Advanced functional analysis

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1 Introduction

This course will mostly deal with the analysis of unbounded operators on a Hilbert or Banach space with a particular focus on Schrödinger operators arising in quantum mechanics. All the abstract notions presented in the course will be motivated and illustrated by concrete examples. In order to be able to present some of the more interesting material, emphasis will be put on the ideas of proofs and their conceptual understanding rather than the rigorous verification of every little detail.

After introducing the basic notions relevant here (adjoint, closed operator, spectrum, etc), we will work towards our first milestone: the spectral decomposition theorem. Once this is established, we will discuss the different types of spectrum (pure point, essential, etc) and present Weyl's criteria which tells us to which category a given point in the spectrum belongs to.

If time permits, we will also discuss some of the basic results in the theory of analytic semigroups and a simplified version of Calderón-Zygmund's interpolation theory.

The second part of the course will be mainly devoted to the study of Schrödinger operators, which are operators of the form $H = -\Delta + V$ where Δ is the Laplacian and V is a potential function. One of the most important abstract results in their study is the Kato-Rellich theorem which gives a very easily verifiable and essentially sharp criterion in terms of V for H to be essentially selfadjoint. We will then apply this criterion to the study of the hydrogen atom.

Another question of interest is to characterise the essential spectrum of a Schrödinger operator in terms of its potential. We will present Weyl's stability theorem for the essential spectrum under relatively compact perturbations as well as Rellich's criterion for the absence of essential spectrum.

1.1 Prerequisites

I will assume that the basic notions of functional analysis have already been mastered. In particular, one should be familiar with the notions of Hilbert and Banach space, reflexivity, separability, the Hahn-Banach theorem, the open mapping theorem, and the spectral decomposition theorem for compact operators.

1.2 References

Most of the material of these notes is taken in some form or the other from one of the following references:

M. Reed and B. Simon, *Methods of Modern Mathematical Physics*
K. Yosida, *Functional Analysis*
T. Katō, *Perturbation Theory for Linear Operators*

2 Unbounded operators

Let $\mathcal{B}$ and $\bar{\mathcal{B}}$ be two Banach spaces.

Definition 2.1 An unbounded operator T from $\mathcal{B}$ to $\bar{\mathcal{B}}$ consists of a linear subspace $\mathcal{D}(T) \subset \mathcal{B}$, called the *domain* of T, as well as a linear map $T\colon \mathcal{D}(T) \to \bar{\mathcal{B}}$, where we make the usual abuse of notation of identifying an operator with the corresponding linear map.

An alternative way of viewing unbounded operators is to identify T with its *graph*, which is the set $\Gamma(T) = \{(x,y) \in \mathcal{B} \times \bar{\mathcal{B}} \,:\, x \in \mathcal{D}(T)\,,\; y = Tx\}$. In this way, an unbounded operator is nothing but a linear subspace T of $\mathcal{B} \times \bar{\mathcal{B}}$ with the property that if $(0,y) \in T$, then $y = 0$.

Remark 2.2 Unless explicitly specified, we will always assume that $\mathcal{D}(T)$ is dense in $\mathcal{B}$ and that $\mathcal{B}$ is separable, i.e. there exists a countable dense subset of $\mathcal{B}$.

One typical example is given by $\mathcal{B} = \bar{\mathcal{B}} = L^2(\mathbf{R})$, $\mathcal{D}(T) = \mathcal{C}_0^\infty(\mathbf{R})$, the space of smooth compactly supported functions, and

$$(Tf)(x) = \frac{d^2 f}{dx^2}(x)\;,$$

for any such smooth function f.

2.1 Closed operators

Typically, just as in the example just given, there is no natural way of extending T to a linear map defined on all of $\mathcal{B}$. This is not to say that it is *impossible* to do so, just that any such extension would have rather strange properties. One way of formulating this rigorously is to introduce the notion of a *closed* operator:

Definition 2.3 An operator T from $\mathcal{B}$ to $\bar{\mathcal{B}}$ is closed if $\Gamma(T)$ is a closed subset of $\mathcal{B} \times \bar{\mathcal{B}}$.

One maybe more intuitive way of stating this is to say that T is closed if, whenever (x_n) is a sequence of elements in $\mathcal{D}(T)$ converging to some element $x \in \mathcal{B}$ is such that the sequence (Tx_n) converges to some $y \in \bar{\mathcal{B}}$, one has $x \in \mathcal{D}(T)$ and $Tx = y$. Equivalently, if $x_n \to 0$ and $Tx_n \to y$, then one necessarily has $y = 0$.

An operator T is *closable*, if the closure of its graph is again the graph of an unbounded operator. We call this new operator the *closure* of T and denote it by $\bar{T}$. By definition, $\bar{T}$ is an *extension* of T in the sense that the graph of $\bar{T}$ contains the graph of T.

Exercise 2.4 *Convince yourself that our definitions are set up in such a way that if T is closable, then $\bar{T}$ is its smallest closed extension. Show furthermore by contradiction that if T is not closable, then it admits no closed extension.*

Note however that a given operator T could have more than one closed extension, even if it already defined on a dense subspace of $\mathcal{B}$! This is illustrated by the following example:

Example 2.5 *Take $\mathcal{H} = L^2([0,1])$ and define an operator $T\colon \mathcal{H} \to \mathcal{H}$ by setting $\mathcal{D}(T) = \mathcal{C}_0^\infty([0,1])$ and setting $(Tf)(x) = f'(x)$. Here, we denote by $\mathcal{C}_0^\infty([0,1])$ the set of smooth functions which vanish at the boundaries of the interval $[0,1]$.*

We first claim that T is closable. Indeed, let f_n be any sequence of elements in $\mathcal{C}_0^\infty$ such that $f_n \to 0$ in $\mathcal{H}$ and such that $g_n \stackrel{def}{=} Tf_n$ converges in $\mathcal{H}$ to some function g. Note now that, for every n, one has the identity

$$f_n(x) = \int_0^x g_n(y)\,dy\;.$$

(In particular, one must have $\int_0^1 g_n(y)\,dy = 0$ for every n.) An elementary estimate then shows that if $g_n \to g$ in $\mathcal{H}$, one also has $f_n \to f$ with $f(x) =$

$\int_0^x g(y)\,dy$. Since f is identically 0 by assumption, it follows at once that g vanishes almost everywhere, so that $g = 0$ as an element in $\mathcal{H}$.

This argument also shows that the domain $\mathcal{D}(\bar{T})$ of the closure $\bar{T}$ of T consists of all functions $f \in \mathcal{H}$ that are absolutely continuous, vanish at 0 and at 1, and have a weak derivative that is itself an element of $\mathcal{H}$. Consider now the operator $\hat{T}$ whose domain consists of all absolutely continuous functions with weak derivative in $\mathcal{H}$ (i.e. without the assumption that they vanish at the boundaries). If we then set $\hat{T}f$ to be the weak derivative of f, a similar calculation to before shows that $\hat{T}$ is also a closed linear operator. Furthermore, it is obviously an extension of $\bar{T}$.

Example 2.6 *Take $\mathcal{H}$ as above and let this time T be the linear operator given by*

$$(Tf)(x) = f(1/2)\,\sin(\pi x)\;,$$

with domain given by $\mathcal{C}_0^\infty$ as before. The operator T is not closable. This is seen very easily by considering the sequence $f_n(x) = \sin^n(\pi x)$. Indeed, one has $f_n \to 0$ in $\mathcal{H}$, but $(Tf_n)(x) = \sin(\pi x)$ independently of n.

We then have the following result:

Proposition 2.7 *An operator $T\colon \mathcal{B} \to \bar{\mathcal{B}}$ with domain $\mathcal{D}(T) = \mathcal{B}$ is bounded if and only if it is closed.*

Proof. The fact that bounded implies closed is trivial, so we only need to prove the converse.

By assumption, $\Gamma(T)$ is closed so that it is itself a Banach space under the norm $\|(x,y)\| = \|x\|_{\mathcal{B}} + \|y\|_{\bar{\mathcal{B}}}$. Consider now the projection operators Π_1 and Π_2 from $\Gamma(T)$ into $\mathcal{B}$ and $\bar{\mathcal{B}}$ respectively, namely

$$\Pi_1(x,y) = x\;, \qquad \Pi_2(x,y) = y\;.$$

Since the domain of T is all of $\mathcal{B}$ by assumption, the map Π_1 is a bijection. Furthermore, since $y = Tx$ for every $(x,y) \in \Gamma(T)$, one has the identity

$$Tx = \Pi_2 \Pi_1^{-1} x\;.$$

Since Π_2 is obviously bounded, the boundedness of T now follows from the boundedness of Π_1. This on the other hand is an immediate consequence of the open mapping theorem. Indeed, the latter states that a bounded linear surjection from a Banach space onto an other one maps open sets into open sets, so that its inverse must necessarily be continuous. □

The following is an extremely important corollary of this fact:

Corollary 2.8 *If $T: \mathcal{B} \to \bar{\mathcal{B}}$ is a closed operator which is a bijection from $\mathcal{D}(T)$ to $\bar{\mathcal{B}}$, then its inverse T^{-1} is a bounded operator from $\bar{\mathcal{B}}$ to $\mathcal{B}$.*

Proof. Note that $\Gamma(T^{-1})$ is obtained from $\Gamma(T)$ by simply switching the two components. □

Remark 2.9 In the case where $\mathcal{B}$ and $\bar{\mathcal{B}}$ are separable (i.e. they contain a countable dense subset), then a rather surprising by L. Schwartz states that if T is a *measurable* linear map defined on all of $\mathcal{B}$, then it is necessarily bounded. Since pretty much every function that can be described unambigously is measurable, this is another example of a statement showing that unbounded operators cannot be extended to the whole space in any reasonable way.

2.2 Dual and adjoint operators

A very important notion is that of the *dual* of a linear operator. Recall that, given a Banach space $\mathcal{B}$, its dual space $\mathcal{B}^*$ consists of all bounded linear functionals from $\mathcal{B}$ to **R**, endowed with the operator norm. With this notation, we have the following:

Definition 2.10 Let $T: \mathcal{B} \to \bar{\mathcal{B}}$ be a densely defined linear operator. Its dual operator $T': \bar{\mathcal{B}}^* \to \mathcal{B}^*$ is defined on the set $\mathcal{D}(T')$ of all $\ell \in \bar{\mathcal{B}}^*$ such that there exists $m \in \mathcal{B}^*$ with the property that the identity

$$m(x) = \ell(Tx)\;, \tag{1}$$

holds for every $x \in \mathcal{D}(T)$. We then set $T'\ell = m$.

