium with height 1 which is stretched over the interval $[a, b]$ and has slopes of the sides equal to $\pm 1$. More precisely $\varphi_{a,b}$ is subject to the constraints: $\varphi_{a,b}(\lambda) = \lambda - a$ on $[a+\varepsilon, a+1-\varepsilon]$, $\varphi_{a,b}(\lambda) = b - \lambda$ on $[b-1+\varepsilon, b-\varepsilon]$, and except as already specified $\varphi_{a,b}$ does not take values in $[\varepsilon, 1-\varepsilon]$. Let $1_A$ denote the indicator of a Borel set $A$. By construction, $1_E \circ \varphi_{a,b} \cdot \varphi'_{a,b} = 1_{a+E} - 1_{b-E}$. Then by Corollary 5.26,

$$\xi_{\varphi_{a,b}}(E) = \xi(a + E) - \xi(b - E) = \mu(a + E) - \mu(b - E).$$

The left hand side is zero, since $\xi_{\varphi_{a,b}}$ is absolutely continuous by Kreĭn's result for trace class perturbations. Hence choosing $b$ such that $b > 2$ and $b - a > 2$, we conclude that $\mu(E) = \mu(b - E) = \mu(a + E)$. □

## 5.5. The absolutely continuous and singular SSF's

This section concerns the Lebesgue decomposition of the infinitesimal spectral shift measure $\Phi$ and its implications for the SSF. Recall that we are assuming $\mathcal{A}$ to be a resolvent comparable rigged affine space. For $H \in \mathcal{A}$ and $V \in \mathcal{A}_0$, the absolutely continuous and singular parts are respectively given by replacing $(\cdot)$ with $(a)$ and $(s)$ in the formula

$$\Phi_H^{(\cdot)}(V)(\varphi) = \operatorname{Tr}\left(E^{(\cdot)}(\operatorname{supp}\varphi)V\varphi(H)\right), \quad \varphi \in C_c(\mathbb{R}), \tag{5.45}$$

where $E^{(\cdot)}$ denotes the absolutely continuous or singular spectral measure of the self-adjoint operator $H$.

Confirming these formulas (5.45) is easy given the properties of $E^{(\cdot)}$. A null support $Z_s$ of $\sigma_s(H)$ is a support of $\Phi^{(s)}$, since for any bounded Borel set $\Delta$ which does not intersect $Z_s$ we have

$$\Phi_H^{(s)}(V)(\Delta) = \operatorname{Tr}\left(E^{(s)}(\Delta)VE(\Delta)\right) = 0.$$

Therefore $\Phi^{(s)}$ is singular. On the other hand $\Phi^{(a)}$ is absolutely continuous, since if $Z$ is any bounded null set then

$$\Phi_H^{(a)}(V)(\Delta) = \operatorname{Tr}\left(E^{(a)}(Z)VE(Z)\right) = 0.$$

The absolutely continuous and singular parts of the infinitesimal spectral shift measure are again 1-forms on $\mathcal{A}$, but they may no longer be smooth. Moreover, they may no longer be exact. A counterexample to the exactness of the singular part is given in [Aza11a, §8.3] and will be reviewed in the next section. However, their integrals along any piecewise $C^1$ path in the affine space $\mathcal{A}$ define absolutely continuous measures, which result in a natural decomposition of the SSF. To show this is the aim of the present section.

Proposition 5.28. *The Poisson kernel is integrable with respect to both the infinitesimal spectral shift measure and the spectral shift measure itself. Their Poisson integrals are respectively given by*

$$\Phi_H(V)(z) := \frac{y}{\pi}\operatorname{Tr}(R_z(H)VR_{\bar{z}}(H)), \tag{5.46}$$

$$\xi(z; H_1, H_0) := \frac{y}{\pi}\int_0^1 \operatorname{Tr}\left(R_z(H_r)\dot{H}_r R_{\bar{z}}(H_r)\right)\, dr, \tag{5.47}$$

*where $y = \operatorname{Im} z$ and $H_r$ is any piecewise $C^1$ path in $\mathcal{A}$ from $H_0$ to $H_1$.*

The Poisson integral of the spectral shift measure will be called the *smoothed SSF.*

Proof. Since $V \mapsto \Phi_H(V)$ is linear, we can assume without loss of generality that $V$ is positive so that $\Phi_H(V)$ is a positive measure. Let $1_n$ denote the indicator function for the interval $[-n, n]$. Then the monotone convergence theorem implies that, whether or not the limit is finite,

$$\begin{aligned}\Phi_H(V)(\operatorname{Im} R_z) &= \lim_{n\to\infty} \Phi_H(V)(1_n \cdot \operatorname{Im} R_z) \\ &= y \lim_{n\to\infty} \operatorname{Tr}\left(1_n(H) R_z(H) V R_{\bar z}(H) 1_n(H)\right),\end{aligned}$$

where in the second line we have used the definition (5.38) and the equality $\operatorname{Im} R_z = y R_z R_{\bar z}$. Lemma 2.19 implies the $\mathcal{L}_1$-convergence

$$1_n(H) R_z(H) V R_{\bar z}(H) 1_n(H) \to R_z(H) V R_{\bar z}(H) \tag{5.48}$$

and it follows that $\operatorname{Im} R_z$ is integrable and (5.46) is the Poisson integral of $\Phi$.

We use a similar argument to establish the fact that 5.47 is the Poisson integral of the spectral shift measure $\xi$.

$$\begin{aligned}\xi(\operatorname{Im} R_z; H_1, H_0) &= \lim_{n\to\infty} \xi(1_n \cdot \operatorname{Im} R_z; H_1, H_0) \\ &= y \lim_{n\to\infty} \int_0^1 \operatorname{Tr}\left(1_n(H_r) R_z(H_r) \dot H_r R_{\bar z}(H_r) 1_n(H_r)\right)\end{aligned}$$

and in this case the result follows by an application of the dominated convergence theorem, which is justified by Proposition 5.21. □

Corollary 5.29. *For any self-adjoint operator $H \in \mathcal{A}$ and perturbation $V \in \mathcal{A}_0$, the density of the absolutely continuous part of the infinitesimal spectral shift measure is for a.e. $\lambda \in \mathbb{R}$ equal to*

$$\Phi_H^{(a)}(V)(\lambda) = \frac{1}{\pi} \lim_{y\to 0^+} y \operatorname{Tr}(R_{\bar z}(H) V R_z(H)). \tag{5.49}$$

*Moreover, if $H_0$ and $H_1$ are two self-adjoint operators from $\mathcal{A}$, then the SSF $\xi(\lambda; H_1, H_0)$ belongs to $L_1(\mathbb{R}, (1+\lambda^2)^{-1}\, d\lambda)$ and for a.e. $\lambda \in \mathbb{R}$ satisfies*

$$\xi(\lambda; H_1, H_0) = \lim_{y\to 0^+} \xi(\lambda + iy; H_1, H_0). \tag{5.50}$$

Proof. This is a direct consequence of Theorem 2.4 □

Consider the function (5.49). Suppose $F$ is the rigging operator, $V = F^* J F$, and put $z = \lambda + iy$. Then there exists the limit

$$\begin{aligned}\lim_{y\to 0^+} \frac{1}{\pi} \Phi_H(V)(\operatorname{Im} R_z) &= \lim_{y\to 0^+} \frac{y}{\pi} \operatorname{Tr}(R_z(H) V R_{\bar z}(H)) \\ &= \lim_{y\to 0^+} \frac{1}{\pi} \operatorname{Tr}(J \operatorname{Im} T_z(H)) \\ &= \frac{1}{\pi} \operatorname{Tr}(J \operatorname{Im} T_{\lambda+i0}(H)),\end{aligned}$$

at every point $\lambda$ from the set of trace-regular points $\Lambda(H, F; \mathcal{L}_1)$, which is a full set by Corollary 3.15. Hence the density of the infinitesimal spectral shift measure is for a.e. $\lambda$ equal to

$$\Phi_H^{(a)}(V)(\lambda) = \frac{1}{\pi} \operatorname{Tr}(J \operatorname{Im} T_{\lambda+i0}(H)). \tag{5.51}$$

LEMMA 5.30. *Let $H_r$, $r \in \mathbb{R}$, be a piecewise analytic path in the resolvent comparable affine space $\mathcal{A}(F)$. Then the set of points $(\lambda, r)$ in the plane for which $\lambda$ is a trace-regular point of $H_r$,*

$$\Gamma(\{H_r\}, F) := \{(\lambda, r) \in \mathbb{R}^2 : \lambda \in \Lambda(H_r, F; \mathcal{L}_1)\},$$

*has full measure in $\mathbb{R}^2$. Moreover a.e. cross section of $\Gamma$ in either the $r$ or $\lambda$ direction has full measure in $\mathbb{R}$. In addition, the function defined on $\Gamma$ by*

$$(\lambda, r) \mapsto \operatorname{Tr}\left(\dot{J}_r \operatorname{Im} T_{\lambda+i0}(H_r)\right), \tag{5.52}$$

*where $\dot{H}_r = F^* \dot{J}_r F$, is locally integrable.*

PROOF. We note that the set $\Gamma$ is measurable as the set of convergence points as $y \to 0^+$ of the two families of continuous functions $T_{\lambda+iy}(H_r)$ and $\operatorname{Im} T_{\lambda+iy}(H_r)$ of the variables $(\lambda, r)$. Further, the function (5.52) is measurable as a limit of measurable functions.

Clearly at any $r \in \mathbb{R}$ the $\lambda$-cross section of $\Gamma$ is the full set $\Lambda(H_r, F; \mathcal{L}_1)$ of trace-regular points of $H_r$. On the other hand since the path $H_r$ is piecewise analytic, at any point $\lambda$ from the full set $\bigcap_j \Lambda(\{H_{r_j}\}, F; \mathcal{L}_1)$, where the intersection is taken over the pieces $H_{r_j}$ of the path $H_r$, the $r$-cross section of $\Gamma$ is equal to the complement of the discrete set of resonance points $\bigcup_j R(\lambda; \{H_{r_j}\})$. The Lebesgue measure of the complement $\mathbb{R}^2 \setminus \Gamma$ can be calculated using Fubini's theorem and must be zero since its cross sections are null sets.

We will now check that (5.52) is integrable over a bounded rectangle, for which it suffices to show that as a function of $\lambda$ on a bounded interval $\Delta$ its $L_1$-norm is locally bounded with respect to $r$.

$$\begin{aligned} \frac{1}{\pi} \int_\Delta \left| \operatorname{Tr}\left(\dot{J}_r \operatorname{Im} T_{\lambda+i0}(H_r)\right) \right| d\lambda &\le \frac{1}{\pi} \int_\Delta \left\| \dot{J}_r \right\| \operatorname{Tr}\left(\operatorname{Im} T_{\lambda+i0}(H_r)\right) d\lambda \\ &= \left\| \dot{J}_r \right\| \Phi_{H_r}^{(a)}(F^* F)(\Delta) \\ &\le \left\| \dot{J}_r \right\| \left\| F 1_\Delta(H_r) \right\|_2^2, \end{aligned}$$

where in the second to last line we have used (5.51) and in the last line $1_\Delta$ denotes a test function equal to 1 on $\Delta$. Since the last expression is a locally bounded function of $r$, the proof is complete. □

Let $H_r$ be a piecewise analytic path in $\mathcal{A}$. It follows from Lemma 5.30 that for any $\varphi \in C_c(\mathbb{R})$, the absolutely continuous part $\Phi^{(a)}(\varphi)$ of the infinitesimal spectral shift measure is integrable along $H_r$. Therefore, the same is true of the singular part. The *absolutely continuous* and *singular* *spectral shift measures* along $H_r$ are respectively defined, as these (path-dependent) integrals, by replacing $(\cdot)$ with $(a)$ and $(s)$ in the formula

$$\xi^{(\cdot)}(\varphi; \{H_r\}) := \int_0^1 \operatorname{Tr}\left(E_r^{(\cdot)}(\operatorname{supp}\varphi)\dot{H}_r\varphi(H_r)\right) dr, \quad \varphi \in C_c(\mathbb{R}). \tag{5.53}$$

These are again real measures which are shown below to be absolutely continuous. Hence they correspond to locally integrable functions, which are known respectively as the *absolutely continuous* and *singular SSF's.*

Note that although the absolutely continuous and singular spectral shift measures in general depend on a curve $\{H_r\}$ (see the next section), they are path-additive in the sense that if $\gamma_1 \sqcup \gamma_2$ is the concatenation of two paths $\gamma_1$ and $\gamma_2$ then

$$\xi^{(\cdot)}(\varphi; \gamma_1 \sqcup \gamma_2) = \xi^{(\cdot)}(\varphi; \gamma_1) + \xi^{(\cdot)}(\varphi; \gamma_2).$$

THEOREM 5.31. *Let $H_r$ be a piecewise analytic path in $\mathcal{A}$ and put $z = \lambda + iy$. The absolutely continuous spectral shift measure along $H_r$ defined by* (5.53) *is an absolutely continuous measure whose density, the absolutely continuous SSF, is for a.e. $\lambda \in \mathbb{R}$ equal to*

$$\xi^{(a)}(\lambda; \{H_r\}) = \frac{1}{\pi}\int_0^1 \lim_{y\to 0^+} y \operatorname{Tr}\left(R_{\bar{z}}(H_r)\dot{H}_r R_z(H_r)\right) dr. \tag{5.54}$$

PROOF. It can be assumed without loss of generality that the path $H_r$ is analytic. Suppose $F$ is the rigging operator. Then for any $\lambda$ from the full set $\Lambda(\{H_r\}, F; \mathcal{L}_1)$, the integrand on the right hand side of (5.54) is equal for a.e. $r$ to the value of the function (5.52). We will show that $\xi^{(a)}$ is absolutely continuous with density equal a.e. to the function

$$\xi^{(a)}(\lambda; \{H_r\}) = \frac{1}{\pi}\int_0^1 \operatorname{Tr}\left(\dot{J}_r \operatorname{Im} T_{\lambda+i0}(H_r)\right) dr, \tag{5.55}$$

which is defined on $\Lambda(\{H_r\}, F; \mathcal{L}_1)$.

For any $\varphi \in C_c(\mathbb{R})$, Lemma 5.30 justifies the following use of Fubini's theorem

$$\int_{\mathbb{R}} \varphi(\lambda) \int_0^1 \frac{1}{\pi} \operatorname{Tr}\left(\dot{J}_r \operatorname{Im} T_{\lambda+i0}(H_r)\right) dr\, d\lambda$$
$$= \int_0^1 \int_{\mathbb{R}} \varphi(\lambda) \frac{1}{\pi} \operatorname{Tr}\left(\dot{J}_r \operatorname{Im} T_{\lambda+i0}(H_r)\right) d\lambda\, dr.$$

The inner integral on the left hand side is equal to $\xi^{(a)}(\lambda; \{H_r\})$ whereas by (5.51) the inner integral on the right hand side is equal to $\Phi_{H_r}^{(a)}(\dot{H}_r)(\varphi)$. Therefore, the same equality can be rewritten as

$$\int_{\mathbb{R}} \varphi(\lambda)\xi^{(a)}(\lambda; \{H_r\})\, d\lambda = \xi^{(a)}(\varphi; \{H_r\})$$

and the result follows. $\square$

Corollary 5.32. *Let $H_r$ be a piecewise analytic path in $\mathcal{A}$. The singular spectral shift measure along $H_r$ defined by* (5.53) *is an absolutely continuous measure whose density, the singular SSF, is for a.e. $\lambda \in \mathbb{R}$ equal to the difference of the SSF and the absolutely continuous SSF*

$$\xi^{(s)}(\lambda; \{H_r\}) = \xi(\lambda; H_1, H_0) - \xi^{(a)}(\lambda; \{H_r\}).$$

## 5.6. Path-dependence of the singular SSF

This section is a review of [Aza11a, §8.3] and is devoted to a proof of the theorem below, which is achieved by presenting a counterexample.

Theorem 5.33. *The singular part of the infinitesimal spectral shift measure is not exact. That is, the singular SSF $\xi^{(s)}(\lambda; \{H_r\})$ in general depends on the path $H_r$ connecting $H_0$ and $H_1$ in a resolvent comparable rigged affine space. Therefore the absolutely continuous SSF $\xi^{(a)}(\lambda; \{H_r\})$ is also path-dependent.*

This also provides an opportunity to review a version of the LAP for the one-dimensional free Hamiltonian.

Theorem 5.34. *Let $H = -\Delta$ be the Laplacian on $L_2(\mathbb{R})$. Let $F$ be the operator of multiplication by the function $\psi(x) = (1 + x^2)^{-1/2}$. Then the LAP holds in the sense that $\Lambda(H, F)$ contains every nonzero real number.*

A few notes: The operator $F$ is a bounded self-adjoint rigging operator on $L_2(\mathbb{R})$. It is also relatively Hilbert-Schmidt with respect to $H = -\Delta$, i.e. $FR_z(H)$ is Hilbert-Schmidt, by Corollary 5.4. Thus the LAP in the form of Corollary 3.14 is applicable here. However, the conclusion of this theorem is more specific. In its proof we will use the following well-known lemma (cf. [RS75, Example 1 in Section IX.7]).

Lemma 5.35. *For nonreal $z$, let $\sqrt{z}$ be chosen with $\operatorname{Im}\sqrt{z} > 0$. Then the resolvent of the Laplacian $R_z(-\Delta)$ is an integral operator with the kernel*

$$K(x, y) = \frac{i}{2\sqrt{z}} e^{i\sqrt{z}|x-y|}. \tag{5.56}$$

Proof. We will use properties of the Fourier transform (see e.g. [Rud91, Chapter 7]). For $f \in L_2(\mathbb{R})$, its Fourier transform is denoted by $\hat{f}$ and its inverse Fourier transform by $\check{f}$. Through the Fourier transform the operator $R_z(-\Delta)$ acts as multiplication by the function $g(\xi) := (\xi^2 - z)^{-1}$. For any $f \in L_2(\mathbb{R})$, we obtain

$$\begin{aligned} R_z(-\Delta) f(x) &= \left(g\hat{f}\right)^{\vee}(x) \\ &= (\check{g} * f)(x) \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \check{g}(x - y) f(y)\, dy. \end{aligned}$$

It remains to see that the inverse Fourier transform $\check{g}$ is given by

$$\frac{1}{\sqrt{2\pi}}\check{g}(x) = \frac{i}{2\sqrt{z}}e^{i\sqrt{z}|x|}. \tag{5.57}$$

To calculate the integral

$$\frac{1}{2\pi}\int_{\mathbb{R}} e^{ix\xi}g(\xi)\,d\xi = \frac{1}{2\pi}\int_{\mathbb{R}} \frac{e^{ix\xi}}{\xi^2 - z}\,d\xi$$

(except if $x = 0$ in which case it can be directly calculated by partial fractions to be $i(2\sqrt{z})^{-1}$ as required), it is convenient to approximate by a contour integral over a large closed rectangle. We distinguish two cases: $x > 0$ and $x < 0$. If $x > 0$, then let $C_R$ denote the positively-oriented rectangle with vertices $(-R, 0)$, $(R, 0)$, $(R, \sqrt{R})$, and $(-R, \sqrt{R})$. It is not difficult to check that the integrals along the top and vertical sides of $C_R$ can be made arbitrarily small for large $R$. Therefore,

$$\frac{1}{\sqrt{2\pi}}\check{g}(x) = \lim_{R\to\infty}\frac{1}{2\pi}\int_{C_R}\frac{e^{ix\xi}}{\xi^2 - z}\,d\xi.$$

The residue theorem can now be applied. Since

$$\frac{e^{ix\xi}}{\xi^2 - z} = \frac{e^{ix\xi}}{2\sqrt{z}}\left(\frac{1}{\xi - \sqrt{z}} - \frac{1}{\xi + \sqrt{z}}\right)$$

and the singularity $\xi = \sqrt{z}$ is within $C_R$, we get (5.57).