In the particular case where $\mathcal{B} = \bar{\mathcal{B}} = \mathcal{H}$ is a separable Hilbert space, we use Riesz's representation theorem to identify $\mathcal{H}^*$ with $\mathcal{H}$. One can then identify the dual of T with an operator from $\mathcal{H}$ to $\mathcal{H}$ which we call the *adjoint* T^* of T. More formally, if we denote by $J: \mathcal{H} \to \mathcal{H}^*$ the map given by Riesz's representation theorem, then we set $T^* = J^{-1}T'J$. Note that the map J is *antilinear* in the sense that $J(\lambda x) = \bar{\lambda} Jx$ for any complex number λ. One can easily see that this is necessary if one wants J to be such that $(Jx)(x) = \|x\|^2$.

Definition 2.11 Given a separable Hilbert space $\mathcal{H}$ and a densely defined closed operator $T: \mathcal{H} \to \mathcal{H}$, we say that T is *selfadjoint* if $T^* = T$.

Remark 2.12 There is subtlety in the above definition, which is that we should not only have $T^*x = Tx$ for every $x \in \mathcal{D}(T)$, but we also impose that $\mathcal{D}(T^*) = \mathcal{D}(T)$. If T is only such that, for every pair (x, y) in $\mathcal{D}(T)$, one has the identity $\langle x, Ty \rangle = \langle Tx, y \rangle$, then we say that T is *symmetric*. As we will see later on, the notion of a symmetric operator is strictly weaker than that of a selfadjoint operator.

Remark 2.13 Since $\mathcal{D}(T)$ is dense, (1) defines m on a dense subset of $\mathcal{B}$. Since by assumption m is furthermore a bounded linear functional, this determines it uniquely, so that T^* is indeed a linear operator.

Remark 2.14 The adjoint of an operator is not necessarily densely defined! Consider indeed Example 2.6. Then, by the usual identification of $\mathcal{H}^*$ with $\mathcal{H}$, $\mathcal{D}(T^*)$ consists of those functions $g \in L^2$ such that there exists $h \in L^2$ with

$$\int_0^1 h(x) f(x)\, dx = f(1/2) \int_0^1 g(x) \sin(\pi x)\, dx \;, \tag{2}$$

for every smooth and compactly supported function f. This is clearly impossible since any such h would have some support away from $\frac{1}{2}$ which in turn means that it is possible to find a smooth f vanishing at $\frac{1}{2}$ and such that the left hand side of (2) doesn't vanish, leading to a contradiction unless the right hand side also vanishes.

As a consequence, $\mathcal{D}(T^*)$ consists only of those elements $g \in \mathcal{H}$ that are orthogonal to $\sin(\pi x)$ and one has $T^*g = 0$.

The previous remark suggests that the problem of T^* not being densely defined and that of T not being closable might be related. This is indeed the case. Before proving it though, we need the following preliminary result. Recall that if $V \subset \mathcal{B}$ is a (not necessarily closed) subspace of some Banach space, then its orthogonal complement $V^\perp$ is defined as the subspace of $\mathcal{B}^*$ given by

$$V^\perp = \{\ell \in \mathcal{B}^* \,:\, \ell(x) = 0 \;\forall x \in V\} \;. \tag{3}$$

Note that this is a straightforward extension of the usual notion of orthogonal complement in Hilbert spaces. The usual result then holds:

Proposition 2.15 *The space $V^\perp$ is always closed. Furthermore, if $\mathcal{B}$ is reflexive, then one has $(V^\perp)^\perp = \bar{V}$, the closure of V.*

Proof. The fact that $V^\perp$ is closed follows immediately from (3). Regarding $(V^\perp)^\perp$, it follows from the reflexivity of $\mathcal{B}$ that we have the identity

$$(V^\perp)^\perp = \{y \in \mathcal{B} \,:\, \ell(y) = 0\ \forall \ell \in V^\perp\}\;.$$

Assume now that there exists some $y \in (V^\perp)^\perp$ which is not in the closure of V. By linearity, we can assume that $\|y\| = 1$ and that there exists $\delta > 0$ such that $\|y - x\| \ge \delta$ for every $x \in V$.

Denote now by W the closure of the space $V + \lambda y$ in $\mathcal{B}$. Note that any $z \in W$ can be written in a unique way as $z = x + \lambda y$ with $x \in \bar{V}$ and $\lambda \in \mathbf{R}$. Furthermore, it follows by assumption that $\|z\|/\lambda \ge \delta$, so that $\lambda \le \|z\|/\delta$. As a consequence, the linear functional $\ell\colon W \to \mathbf{R}$ given by $\ell(x + \lambda y) = \lambda$ is bounded and so can be extended to all of $\mathcal{B}$ by the Hahn-Banach theorem. The resulting element of $\mathcal{B}^*$ belongs to $V^\perp$ by construction, but it satisfies $\ell(y) = 1$, which is in contradiction with the fact that $y \in (V^\perp)^\perp$. □

This result can now be applied to the study of the dual of a closed operator, yielding the following result:

Proposition 2.16 *The dual of a densely defined operator $T\colon \mathcal{B} \to \bar{\mathcal{B}}$ is always a closed operator. Furthermore, if $\mathcal{B}$ and $\bar{\mathcal{B}}$ are reflexive, then T' is densely defined if and only if T is closable.*

Proof. Let us identify the dual of $\mathcal{B} \times \bar{\mathcal{B}}$ with $\bar{\mathcal{B}}^* \times \mathcal{B}^*$ under the duality relation

$$\langle (\ell, m), (x, y)\rangle = \langle \ell, y\rangle - \langle x, m\rangle\;.$$

With this notation, it follows from the definitions that the graph $\Gamma(T')$ of T' is precisely given by $\Gamma(T)^\perp$, so that it is necessarily closed by Proposition 2.15.

Applying Proposition 2.15 again, we also conclude that if the domain of T' is dense, then we can define its dual $(T')'$ and one has

$$\Gamma((T')') = \Gamma(T')^\perp = (\Gamma(T)^\perp)^\perp = \overline{\Gamma(T)}\;.$$

Since $\Gamma((T')')$ is the graph of a linear operator, this shows that T is closable and that $(T')' = \bar{T}$, as required.

It remains to show that $\mathcal{D}(T')$ is dense if T is closable. Assuming by contradiction that it isn't, we can again find an element $\ell \in \bar{\mathcal{B}}^*$ and a value $\delta > 0$ such that $\|\ell\| = 1$ and such that $\|\ell - \bar{\ell}\| \ge \delta$ for every $\bar{\ell} \in \mathcal{D}(T')$. Similarly to before, this implies that we can exhibit an element $y \in (\bar{\mathcal{B}}^*)^* = \bar{\mathcal{B}}$ with the property that

$\ell(y) = 1$, but $\bar{\ell}(y) = 0$ for every $\bar{\ell} \in \mathcal{D}(T')$. This implies that $(0, y) \in \Gamma(T')^\perp$. Since on the other hand we have just seen that $\Gamma(T')^\perp = \overline{\Gamma(T)}$, this implies that $\overline{\Gamma(T)}$ is not the graph of a single-valued operator, which in turn implies that T isn't closable. □

Example 2.17 *Let us consider again Example 2.5. For $f \in \mathcal{C}_0^\infty$ and $g \in \mathcal{C}^\infty$ (i.e. g is not required to vanish at the boundaries), we have the identity*

$$\langle g, Tf \rangle = \int_0^1 g(x) f'(x)\, dx = -\int_0^1 g'(x) f'(x)\, dx = -\langle g', f \rangle \;.$$

It follows that all such functions belong to the domain of T^* and that $T^* g = -g'$ there.

2.3 The spectrum

We now have all the ingredients at hand to define the spectrum of an unbounded operator. There are several characterisations of it, we choose to take the following as our definition:

Definition 2.18 Given a closed operator $T\colon \mathcal{B} \to \mathcal{B}$, a complex number $\lambda \in \mathbf{C}$ belongs to the *resolvent set* $\varrho(T)$ of T if the operator $x \mapsto \lambda x - Tx$ is a bijection between $\mathcal{D}(T)$ and $\mathcal{B}$. The *spectrum* $\sigma(T)$ of T is then defined as the complement of the resolvent set.

Remark 2.19 In principle, the definition given above also makes sense for operators that aren't closed. However, it turns out that in this case one always has $\sigma(T) = \mathbf{C}$, so that the notion of spectrum is rather useless in this case.

Given $\lambda \in \varrho(T)$, the operator $(\lambda - T)^{-1}$, which is bounded by Corollary 2.8, is called the *resolvent* of T at λ. There are various ways in which $\lambda x - Tx$ might fail to be a bijection. For example, it might fail to be injective. By linearity, this then implies the existence of an eigenvector x of T with eigenvalue λ, i.e. a non-zero element $x \in \mathcal{D}(T)$ such that $Tx = \lambda x$. If this is the case, we say that λ belongs to the *point spectrum* $\sigma_{\rm pp}(T)$.

On the other hand, $\lambda x - Tx$ might fail to be surjective. If λ is such that it isn't an eigenvalue of T but the range of $\lambda - T$ is nevertheless not even dense in $\mathcal{B}$, then we say that λ belongs to the *residual spectrum* $\sigma_{\rm re}(T)$. Elements in the residual spectrum are slightly unusual: we will see that they do not exist if T is selfadjoint for example. Elements in $\sigma(T) \setminus \sigma_{\rm re}(T)$ on the other hand behave "almost" like eigenvalues of T in the sense that they admit approximate eigenfunctions:

Proposition 2.20 *One has $\lambda \in \sigma(T) \setminus \sigma_{\rm re}(T)$ if and only if there exists a sequence $x_n \in \mathcal{D}(T)$ with $\|x_n\| = 1$ and*

$$\lim_{n\to\infty} \|Tx_n - \lambda x_n\| = 0 \;.$$

(In general, the sequence x_n does not converge to a limit though...)

Proof. If $\lambda \in \sigma_{\rm pp}(T)$, the statement is trivial, so we can assume that $\lambda - T$ is injective and has dense range (otherwise one would have $\lambda \in \sigma_{\rm re}(T)$). It follows that $(\lambda - T)^{-1}$ is a closed operator with domain given by the range of $\lambda - T$. (It is closed because its graph is just the transpose of the graph of $\lambda - T$ which is closed.)

Since the range of $\lambda - T$ is not all of $\mathcal{B}$ by the definition of the spectrum, it follows from Proposition 2.7 that the operator $(\lambda - T)^{-1}$ is unbounded. As a consequence, one can find a sequence y_n with $\|y_n\| = 1$ and $\|(\lambda - T)^{-1} y_n\| \to \infty$. The claim now follows by setting

$$x_n = \frac{(\lambda - T)^{-1} y_n}{\|(\lambda - T)^{-1} y_n\|} \;,$$

which is easily seen to have the required properties. □

Example 2.21 *Let $\mathcal{H} = L^2(\mathbf{R})$ and let T be the closure of the operator $f \mapsto \frac{d^2 f}{dx^2}$ defined on $\mathcal{C}_0^\infty$. In this case, one has $\sigma(T) = \mathbf{R}_-$.*

We can see that $\lambda \in \mathbf{C} \setminus \mathbf{R}_-$ belongs to the resolvent set by building an explicit inverse to $\lambda - T$. Indeed, denote by $\sqrt{\lambda}$ the square root of λ with strictly positive real part (such a square root exists unless $\lambda \in \mathbf{R}_-$) and let $f_\lambda \colon \mathbf{R} \to \mathbf{C}$ be the function defined by

$$f_\lambda(x) = \frac{e^{-\sqrt{\lambda}|x|}}{2\sqrt{\lambda}} \;.$$

We then define an operator M_λ by

$$(M_\lambda g)(x) = \int_{\mathbf{R}} f_\lambda(x-y) g(y)\, dy \;.$$

Since f_λ is in L^1, it follows from Young's inequality that M_λ is indeed a bounded operator on L^2. Performing two integrations by part, an explicit calculation then shows that, at least for $g \in \mathcal{C}_0^\infty$, one has the identity $(\lambda - T)M_\lambda g = g$, as required.

To show that every $\lambda = -\omega^2 \in \mathbf{R}_-$ lies in the spectrum of T, it suffices to exhibit some g in L^2 such that it is impossible to find f with $(-\omega^2 - T)f = g$.

Take some function g which is compactly supported in $[0,1]$. Then any function f with $(\omega^2+T)f=-g$ must satisfy $Tf=-\omega^2 f$ outside of $[0,1]$. Since for $\omega\in\mathbf{R}$, all solutions to this equation are of the form $A_1\exp(i\omega x)+A_2\exp(-i\omega x)$ for some $A_1,A_2\in\mathbf{C}$, and since these functions are square integrable if and only if they vanish, one must have $f=0$ outside of $[0,1]$. The problem is therefore reduced to solving the equation

$$\frac{d^2f(x)}{dx^2}=-\omega^2 f(x)-g(x)\;, \tag{4}$$

constrained to satisfy $f(0)=f(1)=f'(0)=f'(1)=0$. Since f is determined uniquely on $[0,1]$ by (4) and the initial condition $f(0)=f'(0)=0$, it is straightforward to see that one can find functions g such that the boundary condition at 1 is violated.

Exercise 2.22 *Build explicit sequences of approximate eigenfunctions for $\lambda\in\mathbf{R}_-$ in the previous example.*

Exercise 2.23 *Show that for every $x\in\mathcal{D}(T)$ and every $\lambda\in\varrho(T)$ one has the identity $(\lambda-T)^{-1}(\lambda-T)x=x$.*

Denote from now on the *resolvent* of T by $R_\lambda=R_\lambda(T)=(\lambda-T)^{-1}$, for every $\lambda\in\varrho(T)$. One then has:

Proposition 2.24 *The set $\varrho(T)$ is open and the map $\lambda\mapsto R_\lambda$ is analytic on $\varrho(T)$ in the operator norm. Furthermore, for any two points $\lambda,\mu\in\varrho(T)$ one has the identity*

$$R_\lambda-R_\mu=(\mu-\lambda)R_\mu R_\lambda\;. \tag{5}$$

In particular, the operators R_λ all commute.

Proof. A formal calculation suggests that if we set

$$\tilde R_\mu=R_\lambda\Big(1+\sum_{n=1}^\infty(\lambda-\mu)^n R_\lambda^n\Big)\;, \tag{6}$$

then one actually has $\tilde R_\mu=R_\mu$ for μ sufficiently close to λ. Note first that the right hand side of the above expression does indeed converge as soon as $|\lambda-\mu|<1/\|R_\lambda\|$. Furthermore, one has

$$(\mu-T)\tilde R_\mu=(\mu-\lambda)\tilde R_\mu+(\lambda-T)\tilde R_\mu=(\mu-\lambda)\tilde R_\mu+\Big(1+\sum_{n=1}^\infty(\lambda-\mu)^n R_\lambda^n\Big)$$

$$= (\mu - \lambda) R_\lambda - \sum_{n=2}^\infty (\lambda - \mu)^n R_\lambda^n + 1 + \sum_{n=1}^\infty (\lambda - \mu)^n R_\lambda^n = 1 \;,$$

which is precisely what was claimed. It follows immediately that, given $\lambda \in \varrho(T)$, one also has

$$\{\mu \in \mathbf{C} \,:\, |\lambda - \mu| < 1/\|R_\lambda\|\} \subset \varrho(T) \;,$$

which shows that $\varrho(T)$ is open. Furthermore, R_μ is given by a norm convergent power series there, so it is analytic.

The identity (5) follows immediately from the fact that

$$R_\lambda - R_\mu = R_\lambda (\mu - T) R_\mu - R_\lambda (\lambda - T) R_\mu \;.$$

(The fact that the operators commute is obtained by simply interchanging λ and μ.) □

A useful notion for bounded operators is that of their spectral radius:

$$r(T) = \sup_{\lambda \in \sigma(T)} |\lambda| \;.$$

In general, the spectral radius is less than the norm of T. However, it can be approximated to arbitrary precision by considering the norm of a sufficiently high power of T. More precisely, one has:

Proposition 2.25 *Let $T \colon \mathcal{B} \to \mathcal{B}$ be bounded. Then*

$$r(T) = \lim_{n \to \infty} \|T^n\|^{1/n} = \inf_{n \ge 1} \|T^n\|^{1/n} \;.$$

Furthermore, if T is selfadjoint, then $\|T\| = r(T)$.

Proof. The claim is trivial if $T = 0$, so we assume that $T \neq 0$ from now on. We first show that

$$\lim_{n \to \infty} \frac{1}{n} \log \|T^n\| = \inf_{n \ge 1} \frac{1}{n} \log \|T^n\| \;, \tag{7}$$

which shows that the above expression makes sense. Indeed, given a fixed value n, we can rewrite any integer $m \ge n$ as $m = kn + d$ with $d < n$. One then has

$$\frac{1}{m} \log \|T^m\| \le \frac{\log \|T^n\|^k \|T\|^d}{kn + d} \le \frac{\log \|T^n\|}{n} + \frac{\log \|T\|^d}{m} \;,$$

so that one has the bound

$$\limsup_{m\to\infty} \frac{1}{m} \log \|T^m\| \le \frac{1}{n} \log \|T^n\| \;.$$

This immediately implies that the identity (7) holds.

In order to obtain the relation with the spectral radius, it remains to show that the Laurent series for R_λ around ∞ converges for every $\lambda > \lim_{n\to\infty} \|T^n\|^{1/n}$. This on the other hand follows almost immediately from the explicit identity

$$R_\lambda = \lambda^{-1}\Big(1 + \sum_{n\ge 1} \frac{T^n}{\lambda^n}\Big) \;,$$

which can be checked in a way that is very similar to (6).

For the last statement, note first that if T is selfadjoint, then on the one hand one has $\|T^2\| \le \|T\|^2$, and on the other hand

$$\|T^2\| \ge \sup_{\|x\|=1} \langle x, T^2 x\rangle = \sup_{\|x\|=1} \|Tx\|^2 = \|T\|^2 \;,$$

so that $\|T^2\| = \|T\|^2$. The claim follows at once. □

Example 2.26 *One very nice example illustrating the different kind of spectra is given by the shift operator. Let $\mathcal{B} = \ell^1$ and set*

$$T(x_0, x_1, \ldots) = (x_1, x_2, \ldots) \;.$$

In this case, the dual space $\mathcal{B}^*$ is given by ℓ^∞ and one has the identity

$$T'(x_0, x_1, \ldots) = (0, x_0, x_1, \ldots) \;.$$

It is easy to see that T and T' have norm 1, so that every λ with $|\lambda| > 1$ belongs to the resolvent set. It is clear that every λ with $|\lambda| < 1$ belongs to the spectrum of T since the vector $x_\lambda = (1, \lambda, \lambda^2, \ldots)$ belongs to ℓ^1 and is an eigenvector with eigenvalue λ.

Since the spectrum is closed and since the spectrum of T' equals the spectrum of T, it follows that $\sigma(T) = \sigma(T') = \{\lambda \in \mathbf{C} \,:\, |\lambda| \le 1\}$. One also easily sees that the equation $T'x = \lambda x$ cannot have any non-zero solution in ℓ^∞ for any $\lambda \in \mathbf{C}$, so that T' has no point spectrum at all.

Let now $|\lambda| < 1$ and note that since $(\lambda - T)x_\lambda = 0$, one has $((\lambda - T')y)(x_\lambda) = 0$ for every $y \in \ell^\infty$. Since on the other hand it is easy to find elements $z \in \ell^\infty$

such that $z(x_\lambda) \neq 0$ and since evaluation against x_λ is a continuous operation, this shows that the range of $\lambda - T'$ cannot be dense. As a consequence, every such λ belongs to the residual spectrum of T'.

In order to obtain a full classification of the spectrum of T and T', it remains to consider λ on the unit circle. Clearly, such points do not belong to the point spectrum of T since $x_\lambda \notin \ell^1$. On the other hand, if λ were in the residual spectrum of T, then one could find some element $y \in \ell^\infty$ such that $y((\lambda - T)x) = 0$ for every $x \in \ell^1$. This however would imply that $(\lambda - T')y = 0$, so that λ would be in the point spectrum of T', which we have already shown is empty...