If $x < 0$, then let $C_R$ instead denote the negatively oriented rectangle with vertices $(-R, 0)$, $(R, 0)$, $(R, -\sqrt{R})$, and $(-R, -\sqrt{R})$. Then a similar argument, where now $C_R$ has winding number $-1$ around the singularity $\xi = -\sqrt{z}$, completes the proof. □

Proof of Theorem 5.34. Here we will follow [Kur78, Example 4.1.4]. For nonreal $z$, by Lemma 5.35 the sandwiched resolvent $T_z(H) = FR_z(H)F$ is an integral operator with kernel

$$K(z; x, y) = \frac{i}{2\sqrt{z}}(1 + x^2)^{-1/2}e^{i\sqrt{z}|x-y|}(1 + y^2)^{-1/2}.$$

Then since

$$|K(z; x, y)| \le \frac{1}{2\sqrt{|z|}}(1 + x^2)^{-1/2}(1 + y^2)^{-1/2}$$

and the right hand side as a function of $(x, y)$ belongs to $L_2(\mathbb{R}^2)$, it follows by dominated convergence that $K(\lambda + i\epsilon; x, y)$, for $\lambda \neq 0$, converges in $L_2(\mathbb{R}^2)$ as $\epsilon \to 0^+$ to the function

$$K(\lambda + i0; x, y) = \frac{i}{2\sqrt{\lambda}}(1 + x^2)^{-1/2}e^{i\sqrt{\lambda}|x-y|}(1 + y^2)^{-1/2}.$$

This implies (see e.g. [RS72, Theorem VI.23]) that the corresponding integral operators converge (in the Hilbert-Schmidt class). That is, the limit $T_{\lambda+i0}(H)$ exists for any nonzero real $\lambda$. □

To prove Theorem 5.33 it clearly suffices to present a pair of operators $H_0$ and $H_1$ which can be connected by two different piecewise analytic paths $\gamma_1$ and $\gamma_2$ in a resolvent comparable rigged affine space, so that

$$\xi^{(s)}(\lambda;\gamma_1) \neq \xi^{(s)}(\lambda;\gamma_2).$$

To construct this counterexample to exactness we will consider operators acting on the Hilbert space $\mathcal{H} = L_2(\mathbb{R}) \oplus \mathbb{C}$. A bounded operator $V \in \mathcal{B}(\mathcal{H})$ can be written in block matrix form as

$$V = \begin{pmatrix} V_0 & f \\ \langle g, \cdot\rangle & \alpha \end{pmatrix}, \tag{5.58}$$

where $V_0$ is a bounded operator on $L_2(\mathbb{R})$, $f, g \in L_2(\mathbb{R})$, and $\alpha \in \mathbb{C}$. Here, $f$ and $\langle g, \cdot\rangle$ are being considered in the obvious way as operators acting $\mathbb{C} \to L_2(\mathbb{R})$ and $L_2(\mathbb{R}) \to \mathbb{C}$ respectively. In this sense, $\langle f, \cdot\rangle$ is the adjoint of $f$. We will actually choose $V_0$ to be rank one.

As a rigging we choose the rank-two operator $F = \langle v, \cdot\rangle \oplus 1$, where $v(x) = e^{-x^2/2}$. Then $\mathcal{A}_0(F)$ is isomorphic to the self-adjoint matrices on $\mathcal{K} = \mathbb{C}^2$ and a four dimensional resolvent comparable rigged affine space is defined by

$$\mathcal{A}(F) = -\Delta \oplus 0 + \mathcal{A}_0(F). \tag{5.59}$$

For $r, s \in \mathbb{R}$, we will focus in particular on those operators of the form

$$H_{r,s} := \begin{pmatrix} -\Delta + r\langle v, \cdot\rangle v & rv \\ r\langle v, \cdot\rangle & s \end{pmatrix}. \tag{5.60}$$

LEMMA 5.36. *If $r \neq 0$, then the operator $H_{r,s}$ defined by* (5.60) *is absolutely continuous.*

PROOF. We first check that there is no pure point spectrum. Suppose

$$H_{r,s}\begin{pmatrix} f \\ f_0 \end{pmatrix} = \begin{pmatrix} -f'' + r\langle v, f\rangle v + rf_0 v \\ r\langle v, f\rangle + sf_0 \end{pmatrix} = \lambda \begin{pmatrix} f \\ f_0 \end{pmatrix}. \tag{5.61}$$

Then $-f'' = \lambda f - r(\langle v, f\rangle + f_0)v$ so that $f'' \in L_2(\mathbb{R})$. By taking the Fourier transform of this equality and using the fact that $\hat{v} = v$, we get

$$\hat{f}(\xi) = -r(\langle v, f\rangle + f_0)\frac{v(\xi)}{\xi^2 - \lambda}.$$

Since the function $v(\xi)/(\xi^2 - \lambda)$ does not belong to $L_2(\mathbb{R})$, it follows that $\langle v, f\rangle + f_0 = 0$. Then from (5.61) we see that $f_0 = 0$ and $\langle v, f\rangle = 0$. The last equality implies $f = 0$.

Now we will show that the set $\mathbb{R} \setminus \Lambda(H_{r,s}, F)$, which is a core of singular spectrum by Corollary 3.8, can only contain 0 and hence there can be no singular continuous spectrum either. Let $H_r = -\Delta + r\langle v, \cdot\rangle v$, $r \in \mathbb{R}$, which acts on $L_2(\mathbb{R})$ and should not be confused with the operator $H_{r,s}$ on $\mathcal{H}$. The following two lengthy but straightforward calculations are omitted.

For nonreal $z$, it can be shown using the second resolvent identity (as in (5.11)) that

$$R_z(H_r) = R_z(H_0) - (1 + r\langle v, R_z(H_0)v\rangle)^{-1} r \langle R_{\bar{z}}(H_0)v, \cdot\rangle R_z(H_0)v.$$

Further, it can be checked that the resolvent of $H_{r,s}$ is given by

$$R_z(H_{r,s}) = \begin{pmatrix} R_z(H_r) + r^2 C\langle R_{\bar{z}}(H_r)v, \cdot\rangle R_z(H_r)v & -rCR_z(H_r)v \\ -rC\langle R_{\bar{z}}(H_r)v, \cdot\rangle & C \end{pmatrix},$$

where $C = \left(s - z - r^2\langle v, R_z(H_r)v\rangle\right)^{-1}$. Since $F = \langle v, \cdot\rangle \oplus 1$, we obtain the following sandwiched versions of these formulas

$$T_z(H_r) := \langle v, R_z(H_r)v\rangle = T_z(H_0) - (1 + rT_z(H_0))^{-1} r (T_z(H_0))^2,$$

$$T_z(H_{r,s}) := FR_z(H_{r,s})F^* = \begin{pmatrix} T_z(H_r) + r^2 C(T_z(H_r))^2 & -rCT_z(H_r) \\ -rCT_z(H_r) & C \end{pmatrix}.$$

For $z = \lambda + iy$, the limits as $y \to 0^+$ of $T_z(H_0)$ exist for any nonzero $\lambda \in \mathbb{R}$ as a result of Theorem 5.34 and the fact that $v \in L_2(\mathbb{R}, (1 + x^2)dx)$. Assuming that $T_{\lambda+i0}(H_0)$ has a nonzero imaginary part, it follows that the limit $T_{\lambda+i0}(H_r)$ must also exist and have nonzero imaginary part, which in turn implies the existence of the limit $T_{\lambda+i0}(H_{r,s})$. The assumption can be confirmed using the equality

$$\operatorname{Im} T_{\lambda+i0}(H_0) = \lim_{y\to 0+} \langle v, \operatorname{Im} R_{\lambda+iy}(H_0)v\rangle = \frac{d}{d\lambda}\langle v, E_0(\lambda)v\rangle,$$

which holds as long as the right hand side exists (as follows e.g. from the proof of Theorem 2.4), as it indeed does and is nonzero:

$$\frac{d}{d\lambda}\langle v, E_0(\lambda)v\rangle = \frac{d}{d\lambda}\int_{-\infty}^{\lambda} |\hat{v}(\xi)|^2\, d\xi = |\hat{v}(\lambda)|^2 \neq 0. \qquad \square$$

Proof of Theorem 5.33. We present two paths with common endpoints in the affine space (5.59), for which the corresponding singular SSF's are not equal. Using the notation (5.60), let $\gamma_1$ be the path connecting $H_{0,0}$ and $H_{0,1}$ via the straight line $H_{0,r} = -\Delta \oplus r$, $r \in \mathbb{R}$. Then the singular SSF $\xi^{(s)}(\lambda;\gamma_1)$ can be seen to be the characteristic function of the interval $[0,1]$. Indeed, since the singular spectral measure of $H_{0,r}$ is given by $E_{0,r}(\Delta) = 0 \oplus \chi_\Delta(r)$ and $V := H_{0,1} - H_{0,0} = 0 \oplus 1$, we have

$$\xi^{(s)}(\lambda;\gamma_1) = \frac{d}{d\lambda}\int_0^1 \operatorname{Tr}(VE_{0,r}(\lambda))\, dr = \frac{d}{d\lambda}\int_0^1 \chi_{(-\infty,\lambda]}(r)\, dr = \chi_{[0,1]}(\lambda).$$

On the other hand let $\gamma_2$ be a path which detours through $H_{r,s}$ with nonzero $r$. For example,

$$\gamma_2 \colon r \mapsto \begin{cases} H_{2r,0}, & 0 \le r \le 1/2, \\ H_{2-2r,2r-1}, & 1/2 \le r \le 1. \end{cases}$$

Then by Lemma 5.36 the singular spectral measure of $\gamma_2(r)$ is zero for any $r \in (0,1)$ and hence the singular SSF along $\gamma_2$ must be zero. $\square$

CHAPTER 6

# The singular SSF and the resonance index

This chapter closely follows the preprint [Aza11b]. It consists of two sections. Its main aim is to prove the equality of the singular SSF with the total resonance index and this is achieved using an elegant argument in the first section. Having done so allows the construction of a nontrivial example of singular spectral shift which is reviewed in the second section.

## 6.1. Singular SSF as total resonance index

Throughout this section $\mathcal{A}$ again denotes a resolvent comparable rigged affine affine space. We further restrict our attention to a straight line $H_r$ in $\mathcal{A}(F)$ in the direction $V = F^*JF$. For straight paths we modify previous notation which indicates dependence on a piecewise analytic path by instead writing a pair of endpoints $H_1, H_0$, e.g. $\xi^{(s)}(\lambda; \{H_r\}) \leftrightarrow \xi^{(s)}(\lambda; H_1, H_0)$.

For a fixed essentially regular point $\lambda$ of the path $H_r$, let $r_\lambda \in R(\lambda; \{H_r\})$ be a fixed real resonance point. Let $[a, b]$ be an interval containing $r_\lambda$ and no other resonance points. In a neighbourhood of this interval, and for $z = \lambda + iy$, $y \geq 0$, we consider the meromorphic function

$$r \mapsto \frac{1}{\pi} \operatorname{Im} T_z(H_r)J = \frac{1}{2\pi i}(T_z(H_r)J - T_{\bar{z}}(H_r)J). \tag{6.1}$$

Its poles, namely the poles of $T_z(H_r)$ and the poles of $T_{\bar{z}}(H_r)$, are the resonance and anti-resonance points corresponding to $z$. As $y = 0$ is shifted to small positive values, the resonance point $r_\lambda$ as a pole of $T_{\lambda+i0}(H_r)$ splits into a finite number of nonreal resonance points which constitute the $r_\lambda$-group. On the other hand as a pole of $T_{\lambda-i0}(H_r)$, the same splitting occurs for the anti-resonance points reflected about the real axis (see Figure 6.1).

Let $0 \leq y << 1$ and let $L$ be a contour in $\mathbb{C}$ from $a$ to $b$ which circumvents all resonance and anti-resonance points of the $r_\lambda$-group in $\mathbb{C}_+$, as shown in Figure 6.1. The resonance and anti-resonance points shown in Figure 6.1 represent all nearby poles of the function (6.1). Since $\mathcal{A}$ is resolvent comparable and assuming $\lambda$ is chosen from the full set $\Lambda(\{H_r\}, F; \mathcal{L}_1)$, the function (6.1) takes values in the trace class. Denoting its trace by

$$F_z(r) := \frac{1}{\pi} \operatorname{Tr} (\operatorname{Im} T_z(H_r)J),$$

suppose the integral of $F_z(r)$ over $[a, b]$ is decomposed into the sum of its integrals over $L$ and $C_+(r_\lambda)$. Note that its integral over $[a, b]$ is the smoothed SSF $\xi(\lambda + iy; H_b, H_a)$ given by (5.47). Moreover, Proposition 4.6 implies

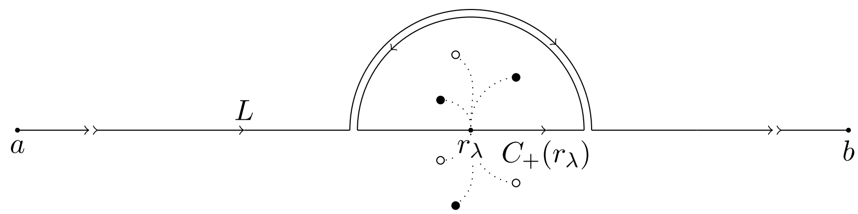


FIGURE 6.1. The coupling parameter plane in the region of $[a, b]$ for small $y$, showing the splitting of the resonance point $r_\lambda$ and two contours. Resonance points are solid dots and anti-resonance points are circles. The contour $C_+(r_\lambda)$ is the positively-oriented closed upper semicircle of a circle enclosing the $r_\lambda$-group. The contour $L$ goes from $a$ to $b$ circumventing resonance and anti-resonance points along the upper rim of $C_+(r_\lambda)$. Note that $C_+(r_\lambda)$ may be tiny in comparison to the interval $[a, b]$.

that for small enough $y$ its integral over $C_+(r_\lambda)$ is equal to the resonance index. Therefore we obtain the equality

$$\xi(\lambda + iy; H_b, H_a) = \int_L F_{\lambda+iy}(r)\, dr + \operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V). \tag{6.2}$$

The smoothed SSF converges for a.e. $\lambda$ to the SSF $\xi(\lambda; H_b, H_a)$ as $y \to 0^+$ (see (5.50)). So it remains to show that the first term on the right hand side of (6.2) converges to the absolutely continuous SSF $\xi^{(a)}(\lambda; H_b, H_a)$. Due to the absence of poles on the contour $L$, the function $F_{\lambda+iy}(r)$ converges uniformly on $L$ to $F_{\lambda+i0}(r)$ as $y \to 0^+$. Thus

$$\lim_{y\to 0^+} \int_L F_{\lambda+iy}(r)\, dr = \int_L F_{\lambda+i0}(r)\, dr. \tag{6.3}$$

We will now use the fact, whose proof is relegated to the lemma below, that the function $F_{\lambda+i0}(r)$ admits analytic continuation to the real axis. This means that it has no poles within a neighbourhood of $C_+(r_\lambda)$. Therefore, by Cauchy's theorem the contour $L$ of the integral on the right hand side of (6.3) can be replaced by the interval $[a, b]$. By Theorem 5.31, the result for a.e. $\lambda$ is $\xi^{(a)}(\lambda; H_b, H_a)$.

For a.e. $\lambda$ from the full set $\Lambda(\{H_r\}, F; \mathcal{L}_1)$ and any interval $[a, b]$ containing a single resonance point $r_\lambda$, we have shown that

$$\xi(\lambda; H_b, H_a) = \xi^{(a)}(\lambda; H_b, H_a) + \operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V).$$

Using additivity along the line $H_r$ proves that for a.e. $\lambda$ belonging to the intersection $\Lambda(H_0, F; \mathcal{L}_1) \cap \Lambda(H_1, F; \mathcal{L}_1)$,

$$\xi(\lambda; H_1, H_0) = \xi^{(a)}(\lambda; H_1, H_0) + \sum_{r_\lambda \in [0,1]} \operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V),$$

where the sum, namely the *total resonance index*, is taken over the finite number of resonance points $r_\lambda$ from the interval $[0, 1]$.

THEOREM 6.1. *Let $H_0$ and $H_1 = H_0 \dotplus V$ be two self-adjoint operators from a resolvent comparable rigged affine space $\mathcal{A}$ and let $H_r = H_0 \dotplus rV$ be the straight path from $H_0$ to $H_1$. For a.e. $\lambda$ from the full set $\Lambda(H_0, F; \mathcal{L}_1) \cap \Lambda(H_1, F; \mathcal{L}_1)$, the singular SSF coincides with the total resonance index:*

$$\xi^{(s)}(\lambda; \{H_r\}) = \sum_{r_\lambda \in [0,1]} \operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V),$$

*where the sum is taken over the finite number of resonance points $r_\lambda$ from the interval $[0, 1]$.*

The missing lemma which completes the proof:

LEMMA 6.2. *Let $H_r$ be an analytic path in $\mathcal{A}$. Then the meromorphic function*

$$r \mapsto \operatorname{Tr}\left(\operatorname{Im} T_{\lambda+i0}(H_r)\dot{J}_r\right)$$

*admits analytic continuation to the real axis, i.e. to real resonance points.*

PROOF. This lemma will be proved later using tools from stationary scattering theory (see the note below Theorem 8.2), but a modified version of the proof is sketched below. Let $H_r = H_0 \dotplus F^* J_r F$ and suppose $\lambda \in \Lambda(H_0, F; \mathcal{L}_1)$. We will use properties of the operator (a modified scattering matrix)

$$\begin{aligned} M(r) &:= (1 + T_{\lambda-i0}(H_0)J_r)(1 + T_{\lambda+i0}(H_0)J_r)^{-1} \\ &= 1 - 2i \operatorname{Im} T_{\lambda+i0}(H_0)J_r(1 + T_{\lambda+i0}(H_0)J_r)^{-1}. \end{aligned}$$

In particular, when $r$ is real and non-resonant this operator is unitary. This can be shown algebraically by applying its adjoint and using the equality (4.7). It follows that except on the discrete resonance set $M(r)$ is bounded and hence admits analytic continuation to the real axis. Its derivative at any non-resonant $r$ can be calculated:

$$M'(r) = -2i(1 + T_{\lambda-i0}(H_0)J_r) \operatorname{Im} T_{\lambda+i0}(H_r)\dot{J}_r(1 + T_{\lambda+i0}(H_0)J_r)^{-1}.$$

It follows that the function

$$\begin{aligned} r \mapsto \frac{i}{2} &\operatorname{Tr}(M'(r)M^*(r)) \\ &= \operatorname{Tr}\left((1 + T_{\lambda-i0}(H_0)J_r) \operatorname{Im} T_{\lambda+i0}(H_r)\dot{J}_r(1 + T_{\lambda-i0}(H_0)J_r)^{-1}\right) \\ &= \operatorname{Tr}\left(\operatorname{Im} T_{\lambda+i0}(H_r)\dot{J}_r\right) \end{aligned}$$

admits analytic continuation to $\mathbb{R}$. □

### 6.2. An example of singular SSF

In this section we will review a nontrivial example of the singular SSF from the preprint [Aza11b], which is allowed by its characterisation as the total resonance index. But let's begin with a trivial example. Let $\mathcal{H}$ be the Hilbert space of complex numbers $\mathbb{C}$ and let $H_0$ and $V$ be the self-adjoint operators of multiplication by 0 and 1 respectively. A rigging operator is unnecessary in the sense that $F = 1$ satisfies the requirements. Moreover, the singular SSF $\xi^{(s)}(\lambda; H_1, H_0)$ can be calculated directly. For $r \in \mathbb{R}$, put $H_r = H_0 + rV = r$. Its spectrum is $\{r\}$ and its purely singular spectral measure $E_r(\Delta) = \chi_\Delta(r)$ tests for the inclusion of $r$. Thus the (singular) spectral shift measure is given by

$$\xi^{(s)}(\Delta; H_1, H_0) = \int_0^1 \operatorname{Tr}(V E_r(\Delta))\, dr = \int_0^1 \chi_\Delta(r)\, dr = |\Delta \cap [0,1]|,$$

hence the singular SSF is equal to

$$\xi^{(s)}(\lambda; H_1, H_0) = \frac{d}{d\lambda} \int_0^1 \operatorname{Tr}(V E_r(\lambda))\, dr = \frac{d}{d\lambda} |(-\infty, \lambda] \cap [0,1]| = \chi_{[0,1]}(\lambda).$$

From the perspective of resonance index, the same calculation proceeds as follows. The operator $V R_z(H_0) = -z^{-1}$ has the single eigenvalue $\sigma_z = -z^{-1}$. So there is a single resonance function $r_z = z$. Obviously to every $\lambda \in \mathbb{R}$ there corresponds a real resonance point, which moves into the upper half-plane as $z = \lambda$ is perturbed to $z = \lambda + iy$, $y > 0$. Hence the resonance index at $\lambda$ is equal to 1 and again we find that

$$\xi^{(s)}(\lambda; H_1, H_0) = \sum_{r_\lambda \in [0,1]} \operatorname{ind}_{res}(\lambda, H_{r_\lambda}, V) = \chi_{[0,1]}(\lambda).$$

This example of a simple moving eigenvalue can be artificially embedded into the essential spectrum of an operator on an infinite-dimensional Hilbert space as follows. Suppose $H$ is an absolutely continuous self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $H_0$ and $V$ be the operators acting on the Hilbert space $\mathcal{H} \oplus \mathbb{C}$ given in block matrix form by

$$H_0 = \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix}, \quad V = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

A rigging operator $F \oplus 1$ is obtained from one on $\mathcal{H}$. Then for any $\lambda \in \Lambda(H, F)$ it is not difficult to see that again $\xi^{(s)}(\lambda; H_1, H_0) = \chi_{[0,1]}(\lambda)$. In this case it may happen that there is also absolutely continuous spectrum within the interval $[0, 1]$, but by construction it lies in a separate layer of the spectrum and doesn't really interact with the singular spectrum.

Two operators $H_0$ and $H_1$ on a Hilbert space $\mathcal{H}$ will be called *irreducible* if the only nonempty closed subspace $\mathcal{U} \subset \mathcal{H}$ which is invariant under both operators is the whole space $\mathcal{H}$, that is, if $H_0 \mathcal{U} = H_1 \mathcal{U} = \mathcal{U}$ implies $\mathcal{U} = \mathcal{H}$. The next example is nontrivial in the sense that the pair of self-adjoint operators $H_0$ and $H_1$ are irreducible and yet the restriction of the singular SSF $\xi^{(s)}(\lambda; H_1, H_0)$ to the essential spectrum is nonzero.