Finally, we show that every λ with $|\lambda| = 1$ does also belong to the residual spectrum of T'. For this, we proceed similarly to the case $|\lambda| < 1$, but we use an approximation argument. Let $\lambda_n = (1 - 2^{-n})\lambda$ (say) so that $|\lambda_n| < 1$ and so that

$$\|x_{\lambda_n}\|_{\ell^1} = \sum_{k\geq 0} |\lambda_n^k| = \frac{1}{1 - |\lambda_n|} = 2^n \;.$$

For any $y \in \ell^\infty$, one then has

$$|((\lambda - T')y)(x_{\lambda_n})| = |(\lambda - \lambda_n)\, y(x_n)| \leq \|y\|_{\ell^\infty} \;,$$

uniformly in n. On the other hand, one has $\|x_{\bar\lambda}\|_{\ell^\infty} = 1$ and

$$|x_{\bar\lambda}(x_{\lambda_n})| = \sum_{k\geq 0} \bar\lambda^k \lambda_n^k = 2^n \;.$$

As a consequence, one has

$$\begin{aligned}\|(\lambda - T')y - x_{\bar\lambda}\|_{\ell^\infty} &= \sup_{\|x\|_{\ell^1}=1} ((\lambda - T')y - x_{\bar\lambda})(x) \\ &\geq \sup_{n\geq 1} 2^{-n} |((\lambda - T')y - x_{\bar\lambda})(x_{\lambda_n})| \\ &\geq \sup_{n\geq 1} (1 - 2^{-n}\|y\|_\infty) = 1 \;,\end{aligned}$$

which shows that $x_{\bar\lambda}$ does not belong to the closure of the range of $(\lambda - T')$.

Exercise 2.27 *Show that it is a general fact that if $\lambda \in \sigma_{\rm re}(T)$ then $\lambda \in \sigma_{\rm pp}(T')$.*

We conclude this section with the following fundamental result about the spectrum of selfadjoint operators.

Proposition 2.28 *If T is selfadjoint, then $\sigma(T) \subset \mathbf{R}$. Furthermore, T cannot have any residual spectrum and any two eigenvectors of T with different eigenvalues are orthogonal.*

Proof. The proof relies on the fact that, for λ and μ real, one has the identity

$$\|(T - \lambda + i\mu)x\|^2 = \|(T - \lambda)x\|^2 + \mu^2\|x\|^2 \geq \mu^2\|x\|^2 \; . \tag{8}$$

In particular, this shows that $T - \lambda + i\mu$ is injective and has closed range. If its range wasn't the whole space then $\lambda - i\mu$ would be in the residual spectrum of T. This however would imply that $\lambda + i\mu$ is in the point spectrum of $T^* = T$, which is again impossible by (8). Therefore, $T - \lambda + i\mu$ is a bijection, so that $\lambda - i\mu \in \varrho(T)$ as required.

The fact that T has no residual spectrum is then an immediate consequence of Exercise 2.27. The last statement is proven in the same way as for finite-dimensional matrices. □

3 The spectral theorem

One of the most important theorems in finite-dimensional linear algebra states that every normal matrix (in particular every Hermitian matrix) can be diagonalised by a unitary change of basis. In other words, if $T\colon \mathbf{C}^n \to \mathbf{C}^n$ is a normal matrix, then there exists a basis $\{x_k\}_{k=1}^n$ of $\mathbf{C}^n$ and complex values $\{\lambda_k\}_{k=1}^n$ such that $Tx_k = \lambda_k x_k$.

In this case, if $F\colon \sigma(T) \to \mathbf{C}$ is *any* function, then there is a natural way of making sense of the expression $F(T)$. Indeed, one would simply set

$$F(T)x_k = F(\lambda_k)x_k \; .$$

Note that this definition is automatically consistent with the intuitive facts that if $F(t) = 1/t$, one obtains the inverse of T (provided that no eigenvalue vanishes), if $F(t) = t^2$, one obtains the square of T in the sense of matrix multiplication, etc. The aim of this section is to provide a far-reaching generalisation of these facts for unbounded selfadjoint operators. The immediate question that arises is: what does it actually mean to "diagonalise" a selfadjoint operator T?

A naïve guess would be to say that one can find an orthonormal basis $\{e_n\}_{n\geq 0}$ of $\mathcal{H}$ such that each of the e_n belongs to $\mathcal{D}(T)$ and such that $Te_n = \lambda_n e_n$ for some values λ_n. However, we have already seen that operators on infinite-dimensional spaces admit values in their spectrum for which there are no corresponding "true" eigenfunctions, only "approximate" eigenfunctions. Consider for example the space $\mathcal{H} = L^2(\mathbf{R})$ and an arbitrary (possibly unbounded) function $\Lambda: \mathbf{R} \to \mathbf{R}$. One can then define the operator "multiplication by Λ" by

$$\mathcal{D}(T) = \{f \in L^2 \,:\, \Lambda f \in L^2\} \;, \qquad (Tf)(x) = f(x)\Lambda(x) \;.$$

It is straightforward to verify that T is selfadjoint. (In general, if Λ is complex-valued, then T is still normal, but we haven't defined this notion for unbounded operators...) In some sense, T is also "diagonal": for every $x \in \mathbf{R}$, δ_x is *formally* an eigenvector with eigenvalue $\Lambda(x)$. Furthermore, and most importantly, for a multiplication operator as above and a function $F: \mathbf{R} \to \mathbf{R}$, it is straightforward to define what we mean by $F(T)$: this should simply be the multiplication operator by $F \circ \Lambda$.

This motivates the following result, which is the main theorem in this section:

Theorem 3.1 *Let T be a selfadjoint operator on some separable Hilbert space $\mathcal{H}$. Then, there exists a measure space (E, μ), a unitary operator $K: \mathcal{H} \to L^2(E, \mu)$, and a function $\Lambda: E \to \mathbf{R}$ such that*

$$\mathcal{D}(T) = \{f \in \mathcal{H} \,:\, \Lambda K f \in L^2(E, \mu)\} \;, \quad (KTf)(\lambda) = \Lambda(\lambda)(Kf)(\lambda) \;, \qquad (9)$$

where $\lambda \in E$.

Remark 3.2 Separability isn't actually needed, but the proof then requires transfinite induction...

3.1 Bounded selfadjoint operators

We first show that if T is a bounded selfadjoint operator, then there is a consistent way of making sense of $F(T)$ as long as the map $F: \sigma(T) \to \mathbf{C}$ is *continuous*. Note that since $\sigma(T)$ is both bounded and closed, it is compact. The idea then is to use the Stone-Weierstrass theorem which states that every continuous function defined on a compact subset of $\mathbf{R}$ can be approximated by polynomials in the supremum norm.

As a consequence, we can build a continuous functional calculus as soon as we have the following result:

Proposition 3.3 *Let $T: \mathcal{H} \to \mathcal{H}$ be a bounded selfadjoint operator and let P be a polynomial. Then, one has the identity $\|P(T)\| = \sup_{\lambda \in \sigma(T)} |P(\lambda)|$.*

Proof. Note first that, similarly to the last argument of Proposition 2.25, one has

$$\|P(T)\|^2 = \|P(T)^* P(T)\| = \|(\bar{P}P)(T)\| \ .$$

It then follows from Proposition 2.25 that

$$\|P(T)\|^2 = \sup_{\lambda\in\sigma((\bar{P}P)(T))} |\lambda| \ .$$

It therefore remains to argue that $\lambda \in \sigma(\bar{P}P(T))$ if and only if there exists $\mu \in \sigma(T)$ such that $\lambda = |P(\mu)|^2$.

Write $Q = \bar{P}P$. If $\mu \in \sigma(T)$, then $Q(x) - Q(\mu) = (x-\mu)\tilde{Q}(x)$ for some polynomial $\tilde{Q}$. As a consequence, $Q(T)-Q(\mu) = (T-\mu)\tilde{Q}(T) = \tilde{Q}(T)(T-\mu)$, so that since $(T-\mu)$ fails to either be surjective or injective, so does $Q(T)-Q(\mu)$, thus implying that $Q(\mu) \in \sigma(Q(T))$.

Conversely, if $\lambda \in \sigma(Q(T))$, then we can factor the polynomial $x \mapsto Q(x)-\lambda$ as

$$Q(x) - \lambda = C(x-\mu_1)\cdots(x-\mu_n) \ ,$$

where n is the degree of Q. We claim that one of the μ_k necessarily belongs to $\sigma(T)$, which then shows the claim since $Q(\mu_k) - \lambda = 0$ by construction. This however follows immediately by contradiction, noting that otherwise the operator $C^{-1}(T-\mu_n)^{-1}\cdots(T-\mu_1)^{-1}$ would provide an inverse for $Q(x)-\lambda$, in contradiction with the fact that $\lambda \in \sigma(Q(T))$. □

Corollary 3.4 *The map $F \mapsto F(T)$ is an isometry from $\mathcal{C}_b(\sigma(T))$ into the space of bounded operators on $\mathcal{H}$. Furthermore, one has the identities $F(G(T)) = (F \circ G)(T)$, $(FG)(T) = F(T)G(T)$, $F(T)^* = \bar{F}(T)$, and $(cF)(T) = cF(T)$. If x and λ are such that $Tx = \lambda x$, then $F(T)x = F(\lambda)x$. Finally, $\sigma(F(T)) = F(\sigma(T))$.*

Proof. Proposition 3.3 shows that $F \mapsto F(T)$ is an isometry when restricted to polynomials. Since these are dense in $\mathcal{C}_b(\sigma(T))$ by Stone-Weierstrass, the first claim follows. The identities in the second claim are stable under norm convergence and hold in the case of polynomials, so they hold for all $F \in \mathcal{C}_b(\sigma(T))$. A similar argument shows that $F(T)x = F(\lambda)x$ if $Tx = \lambda x$.

For the last statement, it is easy to see that $\sigma(F(T)) \subset F(\sigma(T))$. Actually, one verifies the contrapositive, namely that if $\lambda \in \varrho(T)$, then $F(\varrho) \in \varrho(F(T))$. Indeed, it suffices to verify that by approximating the function $G(x) = 1/(x - F(\lambda))$ with bounded continuous functions, one can ensure that the operator $(G \circ F)(T)$ is indeed a bounded inverse for $F(T) - F(\lambda)$.

If $\lambda \in \sigma(T)$, then it follows from Proposition 2.20 and Exercise 2.27 that for every $\varepsilon > 0$ there exists x_ε with $\|x_\varepsilon\| = 1$ such that

$$\|(T - \lambda)x_\varepsilon\| \leq \varepsilon \ .$$

On the other hand, for every $\delta > 0$, there exists a polynomial P_δ such that $\sup_{\lambda\in\sigma(T)} |F(\lambda) - P_\delta(\lambda)| \leq \delta$. It follows that

$$\begin{aligned}\|F(T)x_\varepsilon - F(\lambda)x_\varepsilon\| \leq \|F(T)x_\varepsilon - P_\delta(T)x_\varepsilon\| + \|P_\delta(T)x_\varepsilon - P_\delta(\lambda)x_\varepsilon\| \\ + \|P_\delta(\lambda)x_\varepsilon - F(\lambda)x_\varepsilon\| \leq 2\delta + C_\delta\varepsilon \ ,\end{aligned}$$

where C_δ is a constant obtained as in the proof of Proposition 3.3. Choosing first δ small and then ε small shows that the sequence x_ε is a sequence of approximating eigenvectors for the operator $F(T)$ and the value $F(\lambda)$ as required. □

This is already quite close to building a functional calculus for T. However, in the case of multiplication operators, we had no problems making sense of $F(T)$ as a bounded operator for arbitrary bounded (measurable) functions F, not just continuous functions. In order to similarly extend our functional calculus to arbitrary bounded measurable functions, we first introduce the concept of a *spectral measure* for T.