Let $K$ be a Cantor subset of $[-1, 1]$ which is symmetric with respect to 0 and has Lebesgue measure equal to 1. We can construct such a $K$ by first removing an open interval of length 1/3 from the middle of $[-1, 1]$, then removing an open interval of length 1/9 from the middle of each of the two remaining intervals, removing 1/27 from the remaining intervals, and continuing ad infinitum. The Cantor set left over is $K$, while the removed open set will be denoted $U$. Both $K$ and $U$ have Lebesgue measure 1.

Consider the operator of multiplication by $\lambda$ on the space $L_2(U, d\lambda)$, which is obviously an absolutely continuous self-adjoint operator and its spectrum is $[-1, 1]$. This will be the initial operator $H_0$. For the perturbation $V$ we choose the self-adjoint rank one operator $\langle 1, \cdot \rangle\, 1$, where 1 denotes the constant function $\lambda \mapsto 1$.

PROPOSITION 6.3. *The operators $H_0$ and $V$ are irreducible.*

PROOF. Let $\mathcal{U}$ be a closed subspace which is invariant under both $H_0$ and $V$ and suppose $f \in \mathcal{U}$ is not zero. Since by the Stone-Weierstrass Theorem the set of polynomials is dense in $L_2(U, d\lambda)$, it must be that for some $n = 0, 1, 2, \ldots$ the scalar product $\langle f, \lambda^n \rangle$ is nonzero. Then

$$0 \neq \langle f, \lambda^n \rangle = \langle f, H_0^n 1 \rangle = \langle H_0^n f, 1 \rangle$$

and since $H_0^n f \in \mathcal{U}$ for each $n$, this shows that $\mathcal{U}$ must not be orthogonal to 1. Therefore it must contain 1, since it is invariant under $V$. Then by its invariance under $H_0$, it must also contain all polynomials. Hence the only possibility is that $\mathcal{U} = \mathcal{H}$. □

THEOREM 6.4. *With $H_0$ and $V$ as above, put $H_r = H_0 + rV$. For all large enough $r > 0$ the singular SSF $\xi^{(s)}(H_r, H_0)$ is nonzero on the essential spectrum as an element of $L_1(\mathbb{R})$.*

Note that in this example the essential spectrum $\sigma_{ess} = [-1, 1]$ coincides with the absolutely continuous spectrum, which is also stable by the Kato-Rosenblum Theorem (numbered 7.24 below).

PROOF. By the equality of singular SSF and total resonance index, it suffices to consider the resonance index. Since $V$ has rank one, so does the operator

$$R_z(H_0)V = \langle 1, \cdot \rangle\, (\lambda - z)^{-1},$$

hence there can be only one resonance point $r_z = -\sigma_z^{-1}$. The eigenvalue $\sigma_z$ is given by

$$\sigma_z = \left\langle 1, (\lambda - z)^{-1} \right\rangle = \int_{-1}^{1} (\lambda - z)^{-1}\, d\mu(\lambda),$$

where the spectral measure $\mu$ is the restriction of Lebesgue measure to $U$. Denoting this Cauchy-Stieltjes transform by $\mathcal{C}_\mu(z)$, we have $r_z = -1/\mathcal{C}_\mu(z)$. We are interested in those points $\lambda \in [-1, 1]$ to which there corresponds a (finite) real resonance point $r_\lambda$ and therefore those $\lambda$ for which $\mathcal{C}_\mu(\lambda + i0)$ is real and nonzero. It follows from Theorem 2.7 that for a.e. $\lambda \in K$,

$$\operatorname{Im} \mathcal{C}(\lambda + i0) = \pi \chi_U(\lambda) = 0.$$

Thus for a.e. $\lambda \in K$,

$$\mathcal{C}_\mu(\lambda + i0) = \lim_{y \to 0^+} \int_{-1}^{1} \frac{x - \lambda}{(x - \lambda)^2 + y^2}\, d\mu(x). \tag{6.4}$$

Moreover, by part (ii) of Theorem 2.6 $\mathcal{C}_\mu(\lambda + i0)$ cannot be zero on a subset of $K$ of positive Lebesgue measure. Therefore, for a.e. $\lambda \in K$ there is a real resonance point $r_\lambda$. Since $V$ is positive and rank one, at any such $\lambda$ the resonance index $\operatorname{ind}_{res}(\lambda; H_{r_\lambda}, V)$ must be equal to 1. Further, since $U$ was chosen to be symmetric about 0, it is easy to check that the limit (6.4) is an odd function of $\lambda$. Thus there are positive resonance points $r_\lambda$ for a set of points $\lambda \in K$ of Lebesgue measure $|K|/2 = 1/2$. It follows that for large enough $r$ the singular SSF $\xi^{(s)}(\lambda; H_r, H_0)$ is equal to 1 on a set of positive measure. $\square$

CHAPTER 7

# Constructive stationary scattering theory

Forming an important part of perturbation theory, scattering theory is concerned with the perturbation of the absolutely continuous spectrum of self-adjoint operators on a Hilert space $\mathcal{H}$. It is also the mathematical framework for quantum mechanical scattering and is of course a vast subject most of which is beyond the scope of this document. The main sources used here are the two comprehensive volumes [Yaf92; Yaf10] by D. R. Yafaev.

The basic idea of scattering theory is to investigate the asymptotic behaviour of solutions

$$u(t) = e^{-itH_1} f$$

to the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}u(t) = H_1 u(t), \quad u(0) = f \in \mathcal{H},$$

for a self-adjoint operator $H_1$, in terms of the solutions for another (presumably simpler) self-adjoint operator $H_0$ which is close to $H_1$ in an appropriate sense. (For example they might be assumed to be resolvent comparable.)

In physical terms $H_0$ and $H_1$ are the Hamiltonians respectively describing an initial and a perturbed system. A motivating example is the Laplace operator $H_0 = -\Delta$ on $L_2(\mathbb{R}^\nu)$ considered as the momentum operator describing a free particle, which is perturbed to $H_1 = -\Delta + V$ by a localised potential $V$ whose influence on the particle (to reasonable approximation) occurs within a finite duration of time. In this case the initial, or *free,* operator $H_0$ is well-known in the sense that solutions of its Schrödinger equation are known explicitly. Moreover, it is expected that the solutions for the perturbed operator $H_1$ asymptotically approach those for $H_0$.

It turns out that in many situations, including the above example if the potential $V$ decays sufficiently quickly at infinity (and is not otherwise pathological, e.g. if $V \in L_1(\mathbb{R}^\nu)$), that for any vector $f$ from the absolutely continuous subspace $\mathcal{H}^{(a)}(H_1)$, there exist $f_\pm \in \mathcal{H}^{(a)}(H_0)$ so that

$$\lim_{t\to\pm\infty} \left\| e^{-itH_1} f - e^{-itH_0} f_\pm \right\| = 0.$$

Or equivalently,

$$\lim_{t\to\pm\infty} e^{itH_1} e^{-itH_0} f_\pm = f.$$

The operators defined by the *so*-limits (assuming they exist)

$$W_\pm(H_1, H_0) := \underset{t\to\pm\infty}{s\text{-}\lim}\, e^{itH_1} e^{-itH_0} P^{(a)}(H_0), \tag{7.1}$$

where $P^{(a)}$ is the projection onto the absolutely continuous subspace, are called the *(strong) wave operators.* As long as they exist the wave operators $W_\pm(H_1, H_0)$ are isometric on $\mathcal{H}^{(a)}(H_0)$, due to the continuity of the norm with respect to the *so*-topology. Further, they automatically exhibit the intertwining property (see e.g. [Yaf92, Theorem 2.1.4]):

$$\varphi(H_1)W_\pm(H_1, H_0) = W_\pm(H_1, H_0)\varphi(H_0) \tag{7.2}$$

for any bounded Borel function $\varphi$. It follows that the range of $W_\pm$ belongs to $\mathcal{H}^{(a)}(H_1)$. If $\operatorname{ran} W_\pm(H_1, H_0) = \mathcal{H}^{(a)}(H_1)$, then the wave operators establish a unitary equivalence of the absolutely continuous parts of $H_0$ and $H_1$. In this case they are said to be *complete.*

It is a central problem of scattering theory to determine the existence and completeness of the wave operators. In essence there are two distinct approaches to this problem known as the *smooth method* and the *trace class method.* Quoting [Yaf10, p. 8], "the smooth method makes essential use of an explicit spectral analysis of the unperturbed operator." This generally entails quite stringent assumptions on the form of the initial operator, for example requiring it to have purely absolutely continuous spectrum of constant multiplicity (in an interval). Whereas the trace class method avoids this kind of assumption by instead making use of the fact that, again quoting [Yaf10, p. 9], "in a weak sense an arbitrary Hilbert-Schmidt operator is smooth with respect to an arbitrary self-adjoint operator." This is meant in the sense of Theorems 3.11 and 3.13 and for example, the requirement that the pair of operators $H_0$ and $H_1$ belong to a resolvent comparable affine space constitutes a typical assumption enabling the trace class method. A unifying theory for the smooth and trace class methods remains elusive ([Yaf92; Yaf98]). However as noted in [Yaf92], they are to a certain extent united within the framework of stationary scattering theory.

The stationary approach to scattering theory replaces the time parameter $t$ with the spectral parameter $z = \lambda + iy$ by transitioning from unitary groups $e^{-itH}$ to resolvents $R_{\lambda+iy}(H)$. Then instead of limits as $t$ approaches infinity, there appear limits as $y$ approaches zero. The LAP (see Section 3.2) is the key to the stationary approach. In Section 7.4 it is shown that if $H_0$ and $H_1$ are two self-adjoint operators from a rigged affine space $\mathcal{A}(F)$ and the sets $\Lambda(H_0, F)$ and $\Lambda(H_1, F)$ have full measure, then the wave operators exist and are complete. This is a well-known result, but the proof given here has novel elements. In particular, it can be considered to take a further step toward uniting the smooth and trace class methods in the sense that it provides the trace class method with an explicit spectral representation and 'evaluation operator' $\mathcal{E}_\lambda$, which is discussed further below.

If the wave operators are complete, then the *scattering operator* is defined as the product

$$S(H_1, H_0) = W_+^*(H_1, H_0)W_-(H_1, H_0).$$

It is a partial isometry and unitary on the absolutely continuous subspace $\mathcal{H}^{(a)}(H_0)$. The intertwining property of the wave operators (7.2) implies that

$$\varphi(H_0)S(H_1,H_0) = S(H_1,H_0)\varphi(H_0) \tag{7.3}$$

for any bounded Borel function $\varphi$. From this it follows by Theorems 2.12 and 2.13 that the scattering operator $S(H_1, H_0)$ acts as multiplication by a measurable operator-valued function $S(\lambda; H_1, H_0)$ in any direct integral spectral representation of $H_0$.

Since the scattering operator is zero on the singular subspace of $H_0$, we might as well restrict it to the absolutely continuous subspace and choose a direct integral representation of the absolutely continuous part of $H_0$, which has the spectral type of Lebesgue measure. In this case by Theorem 2.13 there is a unitary operator

$$\mathcal{F}(H_0)\colon \mathcal{H}^{(a)}(H_0) \to \mathscr{H}(H_0) := \int_{\hat{\sigma}(H_0)}^{\oplus} \mathfrak{h}_\lambda(H_0)\, d\lambda. \tag{7.4}$$

which diagonalises the absolutely continuous part of $H_0$ in a direct integral. Here, $\hat{\sigma}(H_0)$ is any core of the absolutely continuous spectrum $\sigma_{ac}(H_0)$ and the fibre Hilbert spaces $\mathfrak{h}_\lambda(H_0)$ are determined up to their dimension. Assuming that $\mathcal{F}(H_0)$ is extended as zero to the singular subspace $\mathcal{H}^{(s)}(H_0)$, it follows from Theorem 2.12 and (7.3) that the scattering operator can be decomposed as

$$\mathcal{F}(H_0)S(H_1,H_0)\mathcal{F}^*(H_0) = \int_{\hat{\sigma}(H_0)}^{\oplus} S(\lambda; H_1, H_0)\, d\lambda. \tag{7.5}$$

The a.e. defined unitary operator $S(\lambda; H_1, H_0)$ on the fibre Hilbert space $\mathfrak{h}_\lambda(H_0)$ is the *scattering matrix.*

One of the most important formulas within stationary scattering theory is the stationary formula for the scattering matrix. For our purposes its main import is in proving the ordered exponential representation of the scattering matrix discussed in Chapter 1, which is the key to its connection with the SSF. Supposing the operators $H_0$ and $H_1$ belong to a rigged affine space $\mathcal{A}(F)$, with the perturbation $V := H_1 - H_0$ factorised as $V = F^*JF$, and assuming the LAP holds in the sense that the sets $\Lambda(H_0, F)$ and $\Lambda(H_1, F)$ have full measure, the stationary formula reads

$$S(\lambda; H_1, H_0) = 1 - 2\pi i Z(\lambda; H_0)(1 + JT_{\lambda+i0}(H_0))^{-1} JZ^*(\lambda; H_0), \tag{1.13}$$

for a.e. $\lambda \in \mathbb{R}$. The operator $Z(\lambda; H_0)$ is, at least intuitively, given by $Z(\lambda; H_0) = \mathcal{F}_\lambda(H_0)F^*$, where

$$\mathcal{F}_\lambda(H_0)\colon \mathcal{H} \ni f \mapsto (\mathcal{F}(H_0)f)(\lambda) \in \mathfrak{h}_\lambda(H_0) \tag{7.6}$$

is the 'evaluation operator' in the direct integral (7.4). This is not a rigorous definition since the full set of values $\lambda$ for which the right hand side of (7.6) is defined depends on $f$ (and a choice of representative within the equivalence class of a.e. equal functions $\mathcal{F}(H_0)f$). Various precise definitions of this operator are discussed below.

A proof of (1.13) given the LAP can be found for example in [Yaf92, Theorem 5.7.1′] (cf. the more specific formulation of [Yaf10, Theorem 0.8.12]). However, since for fixed $\lambda$ we are interested in its dependence on the normally fixed pair of operators $H_0$ and $H_1$, a standard proof of the stationary formula is not sufficient for our purposes. The main aim of this chapter is to rectify the situation.

We begin with an overview of the problem and its solution (also see the introduction of [Aza16]). In order to consider (1.13) for fixed value of the spectral parameter $\lambda$ as a function of the operators $H_0, H_1 \in \mathcal{A}$, it is necessary to ensure that the set of exceptional points $\lambda$ can be contained; although the union of a countable family of such null sets remains a null set, the same can of course not be said of a continuous family of them. Apart from its existence, the full set of values of $\lambda$ for which (1.13) holds is usually not of particular concern and as a result it is left in a very uncertain state. Three questions can be singled out: for which $\lambda$ is the left hand side of (1.13) defined, for which $\lambda$ is the right hand side defined, and when are they equal?

For a start, it won't do to define either side as an equivalence class of a.e. equal operator-valued functions on the direct integral (7.4) – we need specific representatives in order to ask about their value at a point $\lambda$. Close to the heart of the problem is for the direct integral decomposition (7.4) itself to be chosen arbitrarily – a core of absolutely continuous spectrum and the corresponding fibre Hilbert spaces need to be specified in such a way that their dependence on $H_0 \in \mathcal{A}(F)$ becomes manageable. It turns out that the presence of the rigging operator $F$ allows these specifications to be made naturally.

Let's consider in some detail the question of exactly which values of $\lambda$ the right hand side of (1.13) can be defined. In this regard the inverted factor on the right hand side of (1.13) has already been considered in Section 4.1. By definition, the limit $T_{\lambda+i0}(H_0)$ exists for any $\lambda$ from the set $\Lambda(H_0, F)$, which in this context has full measure by Corollary 3.14 and is therefore a core of the absolutely continuous spectrum $\sigma_{ac}(H_0)$ by Corollary 3.8. Then by Proposition 4.3, the factor $(1 + JT_{\lambda+i0}(H_0))^{-1}$ exists as long as $\lambda$ also belongs to $\Lambda(H_1, F)$. In other words, this factor exists as long neither the initial $H_0$ nor the perturbed operator $H_1$ is resonant at $\lambda$.

So it remains to decide for which values of $\lambda$ the operator $Z(\lambda; H_0)$ is defined. Unfortunately, this is not facilitated by its usual definition, which we now briefly review following [Yaf92, Part 1 of Section 5.4]. Beginning with an arbitrary spectral representation (7.4), $Z(\lambda; H_0)$ is built up from arbitrary representatives of a countable collection of functions in the image of $\mathcal{F}(H_0)F^*$ as follows. Suppose $\{\varphi_j\}_{j\in\mathbb{N}}$ is a basis of the auxiliary Hilbert space $\mathcal{K}$. Then by excluding a countable union of null sets, we can for a.e. $\lambda$ define

$$Z(\lambda; H_0)\varphi := (\mathcal{F}(H_0)F^*\varphi)(\lambda), \tag{7.7}$$

for vectors $\varphi$ which are linear combinations of the basis vectors $\varphi_j$. Then $Z(\lambda; H_0)$ can be continuously extended to other vectors once it is shown to be bounded using the fact that

$$(7.8)\quad \langle (\mathcal{F}(H_0)F^*\varphi)(\lambda), (\mathcal{F}(H_0)F^*\varphi)(\lambda)\rangle_{\mathfrak{h}_\lambda(H_0)} = \frac{1}{\pi}\langle \varphi, \operatorname{Im} T_{\lambda+i0}(H_0)\varphi\rangle_{\mathcal{K}},$$

for a.e. $\lambda$, which follows from Corollary 2.10 and the LAP. The point is that it is difficult to say for which values of $\lambda$ the operator $Z(\lambda; H_0)$ is defined, let alone anything about their dependence on $H_0$.

We now contrast the situation within the smooth approach to scattering theory, where the definition of the operator $Z(\lambda; H_0)$ can be made much more explicit. Suppose that the initial operator $H_0$ has purely absolutely continuous spectrum of constant multiplicity $k$ in an interval $I$. In this case, with $E_0$ denoting the spectral measure of $H_0$, the operator $H_0E_0(I)$ can be diagonalised in a direct integral (7.4) of the particularly simple form $\mathcal{H}(H_0E_0(I)) = L_2(I; \mathfrak{h})$, where $\mathfrak{h}$ is a fixed Hilbert space of dimension $k$. Then $F\colon \mathcal{H} \to \mathcal{K}$ is called *strongly $H_0$-smooth* on $I$ if $F_I := FE_0(I)$ is bounded and the operator $\mathcal{F}(H_0)F_I^*$ maps the auxiliary Hilbert space $\mathcal{K}$ continuously into the linear subspace of Hölder continuous functions $C^\alpha(I; \mathfrak{h})$, $\alpha \in (0, 1]$, i.e.

$$\|(\mathcal{F}(H_0)F_I^*\varphi)(\lambda)\|_{\mathfrak{h}} \le \text{const.}\, \|\varphi\|_{\mathcal{K}},$$
$$\|(\mathcal{F}(H_0)F_I^*\varphi)(\lambda) - (\mathcal{F}(H_0)F_I^*\varphi)(\mu)\|_{\mathfrak{h}} \le \text{const.}\, |\lambda-\mu|^\alpha \|\varphi\|_{\mathcal{K}},$$

for any $\lambda, \mu \in I$ and $\varphi \in \mathcal{K}$ (see e.g. [Yaf10, Definition 0.5.6]). Under this assumption, the operator $Z(\lambda; H_0)$ can be unproblematically defined for any $\lambda \in I$ and any $\varphi \in \mathcal{K}$ by the formula (7.7), since in this case the functions on the right hand side can be canonically evaluated at $\lambda$. In this setting the stationary formula (1.13) is known to hold for any $\lambda$ from the intersection $\Lambda(H_0, F) \cap \Lambda(H_1, F)$ (see e.g. [Yaf10, Theorem 0.7.1]).

Finally, we briefly describe how the problems above are overcome in the constructive approach to stationary scattering theory due to N. Azamov. It begins by defining an explicit spectral decomposition (7.4) as follows (the details can be found in Section 7.2). Given the LAP there is an obvious choice of a core of the absolutely continuous spectrum, namely $\Lambda(H_0, F)$, and the rest of the definition can be motivated by the formula (7.8); for $\lambda \in \Lambda(H_0, F)$, the evaluation operator (7.6) is defined on the range of $F^*$ by the formula

$$\mathcal{E}_\lambda(H_0) = \sqrt{\pi^{-1}\operatorname{Im} T_{\lambda+i0}(H_0)}\,(F^*)^{-1},$$

in which case the operator $Z(\lambda; H_0)$ is simply $\sqrt{\pi^{-1}\operatorname{Im} T_{\lambda+i0}(H_0)}$. The closure of its range is by definition the fibre Hilbert space $\mathfrak{h}_\lambda(H_0)$. Then (using Corollary 2.10) it can be shown that the operator

$$\mathcal{E}(H_0) := \int^{\oplus}_{\Lambda(H_0,F)} \mathcal{E}_\lambda(H_0)\, d\lambda\colon\ \operatorname{ran} F^* \to \mathcal{H}(H_0) := \int^{\oplus}_{\Lambda(H_0,F)} \mathfrak{h}_\lambda(H_0)\, d\lambda$$

continuously extends to a unitary operator from $\mathcal{H}^{(a)}(H_0)$ to $\mathcal{H}(H_0)$, which diagonalises $H_0$ (Theorem 7.12). Importantly, the dependence of this representation on the operator $H_0$ is accessible. This approach is constructive in the sense that the wave matrices $w_\pm(\lambda; H_1, H_0)$ and scattering matrix

$S(\lambda; H_1, H_0)$ are able to be explicitly defined for every value of the spectral parameter $\lambda$ from a predefined full set $\Lambda := \Lambda(H_0, F) \cap \Lambda(H_1, F)$. Their well-known properties including the stationary formula (Theorem 7.21) can then be established for every $\lambda \in \Lambda$ without exception. To complete the picture the wave operators and scattering operator can be built up from their fibres, for example considering the scattering operator to be defined by the formula (7.5), and verified to coincide with their usual time-dependent definitions.

Throughout this chapter we will make reference to a rigged affine space of self-adjoint operators $\mathcal{A}(F)$, but unlike other chapters the compactness of the sandwiched resolvent doesn't play a role here and it can be assumed instead that what is meant by $\mathcal{A}(F)$ is an affine space of self-adjoint operators over some linear subspace of $\mathcal{A}_0(F) = F^*\mathcal{B}_{sa}(\mathcal{K})F$ such that the rigging operator $F$ is $|H|^{1/2}$-bounded for any $H \in \mathcal{A}(F)$.

## 7.1. Existence of the wave operators and the stationary approach

In this section some standard results are collected, mostly from [Yaf92].

Since in applications the initial operator $H_0$ is much simpler than the perturbed operator $H_1$, establishing the existence of the wave operator $W_\pm(H_1, H_0)$ can be much easier than the same problem for $W_\pm(H_0, H_1)$. However in the trace class regime the initial assumptions are symmetric in $H_0$ and $H_1$, so that the following proposition reduces the question of the completeness of the wave operators to that of their existence.

PROPOSITION 7.1. *Suppose that the wave operator $W_\pm(H_1, H_0)$ exists. Then it is complete if and only if the wave operator $W_\pm(H_0, H_1)$ exists.*

For a proof, see e.g. [RS79, Proposition 3 of Section XI.3].

A step towards solving the existence problem for the (strong) wave operators (7.1) is to show the existence of the *weak wave operators* defined by

$$w\text{-}W_\pm(H_1, H_0) := w\text{-}\lim_{t\to\pm\infty} P^{(a)}(H_1) e^{itH_1} e^{-itH_0} P^{(a)}(H_0). \tag{7.9}$$

Note that if the strong wave operators $W_\pm$ exist, then so do the weak wave operators $w\text{-}W_\pm$ and $w\text{-}W_\pm = W_\pm$.

THEOREM 7.2. *The existence of the strong wave operators $s\text{-}W_\pm(H_1, H_0)$ is equivalent to the existence of the weak wave operators $w\text{-}W_\pm(H_1, H_0)$ and the equality*

$$w\text{-}W_\pm^*(H_1, H_0) w\text{-}W_\pm(H_1, H_0) = P^{(a)}(H_0). \tag{7.10}$$

This theorem is numbered 2.2.1 in [Yaf92]. The proof is reproduced here for convenience.

PROOF. Since the existence of the strong wave operators clearly implies the existence of the weak wave operators, it suffices to assume the existence of the weak wave operators and show that the existence of the strong wave operators is equivalent to the equality (7.10). So we assume that the weak wave operators $w\text{-}W_\pm := w\text{-}W_\pm(H_1, H_0)$ exist. Consider the equality

$$\begin{aligned}&\left\| e^{itH_1} e^{-itH_0} P^{(a)}(H_0) f - w\text{-}W_\pm f \right\|^2 \\ &= \|P^{(a)}(H_0)f\|^2 - 2\operatorname{Re}\left\langle e^{itH_1} e^{-itH_0} P^{(a)}(H_0) f, w\text{-}W_\pm f \right\rangle + \|w\text{-}W_\pm f\|^2.\end{aligned}$$

Since $w\text{-}W_\pm = P^{(a)}(H_1) w\text{-}W_\pm$, the second term on the right hand side tends to $-2\|w\text{-}W_\pm f\|^2$. Therefore the convergence to zero of the left hand side is equivalent to the equality $\|P^{(a)}(H_0)f\|^2 = \|w\text{-}W_\pm f\|^2$. For this to hold for any $f$ is equivalent to (7.10). □

The next two results are Lemma 5.3.1 and Theorem 5.3.2 in [Yaf92]. Their statements have been specialised to our needs, but the proofs are almost unchanged.

LEMMA 7.3. *Let $H$ be a self-adjoint operator belonging to a rigged affine space $\mathcal{A}(F)$ and suppose that the LAP holds in the sense that $\Lambda(H, F)$ is a full set. Then*

$$\int_{\mathbb{R}} \left\| F e^{-itH} g \right\|^2 \, dt < \infty,$$

*for all $g$ from some dense linear subspace $D$ in $\mathcal{H}^{(a)}(H)$ consisting of vectors of compact support.*

PROOF. Let $E$ denote the spectral measure of $H$ and let $P^{(a)}$ denote the projection onto the absolutely continuous subspace $\mathcal{H}^{(a)}$. Set

$$X_{n,N} = \left\{ \lambda \in \Lambda(H, F) \,:\, |\lambda| \le n,\ \left\| \pi^{-1} \operatorname{Im} T_{\lambda + i0}(H) \right\| \le N \right\}$$

and let $D$ be the set of linear combinations of all elements of the form $E(X_{n,N}) F^* \psi$ for all possible $n, N$, and $\psi \in \operatorname{dom} F^*$. The sets $X_{n,N}$ do not support any singular spectrum (by Theorem 3.7), that is $E(X_{n,N}) = E(X_{n,N}) P^{(a)}$, and from the LAP it follows that

$$\lim_{N \to \infty} |(-n, n) \setminus X_{n,N}| = 0.$$

Therefore for any $g \in \operatorname{ran} F^*$, the element $P^{(a)} g$ can be approximated by elements $E(X_{n,N}) g \in D$. Since the range of $F^*$ is dense in $\mathcal{H}$, the linear subspace $D$ of $\mathcal{H}^{(a)}$ is dense in $\mathcal{H}^{(a)}$. (Note that while $P^{(a)} \operatorname{ran} F^*$ is dense in $\mathcal{H}^{(a)}$, it is not necessarily true that $\mathcal{H}^{(a)} \cap \operatorname{ran} F^*$ is dense in $\mathcal{H}^{(a)}$.)

Let $g = E(X_{n,N}) F^* \psi \in D$. Choose an orthonormal basis $\{\varphi_j\}_{j \in \mathbb{N}}$ of the auxiliary Hilbert space $\mathcal{K}$ from $\operatorname{dom} F^*$ and consider the scalar products (rewritten using Corollary 2.10)

$$\begin{aligned}\left\langle \varphi_j, F e^{-itH} g \right\rangle &= \left\langle F^* \varphi_j, e^{-itH} E(X_{n,N}) F^* \psi \right\rangle \\ &= \int_{X_{n,N}} e^{-it\lambda} \left\langle \varphi_j, \pi^{-1} \operatorname{Im} T_{\lambda + i0}(H) \psi \right\rangle d\lambda.\end{aligned}$$

Note that this is $\sqrt{2\pi}$ times the Fourier transform $\hat{f}_j(t)$ of the function

$$f_j(\lambda) := X_{n,N}(\lambda) \left\langle \varphi_j, \pi^{-1} \operatorname{Im} T_{\lambda+i0}(H)\psi \right\rangle,$$

which is compactly supported and bounded. Therefore by Parseval's equality,

$$\begin{aligned}\int_{\mathbb{R}} \left|\left\langle \varphi_j, Fe^{-itH}g \right\rangle\right|^2 dt &= 2\pi \int_{\mathbb{R}} \left|\hat{f}_j(t)\right|^2 dt = 2\pi \int_{\mathbb{R}} |f_j(\lambda)|^2 \, d\lambda \\ &= 2\pi \int_{X_{n,N}} \left|\left\langle \varphi_j, \pi^{-1} \operatorname{Im} T_{\lambda+i0}(H)\psi \right\rangle\right|^2 d\lambda.\end{aligned}$$

Now summing over $j$ we obtain

$$\int_{\mathbb{R}} \left\|Fe^{-itH}g\right\|^2 dt = 2\pi \int_{X_{n,N}} \left\|\pi^{-1} \operatorname{Im} T_{\lambda+i0}(H)\psi\right\|^2 d\lambda.$$

Thus, by the construction of the set $X_{n,N}$, the integral converges (and does not exceed $4\pi N^2 n \|\psi\|$). □

THEOREM 7.4. *Let $H_0$ and $H_1 = H_0 \dotplus V$ be a self-adjoint operators from a rigged affine space of self-adjoint operators $\mathcal{A}(F)$. If $\Lambda(H_0, F)$ and $\Lambda(H_1, F)$ are full sets, then the weak wave operators $w$-$W_\pm(H_1, H_0)$ exist.*

PROOF. Note first that for any $f, g \in \mathcal{H}$,

$$\begin{aligned}\frac{d}{dt}\left\langle e^{-itH_1}f, e^{-itH_0}g\right\rangle &= \left\langle -iH_1e^{-itH_1}f, e^{-itH_0}g\right\rangle + \left\langle e^{-itH_1}f, -iH_0e^{-itH_0}g\right\rangle \\ &= -iV\left[e^{-itH_1}f, e^{-itH_0}g\right] \\ &= -i\left\langle Fe^{-itH_1}f, JFe^{-itH_0}g\right\rangle,\end{aligned}$$

where the decomposition $V = F^*JF$ was used in the last line. Therefore,

$$\begin{aligned}&\left\langle f, e^{it_2H_1}e^{-it_2H_0}g\right\rangle - \left\langle f, e^{it_1H_1}e^{-it_1H_0}g\right\rangle \\ &\qquad = -i\int_{t_1}^{t_2}\left\langle Fe^{-itH_1}f, JFe^{-itH_0}g\right\rangle dt.\end{aligned}$$

Using the Schwartz inequality, this implies that

$$\begin{aligned}&\left|\left\langle f, e^{it_2H_1}e^{-it_2H_0}g\right\rangle - \left\langle f, e^{it_1H_1}e^{-it_1H_0}g\right\rangle\right| \\ &\qquad \le \|J\|\int_{t_1}^{t_2}\|Fe^{-itH_1}f\|\|Fe^{-itH_0}g\|\,dt \\ &\qquad \le \|J\|\left(\int_{t_1}^{t_2}\|Fe^{-itH_1}f\|^2\,dt\right)^{1/2}\left(\int_{t_1}^{t_2}\|Fe^{-itH_0}g\|^2\,dt\right)^{1/2}.\end{aligned}$$

By Lemma 7.3 the right hand side above tends to zero when $t_1, t_2 \to \pm\infty$, for a dense set of vectors $f$ in $\mathcal{H}^{(a)}(H_1)$ and a dense set of vectors $g$ in $\mathcal{H}^{(a)}(H_0)$. Thus for $f$ and $g$ from these dense sets, there exist the limits

$$\lim_{t\to\pm\infty}\left\langle f, P^{(a)}(H_1)e^{itH_1}e^{-itH_0}P^{(a)}(H_0)g\right\rangle.$$

Hence the weak wave operators $w$-$W_\pm(H_1, H_0)$ exist. □

Later it will be shown using techniques of stationary scattering theory that the premise of Theorem 7.4 also implies the equality (7.10). Then Theorem 7.2 implies the existence of the strong wave operators.

The transition to the stationary scheme of scattering theory is achieved via the relation (see e.g. [Yaf92, (1.4.4)])

$$R_z(H) = \pm i \int_0^\infty e^{\mp it(H-z)}\, dt, \tag{7.11}$$

where $z = \lambda \pm iy$, $y > 0$. Or perhaps more to the point, the transition is made through the lemma below.

LEMMA 7.5. *Let $H_0$ and $H_1$ be self-adjoint operators with $P_0^{(a)}$ and $P_1^{(a)}$ being the projections onto their absolutely continuous subspaces. For any vectors $f_0$ and $f_1$ and any $y > 0$,*

$$\begin{aligned}(7.12)\quad 2y \int_0^\infty e^{-2yt} \left\langle e^{\mp itH_1} P_1^{(a)} f_1, e^{\mp itH_0} P_0^{(a)} f_0 \right\rangle dt \\ = \frac{y}{\pi} \int_{\mathbb{R}} \left\langle R_{\lambda\pm iy}(H_1) P_1^{(a)} f_1, R_{\lambda\pm iy}(H_0) P_0^{(a)} f_0 \right\rangle d\lambda.\end{aligned}$$

PROOF. This is [Yaf92, Lemma 2.7.1] and we only sketch the proof. We apply the vector-valued Parseval equalities

$$\int_{\mathbb{R}} \langle f_1(t), f_0(t) \rangle\, dt = \int_{\mathbb{R}} \langle \hat{f}_1(\lambda), \hat{f}_0(\lambda) \rangle d\lambda,$$

where $\hat{f}_j(\lambda) = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{\pm i\lambda t} f_j(t)\, dt$, $j = 0, 1$, to the functions

$$f_j(t) = \theta(t)\, e^{-yt \mp itH_j} P_j^{(a)} f_j,$$

where $\theta$ denotes the Heaviside step function. Then it remains to use the equality (7.11). □

The limits of (7.12) as $y \to 0^+$, if they exist, define the *weak abelian wave operators,* which we will denote by $\mathcal{W}_\pm(H_1, H_0)$. That is, the weak abelian wave operators are defined by

$$\mathcal{W}_\pm(H_1, H_0) = w\text{-}\lim_{y\to 0^+} 2y \int_0^\infty e^{-2yt} w\text{-}W_\pm(H_1, H_0)\, dt.$$

If the weak wave operators $w$-$W_\pm(H_1, H_0)$ exist then so do the weak abelian wave operators (which coincide), as a consequence of the following abelian limit result.

LEMMA 7.6. *If $f$ is a bounded function on $\mathbb{R}$ and $f(\infty) := \lim_{t\to\infty} f(t)$ exists, then*

$$f(\infty) = \lim_{y\to 0^+} 2y \int_0^\infty e^{-2y} f(t)\, dt.$$

PROOF. Let $y > 0$. Note that the integral of the function $\omega_y(t) = ye^{-yt}$ over the positive real axis is equal to 1. Also, for $N > 0$ its integral over $[0, N]$ converges to 0 as $y \to 0$, while its integral over $[N, \infty)$ converges to 1. Then the result follows from the estimate

$$\left|\int_0^\infty \omega_y(t) f(t)\, dt - f(\infty)\right| \\ \leq \int_0^N \omega_y(t)\, |f(t) - f(\infty)|\, dt + \int_N^\infty \omega_y(t)\, |f(t) - f(\infty)|\, dt,$$

since both terms on the right converge to 0 as $y \to 0$. □

The lemma below is [Yaf92, Lemma 5.2.1], whose proof is also reproduced for convenience.

LEMMA 7.7. *Let $H_0$, $H_1$, be self-adjoint operators with spectral measures $E_0$ and $E_1$ respectively. For any vectors $f_0$ and $f_1$, and for any Borel sets $\Delta_0, \Delta_1 \subset \mathbb{R}$, with intersection $\Delta := \Delta_1 \cap \Delta_0$,*

$$\lim_{y \to 0^+} \frac{y}{\pi} \langle R_{\lambda \pm iy}(H_1) E_1(\Delta_1) f_1, R_{\lambda \pm iy}(H_0) E_0(\Delta_0) f_0 \rangle = 0, \tag{7.13}$$

*for a.e. $\lambda \in \mathbb{R} \setminus \Delta$. Moreover, if the limit*

$$\lim_{y \to 0^+} \frac{y}{\pi} \langle R_{\lambda \pm iy}(H_1) f_1, R_{\lambda \pm iy}(H_0) f_0 \rangle \tag{7.14}$$

*exists for a.e. $\lambda \in \mathbb{R}$, then there also exists for a.e. $\lambda \in \mathbb{R}$ the limit*

$$\lim_{y \to 0^+} \frac{y}{\pi} \langle R_{\lambda \pm iy}(H_1) E_1(\Delta_1) f_1, R_{\lambda \pm iy}(H_0) E_0(\Delta_0) f_0 \rangle \\ = \Delta(\lambda) \lim_{y \to 0^+} \frac{y}{\pi} \langle R_{\lambda \pm iy}(H_1) f_1, R_{\lambda \pm iy}(H_0) f_0 \rangle . \tag{7.15}$$

PROOF. We begin with the inequality

$$\left|\frac{y}{\pi} \langle R_{\lambda \pm iy}(H_1) f_1, R_{\lambda \pm iy}(H_0) f_0 \rangle\right|^2 \\ \leq \frac{y}{\pi} \|R_{\lambda \pm iy}(H_1) f_1\|^2 \frac{y}{\pi} \|R_{\lambda \pm iy}(H_0) f_0\|^2. \tag{7.16}$$

Consider for example

$$\frac{y}{\pi} \|R_{\lambda \pm iy}(H_0) f_0\|^2 = \frac{1}{\pi} \langle f_0, \operatorname{Im} R_{\lambda + iy}(H_0) f_0 \rangle ,$$

which is the Poisson integral of the measure $\langle f_0, E_0 f_0 \rangle$ and hence has a limit as $y \to 0^+$ for a.e. $\lambda$. Moreover, the set of its finite and nonzero limits is a minimal support of the absolutely continuous part of the measure (Theorem 2.7). Putting $f_0$ equal to $E_0(\Delta_0) f_0$, we see that since the measure is supported within $\Delta_0$, the limit of its Poisson integral must be zero a.e. outside of $\Delta_0$. Therefore, with $f_0 = E_0(\Delta_0) f_0$ and $f_1 = E_1(\Delta_1) f_1$, the right hand side and hence the left hand side of inequality (7.16) is zero for a.e. $\lambda \in \mathbb{R} \setminus \Delta$. This proves (7.13).

Using (7.13), it suffices to verify relation (7.15) on the set $\Delta$. For this, denoting the limit (7.14) by $\mathfrak{a}_\pm(f_1, f_0; \lambda)$, we note that

$$\mathfrak{a}_\pm(E_1(\mathbb{R} \setminus \Delta_1)f_1, E_0(\Delta_0)f_0; \lambda) = \mathfrak{a}_\pm(f_1, E_0(\mathbb{R} \setminus \Delta_0)f_0; \lambda) = 0$$

for a.e. $\lambda$ from the set $\Delta$ by (7.13). Thus for a.e. $\lambda \in \Delta$,

$$\begin{aligned} \mathfrak{a}_\pm(f_1, f_0; \lambda) &= \mathfrak{a}_\pm(E_1(\Delta_1)f_1, E_0(\Delta_0)f_0; \lambda) \\ &\qquad + \mathfrak{a}_\pm(E_1(\mathbb{R} \setminus \Delta_1)f_1, E_0(\Delta_0)f_0; \lambda) \\ &\qquad\qquad + \mathfrak{a}_\pm(f_1, E_0(\mathbb{R} \setminus \Delta_0)f_0; \lambda) \\ &= \mathfrak{a}_\pm(E_1(\Delta_1)f_1, E_0(\Delta_0)f_0; \lambda), \end{aligned}$$

which establishes (7.15). □

THEOREM 7.8. *Assuming the weak abelian wave operators exist, the following equality holds for any vectors $f_0$ and $f_1$.*

$$\langle f_1, \mathcal{W}_\pm(H_1, H_0)f_0\rangle = \frac{1}{\pi} \int_{\mathbb{R}} \lim_{y \to 0^+} y \,\langle R_{\lambda \pm iy}(H_1)f_1, R_{\lambda \pm iy}(H_0)f_0\rangle \, d\lambda. \tag{7.17}$$

PROOF. By Lemma 7.5 we have

$$\langle f_1, \mathcal{W}_\pm(H_1, H_0)f_0\rangle = \lim_{y \to 0^+} \frac{y}{\pi} \int_{\mathbb{R}} \left\langle R_{\lambda \pm iy}(H_1)P_1^{(a)} f_1, R_{\lambda \pm iy}(H_0)P_0^{(a)} f_0 \right\rangle d\lambda.$$

Following [Yaf92, Lemma 5.2.2], we will show that the limit and integral on the right hand side can be interchanged. Then Lemma 7.7 implies that the projections onto the absolutely continuous subspaces can be removed resulting in the right hand side of (7.17).