Definition 3.5 Let T be a bounded selfadjoint operator and let $x \in \mathcal{H}$ with $\|x\| = 1$. The associated *spectral measure* μ_x is the unique probability measure on $\sigma(T)$ such that the identity

$$\langle x, F(T)x\rangle = \int_{\sigma(T)} F(\lambda)\,\mu_x(d\lambda) \ , \tag{10}$$

holds for every continuous function $F\colon \sigma(T) \to \mathbf{C}$.

Remark 3.6 The map $F \mapsto \langle x, F(T)x\rangle$ is obviously linear and it is bounded as a functional on $\mathcal{C}_b(\sigma(T))$ by Corollary 3.4. It is also easy to see that $\langle x, F(T)x\rangle \geq 0$ as soon as F is positive since one then has $\langle x, F(T)x\rangle = \|\sqrt{F}(T)x\|^2$. The existence of a positive measure with the required properties thus follows from the Riesz representation theorem. To see that it is automatically a probability measure, just insert $F = 1$ into (10).

Wit this notation at hand, we have

Lemma 3.7 *In the above setting, let $x \in \mathcal{H}$ and let $\mathcal{H}_x$ be the smallest closed subspace of $\mathcal{H}$ containing $T^k x$ for every $k \geq 0$. Then, there is a unitary transformation $U\colon \mathcal{H}_x \to L^2(\sigma(T), \mu_x)$ such that, for any $f \in L^2(\sigma(T), \mu_x)$, one has the identity*

$$(UTU^{-1}f)(\lambda) = \lambda f(\lambda)\;. \tag{11}$$

Proof. Note first that, for every bounded and continuous function $F\colon \sigma(T) \to \mathbf{C}$, one has $F(T)x \in \mathcal{H}_x$. Furthermore, the set of such elements is obviously dense in $\mathcal{H}_x$. We can then *define* U on such elements by $UF(T)x := F$. Using the definition of the spectral measure, one has the identity

$$\|F(T)x\|^2 = \langle x, F(T)F(T)x\rangle = \langle x, |F|^2(T)x\rangle = \int |F(\lambda)|^2\,\mu_x(d\lambda)\;,$$

which shows that U is indeed not only well-defined, but also unitary. To show (11), note that if f is a continuous function, then (11) is satisfied by the definition of U. The extension to arbitrary f again follows by density. □

Lemma 3.8 *Provided that $\mathcal{H}$ is separable, it is possible to find $N \in \mathbf{N} \cup \{\infty\}$ and a sequence $\{x_n\}$ in $\mathcal{H}$ such that $\mathcal{H} = \bigoplus_{n=0}^N \mathcal{H}_{x_n}$.*

Proof. Fix an orthonormal basis $\{e_k\}_{k\geq 0}$, which exists by the separability of $\mathcal{H}$. Then set $x_0 = e_0$. Assuming that we have already constructed $x_0, \ldots, x_n$, we set $\mathcal{H}_n = \bigoplus_{\ell<n} \mathcal{H}_{x_\ell}$ and we denote by P_n the orthogonal projection onto $\mathcal{H}_n$ in $\mathcal{H}$.

We then set

$$x_{n+1} = \frac{(1-P_n)e_{k_n}}{\|(1-P_n)e_{k_n}\|}\;, \qquad k_n = \inf\{k \geq 0\,:\, e_k \not\in \mathcal{H}_n\}\;,$$

with the convention that $e_\infty = 0$. The claim then follows by construction, provided that we let N be the first index such that $k_N = \infty$, or $N = \infty$ if all k_n are finite. □

We now have all the ingredients necessary for a version of Theorem 3.1 for bounded operators:

Theorem 3.9 *Let T be a bounded selfadjoint operator on some separable Hilbert space $\mathcal{H}$. Then, there exists a finite measure space (E, μ), a unitary operator $K\colon \mathcal{H} \to L^2(E, \mu)$, and a function $\Lambda\colon E \to \mathbf{R}$ such that*

$$(KTf)(\lambda) = \Lambda(\lambda)(Kf)(\lambda)\;, \tag{12}$$

where $\lambda \in E$ and $f \in \mathcal{H}$.

Proof. Let $\{x_n\}_{n=0}^N$ be the sequence of vectors in $\mathcal{H}$ given by Lemma 3.8. Then, we set $E = \{0, \ldots, N\} \times \sigma(T)$ and we endow it with the finite measure

$$\mu = \sum_{n=0}^{N} 2^{-2n} E_n^* \mu_{x_n} ,$$

where $E_n\colon \mathbf{R} \to E$ is given by $E_n(\lambda) = (n, \lambda)$.

Denote by U_n the unitary map from $\mathcal{H}_{x_n}$ to $L^2(\mu_{x_n})$ given by Lemma 3.7 and denote by $I_n\colon L^2(\mu_{x_n}) \to L^2(E, \mu)$ the isometry given by

$$(I_n g)(k, \lambda) = 2^n \delta_{k,n} g(\lambda) .$$

Finally, denote by Q_n the orthogonal projection from $\mathcal{H}$ to $\mathcal{H}_{x_n}$. Then, the operator K and the map $\Lambda\colon E \to \mathbf{R}$ are given by

$$K = \sum_{n=0}^{N} I_n U_n P_n , \qquad \Lambda(k, \lambda) = \lambda .$$

It is a straightforward exercise to verify that K is indeed unitary and that, as a consequence of (11), the identity (9) holds. □

This immediately gives us a bounded measurable functional calculus in the sense that, if $F\colon \sigma(T) \to \mathbf{R}$ is any bounded measurable function, then we set

$$F(T)x = K^{-1} F(\Lambda) K x ,$$

where $F(\Lambda)$ denotes the multiplication operator by the function $F \circ \Lambda$. This bounded functional calculus has all the properties one would intuitively expect, as can easily be verified.

Another standard result from finite-dimensional linear algebra is that if two Hermitian matrices commute, then they can be diagonalised simultaneously. In our case, this can be restated as

Proposition 3.10 *Let $T_1, \ldots, T_n$ be a finite family of bounded selfadjoint operators on the separable Hilbert space $\mathcal{H}$ such that $T_i T_j = T_j T_i$ for any $i, j \in \{1, \ldots, n\}$. Then, there exists a finite measure space (E, μ), a unitary operator $K\colon \mathcal{H} \to L^2(E, \mu)$, and functions $\Lambda_i\colon E \to \mathbf{R}$ such that*

$$(K T_i f)(\lambda) = \Lambda_i(\lambda)(K f)(\lambda) . \tag{13}$$

Proof. The proof is essentially the same as in the case of a single operator. The main difference is that instead of considering spectral measures as above, one considers *joint spectral measures* on $\mathbf{R}^n$ which are defined by the identity

$$\langle x, F(T_1,\ldots,T_n)x\rangle = \int_{\mathbf{R}^n} F(\lambda_1,\ldots,\lambda_n)\,\mu_x(d\lambda)\;.$$

Also, given $x \in \mathcal{H}$, the space $\mathcal{H}_x$ is now defined as the smallest space containing $T_1^{k_1}\cdots T_n^{k_n}x$ for any integer-valued vector k. On any such space, one obtains the desired statement with $E = \mathbf{R}^n$, $\mu = \mu_x$, and $\Lambda_i(\lambda) = \lambda_i$. The general statement then follows exactly as before. □

Corollary 3.11 *If T is a bounded normal operator on $\mathcal{H}$, then there exists a finite measure space (E,μ) a unitary operator $K\colon \mathcal{H} \to L^2(E,\mu)$ and a function $\Lambda\colon E \to \mathbf{C}$ such that (12) holds.*

Proof. If T is normal, one can write $T = T_1 + iT_2$ for T_1 and T_2 selfadjoint and commuting. The claim then follows from Proposition 3.10. □

3.2 Decomposition of the spectrum

So far, we have decomposed the spectrum of an arbitrary closed operator into a pure point part, a residual part, and "everything else". In the case of selfadjoint operators, the residual part is always empty, but there is a finer decomposition of "everything else". Recall that a measure μ on $\mathbf{R}$ can always be decomposed uniquely into an atomic part $\mu_{\rm pp}$, an absolutely continuous part $\mu_{\rm ac}$, and a singular continuous part $\mu_{\rm sc}$.

These are furthermore mutually singular and one has the direct sum decomposition

$$L^2(\mathbf{R},\mu) = L^2(\mathbf{R},\mu_{\rm pp}) \oplus L^2(\mathbf{R},\mu_{\rm ac}) \oplus L^2(\mathbf{R},\mu_{\rm sc})\;. \tag{14}$$

Furthermore, an element $\varphi \in L^2(\mathbf{R},\mu)$ belongs to $L^2(\mathbf{R},\mu_{\rm pp})$ if and only if $\varphi(x) = 0$ for $\mu_{\rm ac}$-almost every x and for $\mu_{\rm sc}$-almost every x. Analogous statements hold with $\mu_{\rm pp}$ replaced by $\mu_{\rm ac}$ or $\mu_{\rm sc}$.

One then has the following result:

Proposition 3.12 *Let μ be as above and let T be the operator of multiplication by x. For $\varphi \in L^2(\mathbf{R},\mu)$ of norm 1, denote as before by μ_φ the corresponding spectral measure.*

Then μ_φ is purely atomic iff $\varphi \in L^2(\mathbf{R},\mu_{\rm pp})$, μ_φ is absolutely continuous iff $\varphi \in L^2(\mathbf{R},\mu_{\rm ac})$, and μ_φ is singular continuous iff $\varphi \in L^2(\mathbf{R},\mu_{\rm sc})$.