For brevity we put

$$g_j(\lambda \pm iy) := R_{\lambda \pm iy}(H_j)P_j^{(a)} f_j, \quad j = 0, 1.$$

Let $Y$ be any Borel subset of $\mathbb{R}$. The Schwartz inequality implies

$$\begin{aligned} &\frac{y}{\pi} \int_Y \left|\langle g_1(\lambda \pm iy), g_0(\lambda \pm iy)\rangle\right| d\lambda \\ &\quad \le \frac{y}{\pi} \int_Y \|g_1(\lambda \pm iy)\| \|g_0(\lambda \pm iy)\| \, d\lambda \\ &\quad \le \left(\frac{y}{\pi} \int_Y \|g_1(\lambda \pm iy)\|^2 \, d\lambda\right)^{1/2} \left(\frac{y}{\pi} \int_Y \|g_0(\lambda \pm iy)\|^2 \, d\lambda\right)^{1/2}. \end{aligned} \tag{7.18}$$

By the Vitali convergence theorem, the interchange of limit and integral will be justified if we show that the integral on the left hand side of (7.18) tends to zero uniformly with respect to $y \in (0, 1)$ when $|Y| \to 0$ and when $Y = (-\infty, -N) \cup (N, \infty)$ and $N \to \infty$. Observe that this property is satisfied if $y \ge \epsilon$ for any fixed positive $\epsilon$. Therefore it suffices to show that two the integrands on the right hand side of (7.18) have limits in $L_1(\mathbb{R})$ as $y \to 0^+$. But for $j = 0, 1$, the function

$$\frac{y}{\pi} \|g_j(\lambda \pm iy)\|^2 = \frac{1}{\pi} \left\langle P_j^{(a)} f_j, \operatorname{Im} R_{\lambda + iy}(H_j) P_j^{(a)} f_j \right\rangle$$

is the Poisson integral of the finite measure $\langle f_j, E_j^{(a)} f_j\rangle$ and since this measure is absolutely continuous, its Poisson integral converges in $L_1(\mathbb{R})$ by Theorem 2.3. □

## 7.2. The evaluation operator

In this section we define the explicit spectral decomposition of the absolutely continuous part of $H$ which was discussed at the beginning of the chapter. Throughout this section, $H$ is a self-adjoint operator and $F$ is a rigging operator which is relatively bounded with respect to the operator $|H|^{1/2}$.

PROPOSITION 7.9. *Let $H$ be a self-adjoint operator from a rigged affine space $\mathcal{A}(F)$. Then for any nonreal $z$, the operator $FR_z(H)$ has trivial kernel and cokernel.*

PROOF. The operator $FR_z(H)$ has trivial kernel, since this is true of both $F$ and $R_z(H)$. If $F$ is bounded then $(FR_z(H))^* = R_{\bar z}(H)F^*$ also has trivial kernel. In the case that $F$ is unbounded, we check that the range of $FR_z(H)$ is dense in $\mathcal{K} = \overline{F\operatorname{dom}[H]}$ (see the discussion surrounding (3.26)). Let $\psi(x) = (|x|+1)^{-1/2}$ so that $\operatorname{ran}\psi(H) = \operatorname{dom}[H]$ and $\operatorname{ran}\psi^2(H) = \operatorname{dom} H = \operatorname{ran} R_z(H)$. To any $\varphi \in \mathcal{K}$ there is an arbitrarily close vector $F\psi(H)f$ belonging to the dense set $F\operatorname{dom}[H]$. Then there exists a vector $\psi(H)g \in \operatorname{dom}[H]$ arbitrarily close to $f$ by the density of $\operatorname{dom}[H]$ in $\mathcal{H}$. Hence

$$\begin{aligned}\|\varphi - F\psi^2(H)g\| &\le \|\varphi + F\psi(H)f\| + \|F\psi(H)f - F\psi^2(H)g\| \\ &\le \|\varphi + F\psi(H)f\| + \|F\psi(H)\|\|f - \psi(H)g\|\end{aligned}$$

can be made arbitrarily small. □

For $y > 0$, the range of the operator $\sqrt{\operatorname{Im} T_{\lambda+iy}(H)}$ is dense in the auxiliary Hilbert space $\mathcal{K}$. Indeed, with $z = \lambda + iy$, this can be seen from the equality

$$\sqrt{\operatorname{Im} T_z(H)} = \sqrt{yFR_z(H)(FR_z(H))^*} = \sqrt{y}|(FR_z(H))^*|, \tag{7.19}$$

since the range of the operator $|(FR_z(H))^*|$ coincides with that of $FR_z(H)$ and $(\operatorname{ran} FR_z(H))^\perp = \ker(FR_z(H))^* = \{0\}$. However, for $\lambda \in \Lambda(H,F)$ the range of $\sqrt{\operatorname{Im} T_{\lambda+i0}(H)}$ may no longer be dense and we define

$$\mathfrak{h}_\lambda(H) = \mathfrak{h}_\lambda(H,F) = \overline{\operatorname{ran}\sqrt{\operatorname{Im} T_{\lambda+i0}(H)}}.$$

LEMMA 7.10. *The field of fibre Hilbert spaces*

$$\{\mathfrak{h}_\lambda(H) : \lambda \in \Lambda(H,F)\} \tag{7.20}$$

*is measurable, in the sense that the orthogonal projections onto $\mathfrak{h}_\lambda$ are weakly measurable.*

Proof. Let $P_\lambda$ be the projection onto $\mathfrak{h}_\lambda$. For any $\varphi, \psi \in \mathcal{K}$, we check that the function

$$\Lambda(H,F) \ni \lambda \mapsto \langle \varphi, P_\lambda \psi \rangle = \langle P_\lambda \varphi, P_\lambda \psi \rangle \tag{7.21}$$

is measurable as the limit of measurable functions. Since any vector in the range of $P_\lambda$ by definition belongs to the closure of the range of the operator $\sqrt{\operatorname{Im} T_{\lambda+i0}(H)}$, there exist sequences $\eta_n$, $\chi_n$, $n = 1, 2, \ldots$, from $\mathcal{K}$ such that

$$\sqrt{\operatorname{Im} T_{\lambda+i0}(H)}\, \eta_n \to P_\lambda \varphi, \ \text{ and } \ \sqrt{\operatorname{Im} T_{\lambda+i0}(H)}\, \chi_n \to P_\lambda \psi.$$

Further, for any fixed $n \in \mathbb{N}$, we can find convergent sequences $\eta_{n,k} \to \eta_n$ and $\chi_{n,k} \to \chi_n$ in $\mathcal{K}$, whose terms belong to the dense set $\operatorname{dom} F^*$. For any $n, k \in \mathbb{N}$, the function

$$\lambda \mapsto \left\langle \sqrt{\operatorname{Im} T_{\lambda+i0}(H)}\, \eta_{n,k}, \sqrt{\operatorname{Im} T_{\lambda+i0}(H)}\, \chi_{n,k} \right\rangle \\ = \lim_{y \to 0+} \langle F^* \eta_{n,k}, \operatorname{Im} R_{\lambda+iy}(H) F^* \chi_{n,k} \rangle$$

is measurable as the limit of measurable functions. Hence for any $n \in \mathbb{N}$ the limit as $k \to \infty$ is a measurable function. Finally, taking the limit as $n \to \infty$ shows that the function (7.21) is measurable. □

It follows from Lemma 7.10 (see Section 2.4) that the field (7.20) defines a direct integral of Hilbert spaces

$$\mathcal{H}(H) = \mathcal{H}(H,F) := \int_{\Lambda(H,F)}^{\oplus} \mathfrak{h}_\lambda(H,F)\, d\lambda, \tag{7.22}$$

which can be viewed as the closed subspace of $L_2(\Lambda, \mathcal{K})$ consisting of those functions $f$ such that $f(\lambda) \in \mathfrak{h}_\lambda(H)$ for a.e. $\lambda \in \Lambda(H,F)$.

For any $\lambda \in \Lambda(H,F)$, let the *evaluation operator* $\mathcal{E}_\lambda(H) = \mathcal{E}_\lambda(H,F)$ be defined on the range of $F^*$ by the formula

$$\mathcal{E}_\lambda(H) = \frac{1}{\sqrt{\pi}} \sqrt{\operatorname{Im} T_{\lambda+i0}(H)} (F^*)^{-1}. \tag{7.23}$$

Lemma 7.11. *The family of operators* $\{\mathcal{E}_\lambda(H) : \lambda \in \Lambda(H,F)\}$ *defines a bounded operator* $\mathcal{E}(H) = \mathcal{E}(H,F) \colon \mathcal{H} \to \mathcal{H}(H)$, *which is given for any* $f \in \operatorname{ran} F^*$ *by* $(\mathcal{E}(H)f)(\lambda) := \mathcal{E}_\lambda(H) f$ *and has norm* $\le 1$. *Moreover, the equality*

$$\|\mathcal{E}(H,F) f\|^2_{\mathcal{H}(H)} = \|E(\Lambda(H,F)) f\|_{\mathcal{H}} \tag{7.24}$$

*holds for any* $f \in \mathcal{H}$.

Proof. For any $f$ from $\operatorname{ran} F^*$, the function $\lambda \mapsto \mathcal{E}_\lambda(H) f$ obviously takes values in $\mathfrak{h}_\lambda(H)$ and we will show that it is square integrable and hence belongs to $\mathcal{H}(H)$. Indeed,

$$\begin{aligned}\|\mathcal{E}(H,F)f\|^2_{\mathcal{H}(H)} &= \int_{\Lambda(H,F)} \langle (\mathcal{E}(H)f)(\lambda), (\mathcal{E}(H)f)(\lambda)\rangle_{\mathfrak{h}_\lambda}\, d\lambda \\ &= \frac{1}{\pi}\int_{\Lambda(H,F)} \lim_{y\to 0^+} \langle f, \operatorname{Im} R_{\lambda+iy}(H)f\rangle_{\mathcal{H}}\, d\lambda \\ &= \|E(\Lambda(H,F))f\|^2_{\mathcal{H}}.\end{aligned}$$

The first equality is the definition of the norm on $\mathcal{H}(H)$ and since $f \in \operatorname{ran} F^*$, the second equality is a consequence of the definition (7.23). The third, in which $E$ denotes the spectral measure of $H$, holds due to properties of the Poisson integral (see Corollary 2.10 and Theorem 3.7): the measure $\langle f, Ef\rangle$ is purely absolutely continuous on the set $\Lambda(H,F)$, since its Poisson integral $\pi^{-1}\langle f, \operatorname{Im} R_{\lambda+iy}(H)f\rangle$ has finite limits there, and its density is a.e. equal to the limit of its Poisson integral. It follows that $\mathcal{E}(H,F)\colon \operatorname{ran} F^* \to \mathcal{H}(H)$ is a bounded operator whose norm is $\leq 1$. Therefore by the density of the range of $F^*$ in $\mathcal{H}$, this operator extends to a bounded operator $\mathcal{E}(H)\colon \mathcal{H} \to \mathcal{H}(H)$ with norm $\leq 1$. The equality (7.24) extends by continuity from $f \in \operatorname{ran} F^*$ to any $f \in \mathcal{H}$. In fact this implies all equalities in the above chain remain valid for any $f \in \mathcal{H}$. □

THEOREM 7.12. *Let $H$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $E$ be its spectral measure. Suppose $F$ is a rigging operator which is relatively bounded with respect to $|H|^{1/2}$. The operator $\mathcal{E}(H)\colon \mathcal{H} \to \mathcal{H}(H)$ defined above is a partial isometry with initial space $E(\Lambda(H,F))\mathcal{H}$ and final space $\mathcal{H}(H)$. Moreover, $\mathcal{E}(H)$ diagonalises the operator $E(\Lambda(H,F))H$ in the sense that for all $f \in \operatorname{dom} H$*

$$(\mathcal{E}(H)Hf)(\lambda) = \lambda(\mathcal{E}(H)f)(\lambda) \quad \forall \text{ a.e. } \lambda \in \Lambda(H,F) \tag{7.25}$$

*and if $h$ is a bounded Borel function whose minimal support is a subset of $\Lambda(H,F)$, then for all $f \in \mathcal{H}$*

$$(\mathcal{E}(H)h(H)f)(\lambda) = h(\lambda)(\mathcal{E}(H)f)(\lambda) \quad \forall \text{ a.e. } \lambda \in \Lambda(H,F). \tag{7.26}$$

PROOF. The equality (7.24) implies that $\mathcal{E}(H)$ is a partial isometry with initial space $E(\Lambda(H,F))\mathcal{H}$.

We will now show, for any Borel subset $\Delta \subset \Lambda(H,F)$, that if $E(\Delta)f = 0$ then $(\mathcal{E}(H)f)(\lambda) = 0$ for a.e. $\lambda \in \Delta$. Let $f_n$ be a sequence from the dense range of $F^*$ converging to $f$. Then

$$\begin{aligned}\int_\Delta \|(\mathcal{E}(H)f)(\lambda) - \mathcal{E}_\lambda(H)f_n\|^2\, d\lambda &= \int_\Delta \|(\mathcal{E}(H)(f-f_n))(\lambda)\|^2\, d\lambda \\ &\leq \int_{\Lambda(H,F)} \|(\mathcal{E}(H)(f-f_n))(\lambda)\|^2\, d\lambda \\ &= \|\mathcal{E}(H)(f-f_n)\|^2 \\ &\leq \|f-f_n\|^2 \to 0.\end{aligned}$$

Moreover, since $f_n \in \operatorname{ran} F^*$, for any $n$ we have

$$\int_\Delta \|\mathcal{E}_\lambda(H) f_n\|^2 \, d\lambda = \frac{1}{\pi} \int_\Delta \lim_{y \to 0^+} \langle f_n, \operatorname{Im} R_{\lambda+iy} f_n \rangle \, d\lambda = \|E(\Delta) f_n\|^2.$$

Therefore, if $E(\Delta) f = 0$, then in the limit the above equality becomes

$$\int_\Delta \|(\mathcal{E}(H) f)(\lambda)\|^2 \, d\lambda = 0,$$

which implies that $(\mathcal{E}(H)f)(\lambda) = 0$ for a.e. $\lambda \in \Delta$.

Let $\Delta$ be a Borel subset of $\Lambda(H,F)$ and let $f \in \mathcal{H}$. From above it follows that $(\mathcal{E}(H)E(\Delta)f)(\lambda) = 0$ for a.e. $\lambda \notin \Delta$ and also that for a.e. $\lambda \in \Delta$,

$$(\mathcal{E}(H)E(\Delta)f)(\lambda) = (\mathcal{E}(H)f)(\lambda) - (\mathcal{E}(H)E(\mathbb{R} \setminus \Delta)f)(\lambda) = (\mathcal{E}(H)f)(\lambda).$$

Therefore,

$$(\mathcal{E}(H)E(\Delta)f)(\lambda) = \Delta(\lambda)(\mathcal{E}(H)f)(\lambda), \quad \forall \text{ a.e. } \lambda \in \Lambda(H,F),$$

where $\Delta(\lambda)$ denotes the indicator of $\Delta$. This equality implies that (7.26) holds for step functions $h(\lambda)$, hence by continuity it holds for all bounded Borel functions $h$. And with $h_n(\lambda) \to \lambda$ continuity implies (7.25).

It remains to show that $\mathcal{H}(H)$ is the final space, for which it is enough to show that the range of $\mathcal{E}(H)$ is dense in $\mathcal{H}(H)$. Let $g(\lambda)$ be an element of $\mathcal{H}(H)$ which is orthogonal to the range of $\mathcal{E}(H)$. The equality (7.26) implies that if the range of $\mathcal{E}(H)$ contains a function $f(\lambda)$, then it also contains all functions of the form $h(\lambda)f(\lambda)$, where $h$ is a scalar-valued bounded Borel function. Hence for any $f \in \mathcal{H}$, $g(\lambda)$ must be orthogonal to $h(\lambda)(\mathcal{E}(H)f)(\lambda)$ for any bounded Borel $h$. It follows that $g(\lambda) \perp (\mathcal{E}(H)f)(\lambda)$ in $\mathfrak{h}_\lambda(H)$ for a.e. $\lambda \in \Lambda(H,F)$. Considering $f$ from the range of $F^*$, it must be that $g(\lambda)$ is orthogonal to the range of $\sqrt{\operatorname{Im} T_{\lambda+i0}(H)}$ and hence to the whole fibre Hilbert space $\mathfrak{h}_\lambda(H)$. Therefore $g(\lambda) = 0$ for a.e. $\lambda \in \Lambda(H,F)$. □

COROLLARY 7.13. *Let $H$ be a self-adjoint operator and let $F$ be a $|H|^{1/2}$-bounded rigging operator such that $\Lambda(H,F)$ is a full set. Then the operator $\mathcal{E}(H,F) \colon \mathcal{H} \to \mathcal{H}(H,F)$ diagonalises the absolutely continuous part of $H$.*

The strength of this corollary, which gives an explicit diagonalisation of the absolutely continuous part of an arbitrary self-adjoint operator, is due to its strong premise: the LAP.

## 7.3. The wave and scattering matrices

Throughout this section and for the remainder of this chapter $\mathcal{A}(F)$ denotes a fixed rigged affine space (however see the remark on p. 108). For any $H \in \mathcal{A}(F)$ and any nonreal $z$, consider the polar decomposition:

$$(FR_{\bar{z}}(H))^* = U_z(H,F)|(FR_{\bar{z}}(H))^*|.$$

Since $(FR_{\bar{z}}(H))^*$ has trivial kernel and cokernel by Proposition 7.9, the operator $U_z(H,F) \colon \mathcal{K} \to \mathcal{H}$ is unitary. For any two self-adjoint operators $H_0$

and $H_1$ from $\mathcal{A}(F)$ and for any nonreal $z$, the operator $w(z; H_1, H_0)$ on the auxiliary Hilbert space $\mathcal{K}$ defined by

$$w(z; H_1, H_0) = U_z^*(H_1, F)U_z(H_0, F) \tag{7.27}$$

will be called an *off-axis wave matrix.* Some immediate properties are collected in the proposition below.

PROPOSITION 7.14. *The off-axis wave matrices are unitary, satisfy the multiplicative property $w(z; H_2, H_0) = w(z; H_2, H_1)w(z; H_1, H_0)$, as well as the equalities $w(z; H_0, H_0) = 1$ and $w^*(z; H_1, H_0) = w(z; H_0, H_1)$.*

LEMMA 7.15. *Suppose $H_0$ and $H_1 = H_0 \dotplus V$, where $V = F^*JF$, are two operators from the affine space $\mathcal{A}(F)$. Then with $z = \lambda \pm iy$, $y > 0$, and $z^+ = \lambda + iy$, the off-axis wave matrices satisfy the equalities*

$$\sqrt{\operatorname{Im} T_{z^+}(H_1)}\, w(z; H_1, H_0) \sqrt{\operatorname{Im} T_{z^+}(H_0)} = yFR_{\bar z}(H_1)(FR_{\bar z}(H_0))^*, \tag{7.28}$$

$$\sqrt{\operatorname{Im} T_{z^+}(H_1)}\, w(z; H_1, H_0) = (1 - T_{\bar z}(H_1)J)\sqrt{\operatorname{Im} T_{z^+}(H_0)}, \tag{7.29}$$

$$w(z; H_1, H_0)\sqrt{\operatorname{Im} T_{z^+}(H_0)} = \sqrt{\operatorname{Im} T_{z^+}(H_1)}(1 + JT_z(H_0)). \tag{7.30}$$

PROOF. These equalities follow easily from the resolvent identities. For example, from the equality (7.19) and the definition (7.27) of the off-axis wave matrix, we obtain

$$w(z; H_1, H_0)\sqrt{\operatorname{Im} T_{z^+}(H_0)} = \sqrt{y}\, U_z^*(H_1)(FR_{\bar z}(H_0))^*.$$

Now using the second resolvent identity and then again (7.19),

$$\begin{aligned} w(z; H_1, H_0)\sqrt{\operatorname{Im} T_{z^+}(H_0)} &= \sqrt{y}\, U_z^*(H_1)(FR_{\bar z}(H_1))^*(1 + JT_z(H_0)) \\ &= \sqrt{\operatorname{Im} T_{z^+}(H_1)}(1 + JT_z(H_0)). \end{aligned}$$

Equalities (7.28) and (7.29) are obtained similarly. □

Now we consider what happens as the off-axis spectral parameter $z = \lambda \pm iy$ approaches the real axis. For this purpose we reintroduce the set of regular points $\Pi(H, F)$, defined by (4.2) – in short it consists of all $z = \lambda \pm iy$ for $y \geq 0$, where it is assumed that $\lambda \in \Lambda(H, F)$ if $y = 0$. As in Lemma 7.15, for any $z = \lambda \pm iy \in \Pi(H, F)$, let $z^+ = \lambda + iy$ denote its projection onto the upper half-plane $\Pi_+(H, F)$.

PROPOSITION 7.16. *Let $p = 1$ and $q = 2$, or $p = q = \infty$, accordingly if the rigged affine space $\mathcal{A}(F)$ is resolvent comparable or not. Then for any $z \in \Pi(H, F; \mathcal{L}_p)$, the operator $\sqrt{\operatorname{Im} T_{z^+}(H)}$ belongs to $\mathcal{L}_q(\mathcal{K})$. Moreover, if $\lambda \in \Lambda(H, F; \mathcal{L}_p)$ then in the norm of $\mathcal{L}_q(\mathcal{K})$,*

$$\sqrt{\operatorname{Im} T_{\lambda+iy}(H)} \to \sqrt{\operatorname{Im} T_{\lambda+i0}(H)} \quad \textit{as} \quad y \to 0+\,.$$

PROOF. Since $\operatorname{Im} T_{z^+}(H)$ belongs to $\mathcal{L}_p(\mathcal{K})$, its square root belongs to $\mathcal{L}_q(\mathcal{K})$. The convergence in $\mathcal{L}_p(\mathcal{K})$ of $\operatorname{Im} T_{\lambda+iy}(H) \to \operatorname{Im} T_{\lambda+i0}(H)$ as $y \to 0^+$ follows from Corollary 3.15. Therefore its square root converges in $\mathcal{L}_q(\mathcal{K})$ as a result of the Birman-Koplienko-Solomyak inequality (2.20). □

If $\lambda$ belongs to the intersection $\Lambda(H_0, F) \cap \Lambda(H_1, F)$ then each of the operators (7.28), (7.29), and (7.30) exists as a bounded operator in the limit as $y \to 0^+$. This is clear for (7.29) and (7.30) given Proposition 7.16, while either one of these equalities implies the existence of the limit of (7.28), which is equal to

$$\begin{aligned}\lim_{y\to 0^+} \frac{y}{\pi} F R_{\lambda\mp iy}(H_1)(F R_{\lambda\mp iy}(H_0))^* &= (1 - T_{\lambda\mp i0}(H_1)J)\frac{1}{\pi}\operatorname{Im} T_{\lambda+i0}(H_0)\\ &= \frac{1}{\pi}\operatorname{Im} T_{\lambda+i0}(H_1)(1 + J T_{\lambda\pm i0}(H_0)).\end{aligned}$$

(In [Aza11a, Definition 5.1.4], also cf. [Yaf92, (2.7.4)], this operator is referred to by the notation $\mathfrak{a}_\pm(\lambda; H_1, H_0)$.)

For convenience, for any $z \in \Pi(H, F)$ we put

$$\mathcal{E}_z(H) := \sqrt{\pi^{-1}\operatorname{Im} T_{z^+}(H)}(F^*)^{-1}.$$

Then Proposition 7.16 implies that for any $z = \lambda \pm iy$ with $\lambda \in \Lambda(H, F)$ and any $f \in \operatorname{ran} F^*$, $\mathcal{E}_z(H)f$ converges to $\mathcal{E}_\lambda(H)f$ as $y \to 0^+$. Suppose $z$ is nonreal, in which case we note that the range of $\mathcal{E}_z(H)$ is dense in the auxiliary Hilbert space $\mathcal{K}$. This fact and the equality (7.28) imply that the off-axis wave matrices are determined by the numbers

$$\langle \mathcal{E}_z(H_1)f, w(z; H_1, H_0)\mathcal{E}_z(H_0)g\rangle = \frac{y}{\pi}\langle R_z(H_1)f, R_z(H_0)g\rangle, \quad f, g \in \operatorname{ran} F^*.$$

PROPOSITION 7.17. *Suppose that $H_0$ and $H_1$ are self-adjoint operators from the affine space $\mathcal{A}(F)$. Then for any $\lambda \in \Lambda(H_0, F) \cap \Lambda(H_1, F)$, there exist bounded operators*

$$w(\lambda \pm i0; H_1, H_0) = w_\pm(\lambda; H_1, H_0)\colon \mathfrak{h}_\lambda(H_0, F) \to \mathfrak{h}_\lambda(H_1, F), \tag{7.31}$$

*namely the wave matrices, which have norm $\leq 1$ and are uniquely determined by the numbers*

$$\begin{aligned} w_\pm(\lambda; H_1, H_0)&[\mathcal{E}_\lambda(H_1)f, \mathcal{E}_\lambda(H_0)g]\\ &:= \lim_{y\to 0^+}\frac{y}{\pi}\langle R_{\lambda\pm iy}(H_1)f, R_{\lambda\pm iy}(H_0)g\rangle, \quad f, g \in \operatorname{ran} F^*.\end{aligned} \tag{7.32}$$

PROOF. This proof follows a standard method (cf. [Yaf92, §5.2]). The formula (7.32) defines a form on $\operatorname{ran}\mathcal{E}_\lambda(H_1) \times \operatorname{ran}\mathcal{E}_\lambda(H_0)$, which we will show is bounded, with bound $\leq 1$, and hence defines a bounded operator (7.31) from the closure of $\operatorname{ran}\mathcal{E}_\lambda(H_0)$ to the closure of $\operatorname{ran}\mathcal{E}_\lambda(H_1)$. For $y > 0$ and any $f = F^*\varphi, g = F^*\psi \in \operatorname{ran} F^*$,

$$\begin{aligned}\frac{y}{\pi}|\langle R_{\lambda\pm iy}(H_1)f, R_{\lambda\pm iy}(H_0)g\rangle| &\leq \frac{y}{\pi}\|R_{\lambda\pm iy}(H_1)F^*\varphi\|\|R_{\lambda\pm iy}(H_0)F^*\psi\|\\ &= \frac{1}{\pi}\langle\varphi, \operatorname{Im} T_{\lambda+iy}(H_1)\varphi\rangle^{1/2}\langle\psi, \operatorname{Im} T_{\lambda+iy}(H_0)\psi\rangle^{1/2}\\ &= \|\mathcal{E}_{\lambda+iy}(H_1)f\|\|\mathcal{E}_{\lambda+iy}(H_0)g\|\end{aligned}$$

Then since $\lambda \in \Lambda(H_0, F) \cap \Lambda(H_1, F)$, by taking the limit $y \to 0^+$ we obtain

$$|\langle \mathcal{E}_\lambda(H_1)f, w_\pm(\lambda; H_1, H_0)\mathcal{E}_\lambda(H_0)g\rangle| \leq \|\mathcal{E}_\lambda(H_1)f\|\|\mathcal{E}_\lambda(H_0)g\|.$$

Therefore by continuous linear extension, (7.32) determines a bounded form on $\mathfrak{h}_\lambda(H_1) \times \mathfrak{h}_\lambda(H_0)$, which corresponds to the bounded operator (7.31) with the same bound. □

The next lemma establishes the equalities of Lemma 7.15 in the case that $z = \lambda \pm i0$.

Lemma 7.18. *For $\lambda \in \Lambda(H_0, F) \cap \Lambda(H_1, F)$, the wave matrices satisfy the equalities*

$$\begin{aligned}\sqrt{\operatorname{Im} T_{\lambda+i0}(H_1)}w_\pm(\lambda; H_1, H_0)\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)} \\ = \lim_{y\to 0^+} \frac{y}{\pi} F R_{\lambda\mp iy}(H_1)(F R_{\lambda\mp iy}(H_0))^*,\end{aligned} \tag{7.33}$$

$$\sqrt{\operatorname{Im} T_{\lambda+i0}(H_1)}w_\pm(\lambda; H_1, H_0) = (1 - T_{\lambda\mp i0}(H_1)J)\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}, \tag{7.34}$$

$$w_\pm(\lambda; H_1, H_0)\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)} = \sqrt{\operatorname{Im} T_{\lambda+i0}(H_1)}(1 + J T_{\lambda\pm i0}(H_0)), \tag{7.35}$$

*which are interpreted as equalities of bounded operators acting $\mathcal{K} \to \mathcal{K}$, $\mathfrak{h}_\lambda(H_0) \to \mathcal{K}$, and $\mathcal{K} \to \mathfrak{h}_\lambda(H_1)$, respectively.*

Proof. For any $\varphi, \psi \in \operatorname{dom} F^*$, the definition (7.32) and the equality (7.28) imply

$$\begin{aligned}(E) &:= \left\langle \sqrt{\operatorname{Im} T_{\lambda+i0}(H_1)}\varphi, w_\pm(\lambda; H_1, H_0)\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}\psi \right\rangle \\ &= \lim_{y\to 0^+} \left\langle \sqrt{\operatorname{Im} T_{\lambda+iy}(H_1)}\varphi, w(\lambda \pm iy; H_1, H_0)\sqrt{\operatorname{Im} T_{\lambda\pm iy}(H_0)}\psi \right\rangle.\end{aligned}$$

By applying each of (7.28), (7.29), and (7.30) and then moving the limit back within the scalar product, we obtain

$$\begin{aligned}(E) &= \left\langle \varphi, \lim_{y\to 0^+} \frac{y}{\pi} F R_{\lambda\mp iy}(H_1)(F R_{\lambda\mp iy}(H_0))^*\psi \right\rangle \\ &= \left\langle \varphi, (1 - T_{\lambda-i0}(H_1)J)\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}\psi \right\rangle \\ &= \left\langle \sqrt{\operatorname{Im} T_{\lambda+i0}(H_1)}\varphi, \sqrt{\operatorname{Im} T_{\lambda+i0}(H_1)}(1 + J T_{\lambda+i0}(H_0))\psi \right\rangle.\end{aligned}$$

By the density of $\operatorname{dom} F^*$, the first equality implies (7.33). Similarly, now also using the density of the range of $\operatorname{ran} \mathcal{E}_\lambda(H)$ in $\mathfrak{h}_\lambda(H)$, the second equality implies (7.34) and the third implies (7.35). □

As an aside, the equalities (7.34) can be identified with equations for the stationary scattering states which appear in physics books, in particular [Tay72, (10.8)]. (There are two sign disagreements with [Tay72]; one comes from the traditional difference between physics and mathematics when it comes to the choice of sign for the definition of the wave operators, while the other comes from a difference in sign convention for the resolvent.)

From (7.34) and the second resolvent identity we can easily obtain a version of the Lippman-Schwinger equation ([Tay72, (10.12)])

$$\begin{aligned}&\sqrt{\pi^{-1}\operatorname{Im}T_{\lambda+i0}(H_1)}\,w_\pm(\lambda;H_1,H_0)\\&=\sqrt{\pi^{-1}\operatorname{Im}T_{\lambda+i0}(H_0)}-T_{\lambda\mp i0}(H_0)J\sqrt{\pi^{-1}\operatorname{Im}T_{\lambda+i0}(H_1)}\,w_\pm(\lambda;H_1,H_0).\end{aligned}$$

For a given state $\varphi$ this equation can be suggestively rewritten as

$$\varphi^{(\pm)}(\lambda)=\varphi(\lambda)-T_{\lambda\mp i0}(H_0)J\varphi^{(\pm)}(\lambda),$$

where $\varphi^{(\pm)}(\lambda)=\sqrt{\delta_\lambda(H_1)}\,w_\pm(\lambda;H_1,H_0)\sqrt{\delta_\lambda(H_0)}\,\varphi$, $\varphi(\lambda)=\delta_\lambda(H_0)\varphi$ and $\delta_\lambda(H)=\pi^{-1}\operatorname{Im}T_{\lambda+i0}(H)$.

THEOREM 7.19. *Let $H_0,H_1$ and $H_2$ be self-adjoint operators from a rigged affine space $\mathcal{A}(F)$. Then the wave matrices satisfy the multiplicative property*

$$w_\pm(\lambda;H_2,H_0)=w_\pm(\lambda;H_2,H_1)w_\pm(\lambda;H_1,H_0), \tag{7.36}$$

*for any $\lambda\in\bigcap_j\Lambda(H_j,F)$, $j=0,1,2$. In addition, the wave matrices are unitary and satisfy the equalities $w(\lambda;H_0,H_0)=1$ and $w_\pm^*(\lambda;H_1,H_0)=w_\pm(\lambda;H_0,H_1)$.*

PROOF. To prove (7.36) it is enough to show that for any $f,g\in\operatorname{ran}F^*$

$$\begin{aligned}&\langle\mathcal{E}_\lambda(H_2)f,w_\pm(\lambda;H_2,H_0)\mathcal{E}_\lambda(H_0)g\rangle\\&\qquad=\langle\mathcal{E}_\lambda(H_2)f,w_\pm(\lambda;H_2,H_1)w_\pm(\lambda;H_1,H_0)\mathcal{E}_\lambda(H_0)g\rangle\,.\end{aligned}$$

This can be inferred from the following equality of bounded operators on the auxiliary Hilbert space $\mathcal{K}$.

$$\begin{aligned}&\sqrt{\operatorname{Im}T_{\lambda+i0}(H_2)}w_\pm(\lambda;H_2,H_0)\sqrt{\operatorname{Im}T_{\lambda+i0}(H_0)}\\&=\lim_{y\to0^+}\sqrt{\operatorname{Im}T_{\lambda+iy}(H_2)}w(\lambda\pm iy;H_2,H_0)\sqrt{\operatorname{Im}T_{\lambda+iy}(H_0)}\\&=\lim_{y\to0^+}\sqrt{\operatorname{Im}T_{\lambda+iy}(H_2)}w(\lambda\pm iy;H_2,H_1)w(\lambda\pm iy;H_1,H_0)\sqrt{\operatorname{Im}T_{\lambda+iy}(H_0)}\\&=\sqrt{\operatorname{Im}T_{\lambda+i0}(H_2)}w_\pm(\lambda;H_2,H_1)w_\pm(\lambda;H_1,H_0)\sqrt{\operatorname{Im}T_{\lambda+i0}(H_0)}.\end{aligned}$$

Here, the first equality follows from (7.28) and its analogue (7.33) in the case $y=0$, the second equality uses the multiplicative property of the off-axis wave matrix, while the final equality follows from (7.29) and (7.30) and their analogues (7.34) and (7.35).

The multiplicative property can now be used to prove the remaining properties. Firstly, it follows easily from the definition of the wave matrices (7.32) that $w_\pm(\lambda;H_0,H_0)=1$. Combining this with the multiplicative property, we have

$$\begin{aligned}w_\pm(\lambda;H_1,H_0)w_\pm(\lambda;H_0,H_1)&=w_\pm(\lambda;H_1,H_1)=1,\\w_\pm(\lambda;H_0,H_1)w_\pm(\lambda;H_1,H_0)&=w_\pm(\lambda;H_0,H_0)=1.\end{aligned}$$

From these equalities and the fact that $\|w_\pm(\lambda; H_1, H_0)\| \leq 1$, it follows that the wave matrices have norm 1 and are invertible with norm 1 inverses, from which it can be inferred that they are unitary and hence satisfy the equalities $w_\pm^*(\lambda; H_1, H_0) = w_\pm(\lambda; H_0, H_1)$. □

For any two self-adjoint operators $H_0$ and $H_1$ from $\mathcal{A}(F)$ and for any $z \in \Pi(H_0, F) \cap \Pi(H_1, F)$ the *(off-axis) scattering matrix* is defined by

$$S(z; H_1, H_0) := w^*(z; H_1, H_0) w(\bar{z}; H_1, H_0),$$

The theorem below collects properties of the scattering matrix which follow immediately from its definition and the properties of the wave matrices established in Theorem 7.19.

THEOREM 7.20. *Let $H_j$, $j = 0, 1, 2$, be self-adjoint operators from the rigged affine space $\mathcal{A}$ and let $z \in \bigcap_j \Pi(H_j, F)$ where $j$ varies through $\{0, 1\}$ or $\{0, 1, 2\}$ as appropriate. Then the operator $S(z; H_1, H_0)$ is unitary and satisfies the multiplicative identities*

$$S^*(z; H_1, H_0) = S(\bar{z}; H_1, H_0)$$

$$S(z; H_2, H_0) = w^*(z; H_1, H_0) S(z; H_2, H_1) w(\bar{z}; H_1, H_0),$$

$$S(z; H_2, H_0) = w^*(z; H_1, H_0) S(z; H_2, H_1) w(z; H_1, H_0) S(z; H_1, H_0), \tag{7.37}$$

Considering the symmetry of the scattering matrix expressed in the first equality above, there is little need to consider $z$ in the lower half-plane $\Pi_-(H_0, F) \cap \Pi_-(H_1, F)$ and we write $S(\lambda; H_1, H_0)$ and $S^*(\lambda; H_1, H_0)$ instead of $S(\lambda + i0; H_1, H_0)$ and $S(\lambda - i0; H_1, H_0)$.

The equality (7.37) (cf. [Yaf92, $(7.1.5)_+$]) will be useful in the next chapter.

THEOREM 7.21. *Let $H_0$ and $H_1 = H_0 \dotplus V$, $V = F^* J F$, be two self-adjoint operators from a rigged affine space $\mathcal{A}(F)$. For any $z \in \Pi_\pm(H_0, F) \cap \Pi_\pm(H_1, F)$, the (off-axis) scattering matrix satisfies the formula*

$$S(z; H_1, H_0) = 1 \mp 2i \sqrt{\operatorname{Im} T_z(H_0)} J (1 - T_z(H_1) J) \sqrt{\operatorname{Im} T_z(H_0)}. \tag{7.38}$$

Note that the off-axis scattering matrix is a unitary operator on the auxiliary Hilbert space $\mathcal{K}$, while the scattering matrix $S(\lambda; H_1, H_0)$ itself is a unitary operator on the fibre Hilbert space $\mathfrak{h}_\lambda(H_0)$. However as a consequence of (7.38), if $\lambda$ belongs to the intersection $\Lambda(H_0, F) \cap \Lambda(H_1, F)$, then the limit $S(\lambda + i0; H_1, H_0)$ of the off-axis scattering matrix is equal to $S(\lambda; H_1, H_0) \oplus 1$ acting on $\mathcal{K} = \mathfrak{h}_\lambda(H_0) \oplus \mathfrak{h}_\lambda(H_0)^\perp$.

Also note that using the second resolvent identity the factor $1 - T_z(H_1) J$ can be written as

$$\begin{aligned} 1 - T_z(H_1) J &= (1 + T_z(H_0) J)^{-1} (1 + T_z(H_0) J - (1 + T_z(H_0) J) T_z(H_1) J) \\ &= (1 + T_z(H_0) J)^{-1}. \end{aligned}$$

(Here we are assuming $T_z(H_0)$ is compact so that the proof of Lemma 4.1 implies the existence of the inverted factor.) Similarly, we could instead write $J(1 - T_z(H_1)J) = (1 - JT_z(H_1))J = (1 + JT_z(H_0))^{-1}J$.

With such an alteration so that only the operator $H_0$ and not $H_1$ appears on the right hand side, the equality (7.38) is known as the *stationary formula* for the scattering matrix.

PROOF. Let $z = \lambda + iy$, $y \geq 0$, where we assume $\lambda \in \Lambda(H_0, F) \cap \Lambda(H_1, F)$ if $y = 0$. Using (7.29) and (7.30), or (7.34) and (7.35), we obtain

$$\begin{aligned}\sqrt{\operatorname{Im} T_z(H_0)}&S(z; H_1, H_0)\sqrt{\operatorname{Im} T_z(H_0)} \\ &= (1 + T_{\bar{z}}(H_0)J) \operatorname{Im} T_z(H_1)(1 + JT_{\bar{z}}(H_0)) \\ &= \operatorname{Im} T_z(H_0)(1 - JT_z(H_1))(1 + JT_{\bar{z}}(H_0)).\end{aligned}$$

While it follows from the second resolvent identity that

$$\begin{aligned}(1 - JT_z(H_1))&(1 + JT_{\bar{z}}(H_0)) \\ &= 1 - JT_z(H_1) + J(1 - T_z(H_1)J)T_{\bar{z}}(H_0) \\ &= 1 - J(1 - T_z(H_1)J)T_z(H_0) + J(1 - T_z(H_1)J)T_{\bar{z}}(H_0) \\ &= 1 - 2iJ(1 - T_z(H_1)J) \operatorname{Im} T_z(H_0).\end{aligned}$$

Therefore, for any $f = F^*\varphi, g = F^*\psi \in \operatorname{ran} F^*$ we get

$$\begin{aligned}\langle \mathcal{E}_z(H_0)f, &S(z; H_1, H_0)\mathcal{E}_z(H_0)g\rangle \\ &= \langle \varphi, \operatorname{Im} T_z(H_0)\left[1 - 2iJ(1 - T_z(H_1)J) \operatorname{Im} T_z(H_0)\right] \psi\rangle \\ &= \langle \mathcal{E}_z(H_0)f, (\ldots)\, \mathcal{E}_z(H_0)g\rangle,\end{aligned}$$

where $(\ldots)$ stands for the right hand side of (7.38). This implies (7.38) by the density of the range of $\mathcal{E}_z(H_0)$, which is dense in $\mathcal{K}$ in the case that $y > 0$ and dense in $\mathfrak{h}_\lambda(H_0)$ in the case that $y = 0$. □

## 7.4. Connection to the time-dependent approach

In this section we show how the wave operators and the scattering operator can be built up from the wave matrices and scattering matrix. Let $H_0$ and $H_1$ be two self-adjoint operators from the rigged affine space $\mathcal{A}(F)$. Then with $\Lambda := \Lambda(H_0, F) \cap \Lambda(H_1, F)$, the *(partial) wave operators* $W_\pm(H_1, H_0; \Lambda)$ are defined by

$$\mathcal{E}(H_1)W_\pm(H_1, H_0; \Lambda)\mathcal{E}^*(H_0) = \int_\Lambda^\oplus w_\pm(\lambda; H_1, H_0)\, d\lambda. \tag{7.39}$$

Let $E_j$, $j = 0, 1$, denote the spectral measure of $H_j$. Since $\mathcal{E}(H_j)$ is an isomorphism of the subspace $E_j(\Lambda)\mathcal{H} \subset \mathcal{H}^{(a)}(H_j)$ and the direct integral $\mathcal{H}(H_j)$ by Theorem 7.12, the partial wave operators act

$$W_\pm(H_1, H_0; \Lambda)\colon E_0(\Lambda)\mathcal{H} \to E_1(\Lambda)\mathcal{H}, \tag{7.40}$$

but of course we can always extend them as zero on $E_0(\mathbb{R} \setminus \Lambda)\mathcal{H}$ in order to consider them acting on the main Hilbert space $\mathcal{H}$.