Proof. We claim that μ_φ is the measure given by $\mu_\varphi(dx) = |\varphi(x)|^2\,\mu(dx)$. Indeed, one then has

$$\langle \varphi, F(T)\varphi\rangle = \int |\varphi(x)|^2 F(x)\,\mu(dx) = \int F(x)\,\mu_\varphi(dx)\;.$$

The claim then follows from the fact that if $\nu \ll \mu$ and μ is atomic / a.c. / s.c., then ν is also atomic / a.c. / s.c. □

As a consequence of Proposition 3.12, the decomposition (14) can alternatively by given as

$$L^2(\mathbf{R}, \mu_{\rm ac}) = \{0\} \cup \{\varphi \in L^2(\mathbf{R}, \mu) \,:\, \mu_\varphi \text{ is absolutely continuous}\}\;, \tag{15}$$

and similarly for $L^2(\mathbf{R}, \mu_{\rm pp})$ and $L^2(\mathbf{R}, \mu_{\rm sc})$. We have seen above that *any* bounded selfadjoint operator T on some Hilbert space $\mathcal{H}$ can be written as a (possibly infinite) direct sum of operators of multiplication by x. As a consequence, we obtain a direct sum decomposition

$$\mathcal{H} = \mathcal{H}_{\rm pp} \oplus \mathcal{H}_{\rm ac} \oplus \mathcal{H}_{\rm sc}\;,$$

where this time we *define*

$$\mathcal{H}_{\rm ac} = \{0\} \cup \{\varphi \in \mathcal{H} \,:\, \mu_\varphi \text{ is absolutely continuous}\}\;,$$

and similarly for $\mathcal{H}_{\rm pp}$ and $\mathcal{H}_{\rm sc}$. It is clear from (15) that each of these spaces is invariant under the action of T, so that the restriction of T to any of these subspaces yields a selfadjoint operator on the subspace in question.

This motivates a further decomposition of the spectrum as

$$\sigma_{\rm ac}(T) = \sigma(T \restriction \mathcal{H}_{\rm ac})\;, \quad \sigma_{\rm sc}(T) = \sigma(T \restriction \mathcal{H}_{\rm sc})$$

We also refer to the continuous spectrum as the union of the absolutely continuous and the singular continuous spectrum.

Note that:

- One does have $\sigma_{\rm pp}(T) \cup \sigma_{\rm sc}(T) \cup \sigma_{\rm ac}(T) \subset \sigma(T)$. One would have equality had one defined $\sigma_{\rm pp}(T) = \sigma(T \restriction \mathcal{H}_{\rm pp})$, but this could then yield elements in $\sigma_{\rm pp}(T)$ that are only accumulation points of eigenvalues.
- These sets are not disjoint in general and the intersection between any two of them may be non-empty.

Exercise 3.13 *Show that in the case when T is the multiplication operator by x on $L^2(\mathbf{R}, \mu)$, one has $\sigma_{\rm ac}(T) = \operatorname{supp} \mu_{\rm ac}$, and similarly for $\sigma_{\rm sc}(T)$.*

A quite different, but also natural, decomposition of the spectrum of a selfadjoint operator into two *disjoint* parts is given by the decomposition into *discrete* and *essential* spectrum.

For $A \subset \mathbf{R}$, the *spectral projection* of T onto A is given by

$$P_A = \mathbf{1}_A(T) ,$$

where $\mathbf{1}_A$ denotes the indicator function of the set A. It follows from the spectral representation theorem that P_A is indeed an orthogonal projection operator for every $A \subset \mathbf{R}$ and that $P_A P_B = P_{A\cap B}$. Loosely speaking, one should think of P_A as a continuous analogue to the projection onto the union of all the eigenspaces with eigenvalues in A. Denote then by $\mathcal{H}_A$ the range of P_A.

Exercise 3.14 *Show that the spectrum $\sigma(T)$ can be characterised as the set of $\lambda \in \mathbf{R}$ such that $\mathcal{H}_{[\lambda-\varepsilon,\lambda+\varepsilon]}$ is non-zero for every $\varepsilon > 0$.*

With this notation at hand, the *discrete spectrum* of T is given by the set of $\lambda \in \sigma(T)$ such that $\mathcal{H}_{[\lambda-\varepsilon,\lambda+\varepsilon]}$ is finite-dimensional for some $\varepsilon > 0$. Conversely, the *essential spectrum* of T is given by those values such that $\mathcal{H}_{[\lambda-\varepsilon,\lambda+\varepsilon]}$ is infinite-dimensional for every $\varepsilon > 0$.

We will see below that the reason for the terminology *essential spectrum* is that it is a part of the spectrum that is stable under a large class of perturbations of T.

3.3 Unbounded selfadjoint operators

Before we turn to the proof of Theorem 3.1, we should verify that the operator of multiplication by Λ defined as in (9) does indeed give a selfadjoint operator. This is the content of the following result.

Proposition 3.15 *For any finite measure space (E, μ) and measurable function $\Lambda\colon E \to \mathbf{R}$, the operator T defined by*

$$\mathcal{D}(T) = \{f \in L^2(E, \mu) \,:\, \Lambda f \in L^2(E, \mu)\} , \quad T f(x) = \Lambda(x) f(x) ,$$

is selfadjoint. Furthermore, one has $\sigma(T) = \operatorname{supp} \Lambda^* \mu$.

Proof. It is clear that T is symmetric. To see that it is also selfadjoint is a simple consequence of a standard truncation argument (using the fact that if we set $\chi_N = \mathbf{1}_{|f|\geq N}$, then $\chi_N f \to f$ in $\mathcal{H}$ for every $f \in \mathcal{H}$). The fact that $\sigma(T) = \operatorname{supp} \Lambda^*\mu$ is left as an exercise. □

We now finally have all the elements in place to give the

Proof of Theorem 3.1. Recall first that by Propositions 2.24 and 2.28, we already know that both $T + i$ and $T - i$ have bounded inverses and commute. Since one also has the identity $((T + i)^{-1})^* = (T - i)^{-1}$ and similarly for $T - i$, it follows that $(T + i)^{-1}$ is normal. By Corollary 3.11 we can therefore find a measure space (E, μ), an isometry $K: \mathcal{H} \to L^2(E, \mu)$, and a bounded measurable function $g: E \to \mathbf{C}$ such that

$$K(T + i)^{-1}K^{-1} = g .$$

Since we know that the kernel of $(T + i)^{-1}$ is 0, it follows that $g(x) \neq 0$ for μ-almost every point $x \in E$. We claim that setting $\Lambda(x) = \frac{1}{g(x)} - i$ concludes the proof.

To show that the domain of T can be characterised by (9), note that every $f \in \mathcal{D}(T)$ can be written as $f = (T+i)^{-1}\varphi$ for some $\varphi \in \mathcal{H}$, so that $Kf = gK\varphi$. It immediately follows from the definition of Λ that ΛKf is indeed bounded. Conversely, if f is such that ΛKf is bounded, then in particular $g^{-1}Kf$ is bounded, so that f is in the range of $(T + i)^{-1}$, as required.

Finally, for $f \in \mathcal{D}(T)$, writing $f = (T + i)^{-1}\varphi$ as before, one has

$$KTf = K\varphi - iKf = (g^{-1} - i)Kf = \Lambda Kf ,$$

as required. The function Λ is necessarily real (almost everywhere), for otherwise this would contradict the self-adjointness of T. □

We immediately deduce from this that we can build a functional calculus which gives an unambiguous meaning to $F(T)$ for *any* function $F: \sigma(T) \to \mathbf{R}$; we only require measurability.

In particular, we can define $U(t) = e^{itH}$ for any self-adjoint operator H and any $t \in \mathbf{R}$. This family of operators is particularly important in the context of quantum mechanics since, at least formally, the solution to the Schrödinger equation

$$\partial_t\varphi = iH\varphi ,$$

is given by $\varphi(t) = e^{itH}\varphi(0)$. In this context, the operator H describes the energy of the system and plays a role analogous to that of the Hamiltonian in classical mechanics. We have the following:

Proposition 3.16 *For any selfadjoint operator H, the family $U(t)$ defined above satisfies $U(t+s) = U(t)U(s)$. Furthermore, one has $\lim_{t\to 0} \|U(t)\varphi - \varphi\| = 0$ and $\varphi \in \mathcal{D}(H)$ if and only if $\lim_{t\to 0} t^{-1}(U(t)\varphi - \varphi)$ exists.*

Proof. The proof is left as an exercise in the case where H is a multiplication operator. The general case then follows from the spectral representation theorem. □

3.4 Commuting operators

One natural question is to ask what it means for two selfadjoint operators to commute. In the bounded case, T and U commute if $TU = UT$. What does this mean in the unbounded case? As a matter of fact, what does TU even mean when both T and U are unbounded?

If $U\colon \mathcal{B} \to \mathcal{E}$ and $T\colon \mathcal{E} \to \mathcal{F}$, a natural general definition is to set

$$\mathcal{D}(TU) = \{x \in \mathcal{D}(U) \,:\, Ux \in \mathcal{D}(T)\}\;,$$

and to define TU as the composition of T with U on that set. In this case however, stating that T and U commute if $TU = UT$ as unbounded operators (i.e. with $\mathcal{D}(UT) = \mathcal{D}(TU)$ and $TU = UT$ on this common domain) is not very natural, as the following example shows.

Example 3.17 *Take $\mathcal{H} = L^2(\mathbf{R})$, Let $(Tf)(x) = xf(x)$ with the domain as before that makes it selfadjoint, and let U be the bounded operator given by $(Uf)(x) = f(x)/(1+x^2)$.*

Then, one has $\mathcal{D}(UT) = \mathcal{D}(T)$, while $\mathcal{D}(TU) = \mathcal{H}$, so that $UT \neq TU$. On the other hand, by any "reasonable" definition of "commuting", these two operators do commute...

What this example also shows is that UT need not be closed, even if both U and T are closed. Furthermore, there might well be situations in which UT isn't even densely defined! All this suggests that one should look for a more "robust" version of the statement that U and T commute.

Note first that if U and T are bounded selfadjoint operators that commute, then of course U^n and T^m commute for any two powers n and m. As a consequence, retracing the way we built our bounded functional calculus, one can see that $F(U)$ and $G(T)$ commute for any two bounded functions F and G. In particular, this is true for the indicator functions of any two subsets of $\mathbf{R}$. This on the other hand is a concept that makes sense for *arbitrary* unbounded selfadjoint operators. It suggests that one might use this property to *define* what it means for two operators to commute:

Definition 3.18 Let T and U be two selfadjoint operators on the same Hilbert space $\mathcal{H}$. Then T are said to commute if the bounded operators $\mathbf{1}_A(T)$ and $\mathbf{1}_B(U)$ commute for any two Borel sets $A, B \subset \mathbf{R}$.