THEOREM 7.22. *Let $H_0$, $H_1$, and $H_2$ be self-adjoint operators from a rigged affine space $\mathcal{A}(F)$ and let $\Lambda := \bigcap_j \Lambda(H_j, F)$, where $j$ varies through $\{0,1\}$ or $\{0,1,2\}$ as appropriate. Then the (partial) wave operators are unitary and satisfy the equalities $W_\pm(H_0, H_0; \Lambda) = 1$, $W_\pm^*(H_1, H_0; \Lambda) = W_\pm(H_0, H_1; \Lambda)$, and the multiplicative property*

$$W_\pm(H_2, H_0; \Lambda) = W_\pm(H_2, H_1; \Lambda) W_\pm(H_1, H_0; \Lambda).$$

PROOF. This is a direct result of Theorem 7.19 and the properties of decomposable operators on direct integrals discussed in Section 2.4. □

THEOREM 7.23. *Let $H_0$, $H_1$, and $\Lambda$ be as in Theorem 7.22. For any bounded Borel function $\varphi$ on $\mathbb{R}$ whose support is a subset of $\Lambda$, there holds the intertwining property*

$$\varphi(H_1) W_\pm(H_1, H_0; \Lambda) = W_\pm(H_1, H_0; \Lambda)\varphi(H_0).$$

*Moreover, the wave operators establish a unitary equivalence of the self-adjoint operators $E_j(\Lambda)H_j$, $j = 0, 1$, and if they are extended as 0 to the whole Hilbert space $\mathcal{H}$, then*

$$H_1 W_\pm(H_1, H_0; \Lambda) = W_\pm(H_1, H_0; \Lambda) H_0.$$

PROOF. This result easily follows from the definition (7.39) and Theorem 7.12. For example, the first equality is established via

$$\begin{aligned}
\varphi(H_1) W_\pm(H_1, H_0; \Lambda) &= \varphi(H_1)\mathcal{E}^*(H_1)\mathcal{E}(H_1) W_\pm(H_1, H_0; \Lambda)\mathcal{E}^*(H_0)\mathcal{E}(H_0) \\
&= \mathcal{E}^*(H_1)\left(\int_\Lambda^\oplus \varphi(\lambda) w_\pm(\lambda; H_1, H_0)\, d\lambda\right)\mathcal{E}(H_0) \\
&= \mathcal{E}^*(H_1)\left(\int_\Lambda^\oplus w_\pm(\lambda; H_1, H_0)\, d\lambda\right)\mathcal{E}(H_0)\varphi(H_0) \\
&= W_\pm(H_1, H_0; \Lambda)\varphi(H_0).
\end{aligned}$$

For the last part, we note that the domain of $E_0(\Lambda)H_0$, which is equal to

$$\left\{ f \in \mathcal{H} : \int_\Lambda |\lambda|^2 \|(\mathcal{E}(H_0)f)(\lambda)\|^2\, d\lambda < \infty \right\},$$

is mapped by $W_\pm(H_1, H_0)$ to the domain of $E_1(\Lambda)H_1$ and use the strong convergence of $E(\Lambda_n)H \to E(\Lambda)H$ for bounded subsets $\Lambda_n \to \Lambda$. □

Now we will assume that the LAP holds in the sense that $\Lambda$ is a full set, in which case we write

$$W_\pm(H_1, H_0) := W_\pm(H_1, H_0; \Lambda).$$

In this case the following version of the Kato-Rosenblum Theorem is an immediate consequence of Theorem 7.23.

THEOREM 7.24. *Let $H_0$ and $H_1$ be self-adjoint operators from a rigged affine space $\mathcal{A}(F)$. Suppose $\Lambda(H_0, F)$ and $\Lambda(H_1, F)$ are full sets. Then the absolutely continuous parts of $H_0$ and $H_1$ are unitarily equivalent.*

Note that it follows from Theorem 7.24 and the LAP in the form of Corollary 3.14 that all operators from a resolvent comparable rigged affine space share a common absolutely continuous spectrum.

The next theorem confirms that the wave operators as defined by (7.39) agree with their usual time-dependent definition (7.1).

THEOREM 7.25. *Under the premise of Theorem 7.24, the wave operators* (7.40) *satisfy the equality*

$$W_\pm(H_1, H_0) = \underset{t\to\pm\infty}{s\text{-}\lim}\, e^{itH_1} e^{-itH_0} P^{(a)}(H_0),$$

*where $P^{(a)}(H_0)$ projects onto the absolutely continuous subspace $\mathcal{H}^{(a)}(H_0)$.*

PROOF. The proof employs a standard method, which proceeds as follows. We first check that the weak wave operators, which exist by Theorem 7.4, coincide with the constructive wave operators (7.40). Let $\Lambda := \Lambda(H_0, F) \cap \Lambda(H_1, F)$. It follows from the definition (7.39) of the constructive wave operators $W_\pm(H_1, H_0)$ that for any $f = F^*\varphi$ and $g = F^*\psi$ from the dense range of $F^*$,

$$\begin{aligned} \langle f, W_\pm(H_1, H_0)g\rangle &= \int_\Lambda \langle \mathcal{E}_\lambda(H_1)f, w_\pm(\lambda; H_1, H_0)\mathcal{E}_\lambda(H_0)g\rangle \, d\lambda \\ &= \int_\Lambda \lim_{y\to 0^+} \frac{y}{\pi} \langle R_{\lambda\pm iy}(H_1)f, R_{\lambda\pm iy}(H_0)g\rangle \, d\lambda. \end{aligned}$$

So by Theorem 7.8 the constructive wave operators coincide with the weak abelian wave operators and hence the weak wave operators. Theorem 7.2 now implies the existence of the strong wave operators, since the constructive wave operators satisfy the required multiplicative property by Theorem 7.22. Moreover, the strong wave operators must coincide with the weak and hence also the constructive wave operators. □

We conclude this section with a brief mention of the *scattering operator* $S(H_1, H_0)$, which can be defined constructively by

$$\mathcal{E}(H_0)S(H_1, H_0)\mathcal{E}^*(H_0) = \int_\Lambda^\oplus S(\lambda; H_1, H_0)\, d\lambda,$$

where $\Lambda = \Lambda(H_0, F) \cap \Lambda(H_1, F)$. The proof of the next theorem follows easily from the results already established and has been omitted.

THEOREM 7.26. *The scattering operator is unitary and satisfies the equality*

$$S(H_1, H_0) = W_+^*(H_1, H_0)W_-(H_1, H_0),$$

*as well as properties analogous to those of the scattering matrix given in Theorem 7.20. Also, the scattering operator commutes with $H_0$.*

CHAPTER 8

# The SSF and the scattering matrix

The first aim of this chapter is to establish the ordered exponential representation of the scattering matrix, which can be written as

$$(8.1)\quad S(\lambda; H_1, H_0) = \operatorname{Texp}\left(-2\pi i \int_0^1 w_+(\lambda; H_0, H_r)\mathcal{E}_\lambda(H_r)\dot{V}_r\mathcal{E}_\lambda^*(H_r)w_+(\lambda; H_r, H_0)\,dr\right),$$

where $H_r = H_0 \dotplus V_r$ is a piecewise analytic path connecting the self-adjoint operators $H_0$ and $H_1$ in a rigged affine space $\mathcal{A}(F)$ and $\lambda$ belongs to the intersection $\Lambda(H_0, F) \cap \Lambda(H_1, F)$. This representation is a little formal, because the adjoint $\mathcal{E}_\lambda^*(H_r)\colon \mathfrak{h}_\lambda(H_r) \to \mathcal{H}$ of the evaluation operator is not well-defined and $\dot{V}_r$ is strictly speaking not an operator on $\mathcal{H}$, but it is clarified by means of the decomposition $V_r = F^* J_r F$ via

$$\mathcal{E}_\lambda(H_r)\dot{V}_r\mathcal{E}_\lambda^*(H_r) := \frac{1}{\pi}\sqrt{\operatorname{Im} T_{\lambda+i0}(H_r)}\,\dot{J}_r\sqrt{\operatorname{Im} T_{\lambda+i0}(H_r)}.$$

By Proposition 2.20, the ordered exponential (8.1) is the unique solution to the ordinary differential equation

$$(8.2)\quad \frac{d}{dr}S(\lambda; H_r, H_0) = -2\pi i\, w_+(\lambda; H_0, H_r)\mathcal{E}_\lambda(H_r)\dot{V}_r\mathcal{E}_\lambda^*(H_r)w_+(\lambda; H_r, H_0)S(\lambda; H_r, H_0),$$

with the initial condition $S(\lambda; H_0, H_0) = 1$. Given the results of Chapter 7, proving (8.2) is quite straightforward as outlined in Chapter 1. The proof and its implications for the SSF are the topic of the upcoming section. Finally, in Section 8.2 we will see how the singular SSF can be represented as the singular $\mu$-invariant.

In this final chapter the trace condition introduced in Section 5.2 is reinstated; throughout, $\mathcal{A}(F)$ will denote a resolvent comparable rigged affine space. However we note that if it is merely assumed that $\mathcal{A}(F)$ is a rigged affine space, then Theorems 8.2 and 8.3 can be confirmed to hold when $\mathcal{L}_1$ is replaced with $\mathcal{L}_\infty$, by making obvious modifications to their proofs.

## 8.1. Scattering matrix as an ordered exponential

The group of unitary operators differing from 1 by a trace class operator will be denoted by

$$\mathcal{U}_1(\mathcal{K}) := \left\{U \in 1 + \mathcal{L}_1(\mathcal{K}) : U^* = U^{-1}\right\}$$

and equipped with the complete metric $(U, V) \mapsto \|U - V\|_1$.

Suppose $H_r = H_0 \dotplus F^* J_r F$ is an analytic path in the resolvent comparable rigged affine space $\mathcal{A}(F)$. Let $z = \lambda + iy$, $y \geq 0$, where if $y = 0$ we assume that $\lambda$ belongs to the full set $\Lambda(H_0, F; \mathcal{L}_1)$. For $r \in \mathbb{R}$ such that $z \in \Pi(H_r, F)$, consider the stationary formula

$$S(z; H_r, H_0) = 1 - 2i\sqrt{\operatorname{Im} T_z(H_0)} J_r (1 + T_z(H_0) J_r)^{-1} \sqrt{\operatorname{Im} T_z(H_0)}, \tag{8.3}$$

which follows from Theorem 7.21 and the second resolvent identity. By the resolvent comparability of $\mathcal{A}$, the operator $\sqrt{\operatorname{Im} T_z(H_0)}$ belongs to the Hilbert-Schmidt class $\mathcal{L}_2(\mathcal{K})$ and hence $S(z; H_r, H_0)$ belongs to $\mathcal{U}_1(\mathcal{K})$, provided that (8.3) holds. If $y > 0$, then it holds for all $r$. On the other hand if $y = 0$, then it holds as long as $r$ is not a resonance point of the path $H_r$.

The stationary formula (8.3) allows us to consider the scattering matrix as a function of the coupling parameter

$$r \mapsto S(z; H_r, H_0) \in \mathcal{U}_1(\mathcal{K}). \tag{8.4}$$

Since $H_r$ is analytic, the analytic Fredholm alternative implies that the factor $(1 + T_z(H_0)J_r)^{-1}$ is meromorphic. Hence in a neighbourhood of the real axis (8.4) is a meromorphic function. If $y > 0$ then (8.4) is in fact holomorphic in a neighbourhood of $\mathbb{R}$, since $(1 + T_z(H_0)J_r)^{-1}$ has no poles there by Lemma 4.1. If $y = 0$ then although the factor $(1 + T_{\lambda+i0}(H_0)J_r)^{-1}$ has poles at real resonance points from the discrete set $R(\lambda; \{H_r\})$, the scattering matrix is unitary and hence bounded for all non-resonant real $r$. Therefore (8.4) must admit analytic continuation to each real resonance point and thus the entire real axis.

PROPOSITION 8.1. *Let $H_r$ be a piecewise analytic path in the resolvent comparable rigged affine space $\mathcal{A}(F)$, whose pieces have endpoints which are non-resonant at $\lambda \in \Lambda(H_0, F; \mathcal{L}_1)$. Then with $z = \lambda + iy$, $y \geq 0$, the scattering matrix $S(z; H_r, H_0)$ is a piecewise analytic function of the coupling parameter $r$, with corresponding pieces.*

THEOREM 8.2. *Let $H_r = H_0 \dotplus F^* J_r F$ be a piecewise analytic path in $\mathcal{A}(F)$ whose pieces have endpoints at $r_j$, $j = 1, \ldots, n$. Let $z = \lambda + iy$, $y \geq 0$, where in the case that $y = 0$ it is assumed that $\lambda \in \bigcap_{j=1}^n \Lambda(H_{r_j}, F; \mathcal{L}_1)$. Then at any non-resonant real $r$,*

$$\frac{d}{dr} S(z; H_r, H_0) = \\ - 2iw(z; H_0, H_r)\sqrt{\operatorname{Im} T_z(H_r)}\, \dot{J}_r \sqrt{\operatorname{Im} T_z(H_r)}\, w(z; H_r, H_0) S(z; H_r, H_0), \tag{8.5}$$

*where the derivative is taken in the norm of $\mathcal{L}_1(\mathcal{K})$.*

Proof. We consider the case when $y = 0$; in case $y > 0$, the formula (8.5) holds for any real $r$ and the calculation is identical. Note that if $r$ is non-resonant, then since the resonance set $R(\lambda; \{H_r\})$ is discrete, so is $r + h$ for small $h$. The derivative of the meromorphic function $r \mapsto J_r(1+T_z(H_0)J_r)^{-1}$ appearing in the stationary formula (8.3) can be calculated for any non-resonant $r$ to be

$$\dot{J}_r(1 + T_z(H_0)J_r)^{-1} - J_r(1 + T_z(H_0)J_r)^{-1}T_z(H_0)\dot{J}_r(1 + T_z(H_0)J_r)^{-1},$$

yet since $J_0 = 0$ its derivative at 0 is simply $\dot{J}_0$. Hence it follows from the stationary formula that

$$\frac{d}{dr}\Big|_{r=0} S(\lambda; H_r, H_0) = -2i\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}\,\dot{J}_0\sqrt{\operatorname{Im} T_{\lambda+i0}(H_0)}. \tag{8.6}$$

By the identity (7.37), the scattering matrix satisfies

$$S(\lambda; H_{r+h}, H_0) = w_+(\lambda; H_0, H_r)S(\lambda; H_{r+h}, H_r)w_+(\lambda; H_r, H_0)S(\lambda; H_r, H_0)$$

for any non-resonant $r$ and $r + h$. Thus

$$\frac{d}{dr}S(\lambda; H_r, H_0) = \\ w_+(\lambda; H_0, H_r)\frac{d}{dh}S(\lambda; H_{r+h}, H_r)\Big|_{h=0} w_+(\lambda; H_r, H_0)S(\lambda; H_r, H_0)$$

and the proof is completed by substituting (8.6). □

Using the notation of Theorem 8.2, consider the $\mathcal{L}_1$-valued function of the coupling parameter

$$A(z; r) := w(z; H_0, H_r)\sqrt{\operatorname{Im} T_z(H_r)}\,\dot{J}_r\sqrt{\operatorname{Im} T_z(H_r)}\,w(z; H_r, H_0). \tag{8.7}$$

It follows from (8.5) and the unitarity of the scattering matrix that this function, although only defined for non-resonant values of $r$ in the case that $y = 0$, admits analytic continuation to real resonance points. Thus by taking its trace and using the fact that $w_+(\lambda; H_r, H_0)w_+(\lambda; H_0, H_r) = 1$ we obtain another proof of Lemma 6.2, which was used to show the equality of the singular SSF with the total resonance index.

Theorem 8.2 along with Proposition 2.20 imply an ordered exponential representation of the scattering matrix.

Theorem 8.3. *Let $H_r$ and $z = \lambda + iy$ be as in Theorem 8.2. For non-resonant $r$,*

$$S(z; H_r, H_0) = \operatorname{Texp}\left(-2i\int_0^r A(z; s)\,ds\right),$$

*where the $\mathcal{L}_1$-valued integrand is given by* (8.7).

Because the derivative (8.5) is considered in the trace class norm, we also obtain the following theorem from Proposition 2.22 and the cyclic property of the trace.

THEOREM 8.4. *Let $H_r$ and $z = \lambda + iy$ be as in Theorem 8.2. For non-resonant $r$ there is the formula*

$$\det S(z; H_r, H_0) = \exp\left(-2i \int_0^r \operatorname{Tr}\left(\dot{J}_s \operatorname{Im} T_z(H_s)\right) ds\right). \tag{8.8}$$

This theorem can be interpreted as a variant of the Birman-Kreĭn formula. The original formula can be recovered as follows. For $y > 0$, the formula (8.8) can be rewritten as

$$\det S(z; H_1, H_0) = e^{-2\pi i\, \xi(z; H_1, H_0)}, \tag{8.9}$$

where $\xi(z; H_1, H_0)$ is the smoothed SSF (5.47), whose limit as $y \to 0^+$ is a.e. equal to the SSF $\xi(\lambda; H_1, H_0)$. On the other hand, it follows from the stationary formula that for any $\lambda$ from the set $\Lambda(H_0, F; \mathcal{L}_1) \cap \Lambda(H_1, F; \mathcal{L}_1)$, the off-axis scattering matrix $S(\lambda + iy; H_1, H_0)$ converges in $\mathcal{U}_1(\mathcal{K})$ to $S(\lambda; H_1, H_0) \oplus 1$ as $y \to 0^+$. Therefore, taking the limit of (8.9) as $y \to 0^+$ proves

COROLLARY 8.5. *For any two operators $H_0$ and $H_1$ from a resolvent comparable rigged affine space $\mathcal{A}$ and for a.e. $\lambda \in \mathbb{R}$, the SSF is and the scattering matrix are related by the formula*

$$\det S(\lambda; H_1, H_0) = e^{-2\pi i \xi(\lambda; H_1, H_0)}. \tag{8.10}$$

In addition to the classical Birman-Kreĭn formula (8.10), Theorem 8.4 explicitly gives the formula

$$\det S(\lambda; H_1, H_0) = \exp\left(-2i \int_0^1 \operatorname{Tr}(\dot{J}_r \operatorname{Im} T_{\lambda+i0}(H_r))\, dr\right).$$

for any $\lambda \in \bigcap_{j=1}^n \Lambda(H_{r_j}, F; \mathcal{L}_1)$. In view of Theorem 5.31, we obtain

COROLLARY 8.6. *For any piecewise analytic path $H_r$ in resolvent comparable rigged affine space $\mathcal{A}$ and a.e. $\lambda \in \mathbb{R}$, the absolutely continuous SSF and the scattering matrix are related by the formula*

$$\det S(\lambda; H_1, H_0) = e^{-2\pi i \xi^{(a)}(\lambda; \{H_r\})}. \tag{8.11}$$

Combining (8.10) and (8.11) gives the equality

$$e^{-2\pi i\, \xi^{(s)}(\lambda; \{H_r\})} = 1.$$

Thus we have again proved the integer-valuedness of the singular SSF, this time along any piecewise analytic path $H_r$.

COROLLARY 8.7. *For any piecewise analytic path $H_r$ in a resolvent comparable rigged affine space $\mathcal{A}$ and for a.e. $\lambda \in \mathbb{R}$, the value of the singular SSF $\xi^{(s)}(\lambda; \{H_r\})$ belongs to $\mathbb{Z}$.*

## 8.2. Singular SSF as singular $\mu$-invariant

The ordered exponential representation of the scattering matrix allows the equality of the singular SSF and the so called singular $\mu$-invariant to be proved using (a simplified version of) the argument appearing in [Aza11a]. We conclude this document by sketching the proof, which relies on properties of the spectral flow of unitary operators in $\mathcal{U}_1(\mathcal{K})$.

Note that any unitary operator $S \in \mathcal{U}_1(\mathcal{K})$ has its spectrum lying on the unit circle $\mathbb{T}$ and by Weyl's theorem (Theorem 2.18) its essential spectrum is the singleton $\{1\}$. The countable set of isolated eigenvalues of finite multiplicity forming its discrete spectrum can thus only accumulate at 1. Intuitively, if $S$ varies continuously then its eigenvalues should trace out continuous but possibly overlapping paths. This is supported by the theorem below, which provides a convenient approach to the definition of spectral flow.

THEOREM 8.8. *Suppose $S = S(r)$ is a continuous path of operators in $\mathcal{U}_1(\mathcal{K})$. Then the eigenvalues of $S$ can be continuously enumerated in the sense that there exists a (non-unique) sequence of continuous functions $z_j$, $j = 1, 2, \dots,$ such that for all $r$ the multiset $\{z_1(r), z_2(r), \dots\}^*$ coincides with the spectrum of $S(r)$, counting multiplicities of all points except 1.*

A multiset is in essence a set allowing repetitions or multiplicities of its elements, in this case equivalent to an unordered sequence. The multiplicity of the point 1 is assumed to be infinite. The spectra of operators in $\mathcal{U}_1(\mathcal{K})$ can obviously be modelled by such multisets.

Theorem 8.8 can be divided into two parts, one of which can be seen as an infinite-dimensional analogue of Theorem II-5.2 in [Kat84] on the continuous enumeration of paths in the space $\mathbb{C}^n_{\mathrm{sym}}$ of unordered $n$-tuples of complex numbers. For a detailed proof of this result see e.g. [ADT15] (also [Aza10]). The proof is not as straightforward as its statement might suggest, nevertheless the problem can be reduced to the finite-rank case by focusing first on those eigenvalues outside of a neighbourhood of the accumulation point. The argument applies to continuous paths in the space $\mathcal{S}_p(\mathbb{X}, x_0)$, which consists of countable multi-subsets of a metric space $\mathbb{X}$, each of which is assumed to contain the fixed point $x_0$ with infinite multiplicity while all other multiplicities are finite. Moreover, each multiset $S \in \mathcal{S}_p(\mathbb{X}, x_0)$ is required to be $p$-summable in the sense that

$$\left\| \{d(x_0, z_j)\}_{j\in\mathbb{N}} \right\|_p := \left( \sum_{j=1}^{\infty} d(x_0, z_j)^p \right)^{1/p} < \infty,$$

where $d$ is the metric of $\mathbb{X}$ and $\{z_j\}$ is some enumeration of $S$. (In fact the $p$-norm can be replaced by any symmetric norm, see e.g. [GK69] for a definition.) The space $\mathcal{S}_p(\mathbb{X}, x_0)$ is equipped with the metric given by

$$d_p(S_1, S_2) = \inf \left\| \left\{ d(z_j^1, z_j^2) \right\}_{j\in\mathbb{N}} \right\|_p ,$$

where the infimum is taken of all enumerations $\{z_j^1\}$ and $\{z_j^2\}$ of the multisets $S_1$ and $S_2$.

The continuity of a path $S = \{z_1, z_2, \ldots\}^*$ in $\mathcal{S}_p(\mathbb{X}, x_0)$ implies the uniform convergence

$$\Big\| \{d(x_0, z_{n+j})\}_{j\in\mathbb{N}} \Big\|_p \to 0, \quad \text{as} \quad n \to \infty. \tag{8.12}$$

Briefly, the continuity of $S$ implies that of $S_n = \{z_{n+1}, z_{n+2}, \ldots\}^*$ which in turn implies that of each function of the sequence (8.12). Hence this decreasing sequence of continuous functions, which converges to 0 pointwise, must converge uniformly by Dini's Theorem. (Assuming the symmetric norm is regular, as e.g. are the $p$-norms, then the converse also holds; see [ADT15] for details.) Since $\|\cdot\|_\infty \leq \|\cdot\|_p$, it follows from (8.12) that all but finitely many of the paths $z_j$ have their images contained in an arbitrarily small neighbourhood of the fixed point $x_0$.

In obvious analogy to the case when $p = 1$ we can define the space of unitary operators $\mathcal{U}_p(\mathcal{K})$. The remaining part of Theorem 8.8 is the fact that for any two operators $S_1$ and $S_2$ from $\mathcal{U}_p(\mathcal{K})$, there exist enumerations $\{z_j^1\}$ and $\{z_j^2\}$ of their eigenvalues, such that

$$\Big\| \big\{ |z_j^1 - z_j^2| \big\}_{j\in\mathbb{N}} \Big\|_p \leq \text{const.}\, \|S_1 - S_2\|_p.$$

For a proof of this inequality see e.g. [BS88] (also [Aza10]). It follows that as $S$ varies continuously in the space of unitary operators $\mathcal{U}_p(\mathcal{K})$, its spectrum $\sigma(S)$ varies continuously in the multiset space $\mathcal{S}_p(\mathbb{T}, 1)$.

Suppose that $S$ is a continuous path in $\mathcal{U}_p(\mathcal{K})$. The functions $z_j$ from a continuous enumeration of $S$ can be used to define the spectral flow. We will only need to consider paths which begin at 1, so suppose $S(0) = 1$. It is convenient to lift the functions $z_j$ on $\mathbb{T}$ to the functions $\theta_j$ on $\mathbb{R}$ which are chosen so that $\theta_j(0) = 0$. Let $\lceil x \rceil$ denote the smallest integer greater or equal to $x \in \mathbb{R}$. Then for $\theta \in (0, 2\pi)$ the *spectral flow* can be defined by the formula

$$\mu(\theta; S) := \sum_{j=1}^{\infty} \left\lceil \frac{\theta_j(1) - \theta}{2\pi} \right\rceil, \tag{8.13}$$

which counts the number of times the eigenvalues $z_j(r)$ of $S(r)$ cross a given point $e^{i\theta} \in \mathbb{T}$ as the path is traversed. This definition is correct in the sense that the sum is finite, as implied by (8.12), and therefore it does not depend on the continuous enumeration. Note also that if $S(0) = S(1) = 1$, then $\mu(\theta; S)$ does not depend on the angle $\theta$.

As an aside, it is of course unnecessary to assume that $S(0) = 1$ in order to define the spectral flow. For the formula (8.13) to be valid it must be assumed that $\theta_j(0) \in (\theta - 2\pi, \theta]$, but an alternative description is

$$\mu(\theta; S) = \sum_{j=1}^{\infty} \begin{pmatrix} \#\{k \in \mathbb{Z} : \theta_j(0) < \theta + 2k\pi \le \theta_j(1)\} \\ \qquad - \#\{k \in \mathbb{Z} : \theta_j(1) \le \theta + 2k\pi < \theta_j(0)\} \end{pmatrix},$$

where $\#$ denotes cardinality. The spectral flow of a continuous path $S$ in $\mathcal{U}_p(\mathcal{K})$ has the following properties (for proof see e.g. [ADT15; Aza10]). It is path additive: if $S_1 \sqcup S_2$ is the concatenation of two paths $S_1$ and $S_2$, then $\mu(\theta; S_1 \sqcup S_2) = \mu(\theta; S_1) + \mu(\theta; S_2)$. It is a homotopy invariant: if two paths $S_1$ and $S_2$ are homotopic relative to their endpoints, then $\mu(\theta; S_1) = \mu(\theta; S_2)$. (In fact it can be shown to define a group isomorphism, under appropriate assumptions on $\mathbb{X}$, from the fundamental group $\pi_1(\mathcal{S}_p(\mathbb{X}, x_0), \{x_0\}^*)$ to the first singular homology group $H_1(\mathbb{X})$.)

Our focus will now be on a continuous path $S$ in the space $\mathcal{U}_1(\mathcal{K})$. In this case the series $\sum_j |z_j - 1|$, is uniformly convergent. Indeed, it is continuous due to the continuity of $\{z_1, z_2, \dots\}^*$ in $S_1(\mathbb{T}, 1)$ and the inequality

$$\left| \sum_{j=1}^{\infty} |z_j(r) - 1| - \sum_{j=1}^{\infty} |z_j(s) - 1| \right| \le \sum_{j=1}^{\infty} |z_j(r) - z_j(s)|,$$

and therefore its sequence of partial sums converges uniformly by Dini's Theorem. Because only finitely many eigenpaths $z_j$ may leave a neighbourhood of 1 and since $|\theta| \le |e^{i\theta} - 1|$ for small enough $\theta$, it follows that the series $\sum_j \theta_j$ is uniformly absolutely-convergent and hence continuous.

The average spectral flow $\xi(S)$ of the path $S$ will be denoted

$$\xi(S) = -\frac{1}{2\pi} \int_0^{2\pi} \mu(\theta; S)\, d\theta.$$

Proposition 8.9. *Let $S$ be a path in $\mathcal{U}_1(\mathcal{K})$ with $S(0) = 1$ and let $z_j = e^{i\theta_j}$, with $\theta_j(0) = 0$, $j = 1, 2, \dots$, be a continuous enumeration of the eigenvalues of $S$. Then the average spectral flow of $S$ can be written as*

$$\xi(S) = -\frac{1}{2\pi} \sum_{j=1}^{\infty} \theta_j(1). \tag{8.14}$$

*Let $S_r$ denote the restriction of the path $S$ in $\mathcal{U}_1(\mathcal{K})$ to the interval $[0, r]$. Then it follows that the function $r \mapsto \xi(S_r)$ is continuous.*

Proof. In this proof we follow [Aza10, Lemma 5.10]. For any $j$, suppose $\alpha_j \in [0, 2\pi)$ and $k \in \mathbb{Z}$ are such that $\theta_j(1) = \alpha_j + 2k\pi$, in which case $\theta_j$ makes $k$ windings around $\mathbb{T}$ as the path is traversed. Then we find that

$$\int_0^{2\pi} \left\lceil \frac{\theta_j(1) - \theta}{2\pi} \right\rceil d\theta = \alpha_j(k+1) + (2\pi - \alpha_j)k = \theta_j(1), \tag{8.15}$$

since the integrand is equal to $k + 1$ if $\theta < \alpha_j$ and $k$ otherwise. Note that the series $\sum_j \theta_j(1)$ is absolutely convergent and further that the absolute value of (8.15) can be moved inside the integral. Therefore, an interchange of sum and integral is justified and the result is

$$\int_0^{2\pi} \mu(\theta; S)\, d\theta = \int_0^{2\pi} \sum_{j=1}^{\infty} \left\lceil \frac{\theta_j(1) - \theta}{2\pi} \right\rceil d\theta = \sum_{j=1}^{\infty} \theta_j(1). \qquad \square$$

By the equality (2.24), the determinant of any $S(r) \in \mathcal{U}_1(\mathcal{K})$ with eigenvalues $z_j(r) = e^{i\theta_j(r)}$, $j = 1, 2, \ldots$, is given by

$$\det S(r) = \prod_{j=1}^{\infty} e^{i\theta_j(r)} = \exp\left( i \sum_{j=1}^{\infty} \theta_j(r) \right).$$

Therefore by combining this with equality (8.14), we arrive at another representation of the average spectral flow.

LEMMA 8.10. *Let $S$ be a continuous path in $\mathcal{U}_1(\mathcal{K})$ with $S(0) = 1$ and let $S_r$ be its restriction to $[0, r]$. Then its average spectral flow is given by the formula*

$$\xi(S_r) = -\frac{1}{2\pi i} \log \det S(r), \tag{8.16}$$

*where the branch of the logarithm is chosen so that the right hand side is continuous.*

Returning now to the scattering matrix, suppose $H_0$ and $H_1$ are two self-adjoint operators from the resolvent comparable rigged affine space $\mathcal{A}(F)$. For any $\lambda$ from the full set $\Lambda(H_0, F; \mathcal{L}_1) \cap \Lambda(H_1, F; \mathcal{L}_1)$, the scattering matrix $S(\lambda; H_1, H_0)$ can be naturally connected with the identity in two different ways. One way is to send the imaginary part of the spectral parameter $\lambda$ from 0 to $+\infty$. Let $S_1$ denote the path

$$S_1 \colon [0, 1] \ni t \mapsto S(\lambda + iy(t); H_1, H_0) \in \mathcal{U}_1(\mathcal{K}), \quad y(t) = (1 - t)t^{-1}.$$

Note that the stationary formula (7.38) and Corollary 3.6 imply that this path is indeed continuous at $t = 0$, where its value is the identity. Following A. B. Pushnitski ([Pus01]), we define the *$\mu$-invariant* as the spectral flow

$$\mu(\theta, \lambda; H_1, H_0) := \mu(\theta; S_1).$$

Consider applying the formula (8.16) to the path $S_1$. Let $z = \lambda + iy$ for $y > 0$ and let $\mu(\theta, z; H_1, H_0)$ denote the spectral flow of the path $S_1$ restricted to the interval $[0, r]$ with $r = (y + 1)^{-1}$. In other words, $\mu(\theta, z; H_1, H_0)$ is the spectral flow of the off-axis scattering matrix as the spectral parameter changes from $\infty$ to $z$. Then from Theorem 8.4 and Lemma 8.10 we obtain a formula for the smoothed SSF:

$$\begin{aligned} \xi(z; H_1, H_0) &= -\frac{1}{2\pi i} \log \det S(z; H_1, H_0) \\ &= -\frac{1}{2\pi} \int_0^{2\pi} \mu(\theta, z; H_1, H_0)\, d\theta. \end{aligned}$$

Moreover, since the smoothed SSF converges a.e. to the SSF $\xi(\lambda; H_1, H_0)$ by (5.50), it follows that for a.e. $\lambda \in \mathbb{R}$

$$\xi(\lambda; H_1, H_0) = -\frac{1}{2\pi} \int_0^{2\pi} \mu(\theta, \lambda; H_1, H_0)\, d\theta. \tag{8.17}$$

Since the right hand side of the equality (8.17) is defined for any $\lambda$ from the full set $\Lambda(H_0, F; \mathcal{L}_1) \cap \Lambda(H_1, F; \mathcal{L}_1)$, it can be considered as an explicit representation of the SSF.

Another way to connect $S(\lambda; H_1, H_0)$ with 1 is to send $H_1$ to $H_0$ along a piecewise analytic path $H_r$ in the affine space $\mathcal{A}(F)$, whose endpoints are not resonant at $\lambda$. Let $S_2 = S_2(\{H_r\})$ be the path

$$S_2 \colon [0,1] \ni r \mapsto S(\lambda; H_r, H_0) \in \mathcal{U}_1(\mathcal{K}),$$

which is continuous by Proposition 8.1. As in [Aza11a], we define the *absolutely continuous $\mu$-invariant* as the spectral flow

$$\mu^{(a)}(\theta, \lambda; \{H_r\}) := \mu(\theta; S_2).$$

The difference $\mu^{(s)}(\lambda; \{H_r\}) := \mu(\theta; S_1) - \mu(\theta; S_2)$, which does not depend on $\theta$, is by definition the *singular $\mu$-invariant.*

By applying formula (8.16) to the path $S_2$ and using Theorem 8.4, we arrive at the equality

$$\xi^{(a)}(\lambda; \{H_r\}) = -\frac{1}{2\pi} \int_0^{2\pi} \mu^{(a)}(\theta, \lambda; \{H_r\})\, d\theta, \tag{8.18}$$

which holds for any $\lambda \in \bigcap_{j=1}^n \Lambda(H_{r_j}, F; \mathcal{L}_1)$, where the intersection is taken over the endpoints $H_{r_j}$ of the pieces of the path $H_r$. This can be considered as an explicit representation of the absolutely continuous SSF. Combining it with (8.17) also provides an explicit representation of the singular SSF.

THEOREM 8.11. *Let $H_r$ be a piecewise analytic path of self-adjoint operators from a resolvent comparable rigged affine space $\mathcal{A}$. Then for a.e. $\lambda \in \mathbb{R}$ the singular SSF coincides with (the negative of) the singular $\mu$-invariant*

$$\xi^{(s)}(\lambda; \{H_r\}) = -\mu^{(s)}(\lambda; \{H_r\}).$$

PROOF. Suppose the SSF and the absolutely continuous SSF are explicitly represented by (8.17) and (8.18) for $\lambda$ from the full set $\bigcap_j \Lambda(H_{r_j}, F; \mathcal{L}_1)$, where $H_{r_j}$, $j = 1, \ldots, n$, are the endpoints of the pieces of the path $H_r$. Combining these equalities, we find that

$$\begin{aligned}
\xi^{(s)}(\lambda; \{H_r\}) &= -\frac{1}{2\pi} \int_0^{2\pi} \Big(\mu(\theta, \lambda; H_1, H_0) - \mu^{(a)}(\theta, \lambda; \{H_r\})\Big)\, d\theta \\
&= -\frac{1}{2\pi} \int_0^{2\pi} \mu^{(s)}(\lambda; \{H_r\})\, d\theta \\
&= -\mu^{(s)}(\lambda; \{H_r\}),
\end{aligned}$$

which completes the proof not only this last theorem, but also of Theorem 1.1. □

# Index of Notation


| | | |
|---|---|---|
| $\mathcal{A}_0$ | real Banach space of perturbations of the form $V = F^*JF$ associated with $\mathcal{A}$ | 49 |
| $\mathcal{A}$ | rigged affine space of self-adjoint operators over $\mathcal{A}_0$ | 49 |
| $C_c(\mathbb{R})$ | space of compactly-supported continuous functions with inductive limit topology | 15 |
| $C_c^\infty(\mathbb{R})$ | space of test functions | 16 |
| $\mathbb{C}$ | field of complex numbers | |
| $\mathbb{C}_+$ | open upper half-plane | |
| $\mathbb{C}_-$ | open lower half-plane | |
| $E$ | (with possible subindices) spectral measure of $H$ | |
| $\mathcal{E}(H)$ | $= \int_\Lambda^\oplus \mathcal{E}_\lambda(H)\,d\lambda$ unitary operator $\mathcal{H} \to \mathcal{H}(H)$ which diagonalises the absolutely continuous part of $H$ | 115 |
| $\mathcal{E}_\lambda(H)$ | evaluation operator $\operatorname{ran} F^* \to \mathfrak{h}_\lambda(H)$ | 115 |
| $F$ | rigging operator $\mathcal{H} \to \mathcal{K}$ | 37 |
| $H$ | (with possible subindices) self-adjoint operator on $\mathcal{H}$ | |
| $H_r$ | path of self-adjoint operators | |
| $\mathcal{H}$ | main Hilbert space | |
| $\mathcal{H}(H)$ | $= \int_\Lambda^\oplus \mathfrak{h}_\lambda(H)\,d\lambda$ direct integral in which the absolutely continuous part of $H$ acts as multiplication by $\lambda$ | 115 |
| $\mathfrak{h}_\lambda(H)$ | fibre Hilbert space of $\mathcal{H}(H)$ | 114 |
| $\operatorname{ind}_{res}$ | resonance index | 58 |
| $J$ | bounded self-adjoint operator on $\mathcal{K}$ | |
| $\mathcal{K}$ | auxiliary Hilbert space | |
| $L_p$ | space of $p$-integrable functions | |
| $\mathcal{L}_p$ | $p$-th Schatten ideal of compact operators | 28 |
| $r$ | coupling parameter of $H_r = H_0 + rV$ (or a more general path $H_r$) | |
| $r_z$ | resonance point corresponding to $z$ | 57 |
| $R_z(H)$ | $= (H - z)^{-1}$ resolvent of $H$ | |
| $\mathbb{R}$ | field of real numbers | |

| | | |
|---|---|---|
| $S(z)$ | (off-axis) scattering matrix | 122 |
| $T_z(H)$ | $= FR_z(H)F^*$ sandwiched resolvent | 38 |
| $U_z(H)$ | unitary operator in the polar decomposition of $R_z(H)F^*$ | 117 |
| $\mathcal{U}_1$ | group of unitary operators from $1 + \mathcal{L}_1$ | 128 |
| $V$ | symmetric perturbation | |
| $w(z)$ | (off-axis) wave matrix | 118 |
| $y$ | imaginary part of the spectral parameter $z$ | |
| $z$ | spectral parameter $z = \lambda \pm iy$ | |
| $\lambda$ | real part of the spectral parameter $z$ | |
| $\Lambda$ | set of regular points $\lambda$ | 43 |
| $\mu(\theta; S)$ | spectral flow on $\mathcal{U}_1$ | 132 |
| $\mu^{(s)}$ | singular $\mu$-invariant | 135 |
| $\xi(\lambda)$ | spectral shift function | 85 |
| $\xi(\varphi)$ | spectral shift measure | 85 |
| $\xi(z)$ | smoothed spectral shift function | 88 |
| $\xi^{(a)}(\lambda)$ | absolutely continuous spectral shift function | 90 |
| $\xi^{(a)}(\varphi)$ | absolutely continuous spectral shift measure | 90 |
| $\xi^{(s)}(\lambda)$ | singular spectral shift function | 90 |
| $\xi^{(s)}(\varphi)$ | singular spectral shift measure | 90 |
| $\Pi$ | domain of the spectral parameter $z$; union of $\mathbb{C} \setminus \mathbb{R}$ with two copies of the set of regular points $\Lambda$ | 54 |
| $\Pi_+$ | union of $\mathbb{C}_+$ and $\Lambda$ | 54 |
| $\Pi_-$ | union of $\mathbb{C}_-$ and $\Lambda$ | 54 |
| $\rho(H)$ | resolvent set of $H$ | |
| $\sigma(H)$ | spectrum of $H$ | |
| $\sigma_{ess}$ | common essential spectrum of operators from $\mathcal{A}$ | 50 |
| $\Phi$ | infinitesimal spectral shift measure $\Phi$ | 82 |
| $\Phi^{(a)}$ | absolutely continuous part of $\Phi$ | 88 |
| $\Phi^{(s)}$ | singular part of $\Phi$ | 88 |

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