While this definition is *a posteriori* a very natural one, it is surprisingly difficult to find sufficent conditions for two operators to commute without computing their spectral representation. In particular, the following statement which seems like a reasonable conjecture is *false*:

Proposition 3.19 (THIS IS FALSE) *Let $\mathcal{D} \subset \mathcal{H}$ be invariant under both U and T and such that $\overline{T \restriction \mathcal{D}} = T$ and $\overline{U \restriction \mathcal{D}} = U$. If $UTx = TUx$ for every $x \in \mathcal{D}$, then U and T commute.*

Explain Nelson's counterexample.

3.5 Selfadjoint and symmetric operators

As we have already seen, a closed operator can be symmetric without being selfadjoint. In general, the adjoint of a symmetric operator T is an extension of T. On the other hand, if we consider some operator U which is itself an extension of T, then it is straightforward to verify that T^* is necessarily an extension of U^*. In other words, the larger the domain of an operator, the smaller the domain of its dual. This suggests that it might be the case that even though T itself is not selfadjoint, it admits an extension which is.

The following two examples show that while this *might* indeed be the case, it does not in general *have* to be the case.

Example 3.20 *Take again for T the second derivative operator defined by $Tf = f''$, this time on $\mathcal{H} = L^2([0,1])$ and with domain $\mathcal{D}(T)$ consisting of smooth functions vanishing at 0 and 1, together with their derivative. (In fact, consider T to be the closure of that operator.) By integrating by parts twice, it is easy to see that T is indeed symmetric. However, T is certainly not selfadjoint since the domain of its adjoint contains every smooth function, not only those vanishing to high enough order at the boundary.*

Let us now try to look for selfadjoint extensions of T. The largest possible "reasonable" extension is given by the adjoint of T, so selfadjoint extensions of T are the same as selfadjoint restrictions of T^*. The only way in which the domains of T and T^* differ is through the boundary conditions imposed on their elements, so it is natural to look for extensions of T that are obtained by relaxing its boundary conditions. Take smooth functions f and g that do not obey any specific boundary conditions. Then, one has the identity

$$\langle f, T^* g\rangle = \bar f(1)g'(1) - \bar f(0)g'(0) - \bar f'(1)g(1) + \bar f'(0)g(0) + \langle T^* f, g\rangle \;. \tag{16}$$

Denote by $E\colon \mathcal{D}(T^*) \to \mathbf{C}^4$ the (bounded!) operator that maps a function g into its boundary data: $Eg = (g(0), g(1), g'(0), g'(1))$. One can then verify that one has the following relation between the domains of T and T^*:

$$\mathcal{D}(T) = \{f \in \mathcal{D}(T^*) \,:\, Ef = 0\} \;.$$

With this notation in place, we see that (16) can be rewritten as

$$\langle f, T^* g\rangle = i\langle Ef, AEg\rangle + \langle T^* f, g\rangle \;, \tag{17}$$

where A is some Hermitian 4×4 matrix and the first scalar product on the right hand side denotes the canonical scalar product on $\mathbf{C}^4$.

Explicit inspection of the matrix A shows that its eigenvalues are given by $\{\pm 1\}$, and that each of these has an eigenspace $V_\pm$ of dimension 2. For any $x \in \mathbf{C}^4$, denote henceforth by $x_\pm$ the orthogonal projection of x onto $V_\pm$, so that

$$\langle x, Ay\rangle = \langle x_+, y_+\rangle - \langle x_-, y_-\rangle \;. \tag{18}$$

Denote now by U an arbitrary unitary operator with $U\colon V_+ \to V_-$ and let T_U be the extension of T (and restriction of T^*) with domain given by

$$\mathcal{D}(T_U) = \{f \in \mathcal{D}(T^*) \,:\, (Ef)_- = U(Ef)_+\} \;. \tag{19}$$

Since components of E are not bounded operations in $\mathcal{H}$, it follows from (17) that the domain of T_U^* is given by the set of functions $g \in \mathcal{D}(T^*)$ such that $\langle Ef, AEg\rangle = 0$ for all $f \in \mathcal{D}(T_U)$. Combining (18) with the definition (19) of the domain of T_U then implies that the functions g are such that

$$\langle x, (Eg)_+\rangle = \langle Ux, (Eg)_-\rangle = \langle x, U^*(Eg)_-\rangle \;,$$

for every $x \in V_+$. This immediately implies that $(Eg)_+ = U^*(Eg)_-$ which, since U is unitary, is equivalent to the fact that $(Eg)_- = U(Eg)_+$, so that one does indeed have $\mathcal{D}(T_U^*) = \mathcal{D}(T_U)$, as required.

3.6 Criteria for selfadjointness

In the absence of an explicit spectral representation, checking whether a given operator is selfadjoint (or essentially selfadjoint in the sense that its closure is selfadjoint) can be a difficult task. It is therefore very useful to have criteria ensuring that a given symmetric operator is selfadjoint. The most basic criterion is given by the following:

Proposition 3.21 *A symmetric operator T on a Hilbert space $\mathcal{H}$ is selfadjoint if and only if its resolvent set contains μ and $\bar{\mu}$ for some complex number μ with non-zero imaginary part.*

Proof. We have already seen that selfadjoint operators have real spectrum, so it remains to show the other implication.

Assume that the resolvent set of T contains μ and $\bar{\mu}$ with Im$\mu \neq 0$. Replacing T by $aT+b$ for two suitably chosen real numbers a and b and noting that this does not affect selfadjointness, we can assume without loss of generality that $\mu = i$. Since $\pm i$ belong to the resolvent set, both $T+i$ and $T-i$ have full range. As a consequence, for any $\varphi \in \mathcal{D}(T^*)$, we can find $\psi \in \mathcal{D}(T)$ such that

$$(T-i)\psi = (T^*-i)\varphi \qquad \Rightarrow \qquad (T^*-i)(\psi - \varphi) = 0 \;,$$

due to the fact that T^* is always an extension of T. Since, by assumption, $T+i$ also has full range, this implies that the kernel of T^*-i is zero, so that $\psi = \varphi$. This shows that $\mathcal{D}(T^*) = \mathcal{D}(T)$, so that T is indeed selfadjoint. □

A simple consequence of this criterion is the following perturbation result for selfadjoint operators.

Proposition 3.22 *Let A be selfadjoint and let B be a symmetric operator on $\mathcal{H}$ with $\mathcal{D}(A) \subset \mathcal{D}(B)$ and such that there exist constants $\varepsilon < 1$ and $C > 0$ such that the bound*

$$\|Bx\| \le \varepsilon \|Ax\| + C\|x\| \;,$$

holds for every $x \in \mathcal{D}(A)$. Then, the operator $Tx = Ax + Bx$ with domain $\mathcal{D}(A)$ is also selfadjoint.

Proof. If we can show that iK belongs to the resolvent set of $T+iK$ for $|K|$ large enough, then we are done, since it is obvious that T is symmetric. The trick is to write

$$T + iK = A + B + iK = (1 + B(A+iK)^{-1})(A+iK)^{-1} \;,$$

so it remains to show that $\|B(A+iK)^{-1}\| < 1$ for large enough K since we can then build the inverse of $1 + B(A+iK)^{-1}$ by its convergent Neumann series.

By assumption, we have the bound

$$\|B(A+iK)^{-1}x\| \leq \varepsilon\|A(A+iK)^{-1}x\| + C\|(A+iK)^{-1}x\| \leq \varepsilon\|x\| + \frac{C}{K}\|x\| \ .$$

Here, we have used the spectral representation theorem, combined with the fact that $|a/(a+iK)| \leq 1$ and $1/|a+iK| \leq 1/K$, uniformly over $a \in \mathbf{R}$. The claim then follows by taking K larger than $C/(1-\varepsilon)$. □

As a consequence of Proposition 3.22, it is quite straightforward to show that the Schrödinger operator with Coulomb potential in $\mathbf{R}^3$ is indeed selfadjoint. To show this, we will make use of the following Sobolev embedding theorem which we state without proof:

Lemma 3.23 *In dimensions $d < 4$, one has $W^{2,2}(\mathbf{R}^d) \subset \mathcal{C}_b(\mathbf{R}^d)$.*

Corollary 3.24 *In $L^2(\mathbf{R}^3)$, multiplication by $V(x) = 1/|x|$ is relatively bounded with respect to $-\Delta$.*

Proof. Note first that, by writing everything in Fourier space, one sees that there exists a constant such that

$$c(\|\varphi\|^2 + \|\Delta\varphi\|^2) \leq \|\varphi\|^2_{W^{2,2}} \leq \frac{1}{c}(\|\varphi\|^2 + \|\Delta\varphi\|^2) \ ,$$

so that in particular there exists a constant $C > 0$ such that

$$\|\varphi\|^2_\infty \leq C(\|\Delta\varphi\|^2 + \|\varphi\|^2) \ ,$$

uniformly over all $\varphi \in W^{2,2}(\mathbf{R}^3)$. □

3.7 Deficiency indices

We have seen in Proposition 3.21 that a symmetric operator is selfadjoint if and only if its resolvent set contains some points in both halves of the complex plane. Actually, one can be much more precise than that. It turns out that a relatively straightforward perturbation argument shows that the dimension of $\ker(\lambda - T^*)$ is necessarily constant for all λ located on the same side of the real axis:

Proposition 3.25 *Let T be a symmetric operator. Then* $\dim\ker(\lambda - T^*) = \dim\ker(\mu - T^*)$ *if* $\operatorname{sgn}\mathrm{Im}\lambda = \operatorname{sgn}\mathrm{Im}\mu$.

Proof. Our aim is to show that $\dim\ker(\lambda - T^*)$ is locally constant in the sense that $\dim\ker(\lambda - T^*) = \dim\ker(\mu - T^*)$ for all μ such that $|\mu - \lambda| \leq |\mathrm{Im}\mu|/2$. The claim then follows immediately by a patching argument. Actually, it is sufficient to show that $\dim\ker(\mu - T^*) \leq \dim\ker(\lambda - T^*)$ for $|\mu - \lambda| \leq |\mathrm{Im}\mu|$, since the reverse inequality is then obtained by exchanging the roles of μ and λ.

Since T is symmetric, one has

$$\begin{aligned}\|(\bar\lambda - T)y\|^2 &= \langle \bar\lambda y - Ty, \bar\lambda y - Ty\rangle = |\lambda|^2\|y\|^2 - (\lambda + \bar\lambda)\langle y, Ty\rangle + \|Ty\|^2 \\ &\geq |\lambda|^2\|y\|^2 - |\mathrm{Re}\lambda|^2\|y\|^2 = |\mathrm{Im}\lambda|^2\|y\|^2 \;. \end{aligned} \tag{20}$$

Recall furthermore that if U and V are two closed subspaces of $\mathcal{H}$ such that $\dim U > \dim V$, then there exists $x \in U \cap V^\perp$ with $\|x\| = 1$. Indeed, denote by $\bar U$ the orthogonal projection of U onto V. If $U \cap V^\perp = \{0\}$, then the projection of a basis of U yields a basis of $\bar U$, so that $\dim \bar U = \dim U$, which is a contradiction with the fact that $\dim U > \dim V$.

We now use this fact with $U = \ker(\mu - T^*)$ and $V = \ker(\lambda - T^*)$. We want to show that $\dim U \leq \dim V$, so we assume by contradiction that $\dim U > \dim V$. By the above argument, there exists some x with $\|x\| = 1$ and such that on the one hand $T^* x = \mu x$ and on the other hand $x \in \ker(\lambda - T^*)^\perp = \mathrm{ran}(\bar\lambda - T)$, so that there exists y with $x = (\bar\lambda - T)y$. We then have

$$0 = \langle \mu x - T^* x, y\rangle = \langle x, (\bar\mu - T)y\rangle = \|x\|^2 + (\bar\lambda - \bar\mu)\langle x, y\rangle \;.$$

As a consequence of (20), we know however that $|\langle x, y\rangle| \leq \|x\|^2/|\mathrm{Im}\lambda|$, which leads to a contradiction if $|\bar\lambda - \bar\mu| < |\mathrm{Im}\lambda|$, as required. □

As a consequence of this statement, the spectrum of a closed symmetric operator is either a subset of **R** (if and only if the operator is selfadjoint), or all of **C**, or one of the two closed half-spaces.

In the particular case when $\langle x, Tx\rangle \geq 0$ (say), one can strengthen (20) to obtain

$$\|(\bar\lambda - T)y\|^2 \geq |\lambda|^2\|y\|^2 \;,$$

as soon as $\mathrm{Re}\lambda \leq 0$. This allows to show that in this case on has $\dim\ker(\lambda - T^*) = \dim\ker(\mu - T^*)$ for *any* two complex numbers μ and ν in $\mathbf{C} \setminus \mathbf{R}_+$. This yields the following corollary:

Corollary 3.26 *If T is symmetric and positive, then T is selfadjoint if and only if* $\ker(1 + T^*) = \{0\}$.

The dimensions of the kernels of $T^* \pm i$ are called the *deficiency indices* of the closed symmetric operator T. In general, the deficiency indices can take any two values, including $+\infty$.

Remark 3.27 A symmetric operator T has selfadjoint extensions if and only if its two deficiency indices are equal. In this case, the set of all selfadjoint extensions is in one-to-one correspondence with the set of unitary transformations between $\ker(T + i)$ and $\ker(T - i)$. This is a generalisation of Example 3.20.

The following example is very instructive:

Example 3.28 *Consider $\mathcal{H} = L^2(\mathbf{R}_+)$ and T such that $Tf(x) = if'(x)$ for $f \in \mathcal{C}_0^\infty(\mathbf{R}_+)$. Then it is easy to see that T is symmetric. Its closure has domain given by*

$$\mathcal{D}(T) = \{f \in H^1 \,:\, f(0) = 0\} .$$

In this case, the domain of T^* is given by H^1 and T^* acts on these functions by $T^* f(x) = if'(x)$. As a consequence, the kernel of $T^* + i$ is given by the span of e^{-x}, while the kernel of $T^* - i$ is empty. As a consequence, the deficiency indices of T are $(1, 0)$, and T has no selfadjoint extensions at all.

If we change $\mathbf{R}_+$ to $\mathbf{R}_-$, then the indices are $(0, 1)$. By forming tensor products of these two examples, one can easily construct operators with arbitrary deficiency indices.

4 Quadratic forms

We have already seen in Proposition **??** that closed positive quadratic forms are in one-to-one correspondence with positive selfadjoint operators. In can be very useful to be able to switch between these two points of view. As a consequence, it will come as little surprise that many results available at the level of symmetric / selfadjoint operators have analogues at the level of quadratic forms. However, it turns out that these analogues often cover slightly different situations. For example, the analogue to Proposition **??** is:

Proposition 4.1 *Let q be a closed symmetric and positive quadratic form. Let furthermore β be a symmetric quadratic form defined on $\mathcal{Q}(q)$ and such that*

$$|\beta(x, x)| \le \varepsilon q(x, x) - C\|x\|^2 , \tag{21}$$

for some constants $\varepsilon \in (0,1)$ and $C \in \mathbf{R}$. Then, the form $q+\beta$ is closed and bounded from below.

Proof. Set $\bar{q} = q + \beta$. Then, one has

$$\bar{q}(x,x) \geq q(x,x) - \varepsilon q(x,x) - C\|x\|^2 ,$$

which immediately shows that $\bar{q}$ is indeed bounded from below. Furthermore, for K large enough, the norm $\bar{q}(x,x) + K\|x\|^2$ is equivalent to $q(x,x) + \|x\|^2$, so that $\bar{q}$ is closed. □

Note that there is no requirement on β being either positive or closed! As a consequence of this result, we can define an operator "$-\partial_x^2 + c\delta_0$" on $L^2(\mathbf{R})$, as seen in the following example:

Example 4.2 *Let $\mathcal{H} = L^2(\mathbf{R})$ and let q be the form with domain $\mathcal{Q}(q) = H^1$ given by*

$$q(f,f) = \int |f'(x)|^2\,dx .$$

Let furthermore β be given by

$$\beta(f,f) = c|f(0)|^2 , \qquad c \in \mathbf{R} .$$

Note that, given any $f \in H^1$, for any $K > 0$ there must be some value $x_K \in \mathbf{R}$ with $|x_K| \leq 1/\sqrt{2K}$ such that $|f(x)| \leq K\|f\|$. One then has

$$|f(0)| \leq K\|f\| + \Big|\int_{x_K}^0 f'(y)\,dy\Big| \leq K\|f\| + \sqrt{|x_K| \int |f'(y)|^2\,dy} ,$$

which shows that the bound (21) holds provided that we choose K large enough. This shows that there is indeed a unique selfadjoint operator associated to the quadratic form $\int |f'(x)|^2\,dx + |f(0)|^2$ with domain H^1. It is a good exercise to determine the expression and domain of that operator.

Another nice example is the following, which shows that the borderline case for having a well-defined meaning for $-\Delta + c|x|^{-\alpha}$ is given by $\alpha = 2$. This is not so surprising since one would expect, at least at a formal level, that $|x|^{-2}$ has the same "strength" as $-\Delta$. For example, both act in very similar ways when applied to polynomials.

Example 4.3 *In dimension $d \geq 3$, the inequality*

$$\int \frac{|f(x)|^2}{|x|^2}\,dx \leq \frac{4}{(d-2)^2} \int |\nabla f(x)|^2\,dx\;,$$

is valid for every smooth compactly supported function f. To show this, one actually shows the slightly stronger statement that

$$\int \frac{|f(x)|^2}{|x|^2}\,dx \leq \frac{4}{(d-2)^2} \int |\partial_r f(x)|^2\,dx\;,$$

where $\partial_r f$ denotes the derivative of f in the radial direction. One then makes use of the identity

$$\partial_r f = |x|^{-\beta}\partial_r(|x|^\beta f) - \frac{\beta}{|x|} f\;,$$

noting that the particular choice $\beta = \frac{d-2}{2}$ leads to a cancellation of the cross-term that appears when integrating the square of the right hand side of this expression.

One nice thing about positive closed forms is that their sum is *always* a positive closed form. Indeed, one has:

Proposition 4.4 *Let q_1 and q_2 be two symmetric positive closed forms and set $q = q_1 + q_2$ with form domain given by $\mathcal{Q}(q) = \mathcal{Q}(q_1) \cap \mathcal{Q}(q_2)$. Then, q is again a symmetric positive closed form.*

Proof. We only need to show that q is closed. Let $\{x_n\}$ be a sequence of elements of $\mathcal{H}$ which is Cauchy in the norm $\|x\|_q^2 = q(x,x) + \|x\|^2$. In particular, the sequence $\{x_n\}$ is Cauchy in the norm $\|\cdot\|_{q_1}$ so that, since q_1 is closed, there exists an element $x \in \mathcal{Q}(q_1)$ such that $\|x_n - x\|_{q_1} \to 0$. Similarly, there exists an element $\bar{x} \in \mathcal{Q}(q_2)$ such that $\|x_n - \bar{x}\|_{q_2} \to 0$.

However, one must have $x = \bar{x}$ since we also know that $\{x_n\}$ is Cauchy in $\mathcal{H}$ and that the limit must coincide with the limit in $\mathcal{H}$. □

This result allows to give a meaning to the operator $-\Delta + V$ on $\mathbf{R}^n$ for *any* potential V that is measurable and bounded from below. However, it might in general be exceedingly difficult to obtain a good characterisation for the domain of such an operator.

Note that one crucial assumption in the study of quadratic forms is that the form in question is closed. Indeed, as the example $q(f,f) = |f(0)|^2$ shows, non-closed quadratic forms do not in general come from any linear operator. However, one could hope that the situation is improved if we consider a quadratic form q that is defined with the help of a symmetric (but not necessarily selfadjoint) operator T. If such a form were to be closable, then this would give us a canonical way of finding a selfadjoint extension for any symmetric operator that is bounded from below. For once, life is kind and this is indeed the case:

Proposition 4.5 *Let T be a positive symmetric operator on $\mathcal{H}$ and let q be the corresponding quadratic form with domain $\mathcal{Q}(q) = \mathcal{D}(T)$. Then q is closable in $\mathcal{H}$.*

Remark 4.6 The selfadjoint operator $\hat{T}$ associated to q is called the Friedrichs extension of T. It is in general strictly larger than the closure of T. For example, if we take for T the Laplacian on $(0,1)$ with domain $\mathcal{C}_0^\infty$, then $\hat{T}$ is the Dirichlet Laplacian.

Proof. Denote by $\mathcal{H}_+$ the (abstract) closure of $\mathcal{D}(T)$ under the norm

$$\|x\|_+^2 = \langle x, Tx\rangle + \|x\|^2 \;.$$

Then all we need to show is that $\mathcal{H}_+ \subset \mathcal{H}$ in a canonical way. Denoting by $\iota\colon \mathcal{D}(T) \to \mathcal{H}$ the identity map, it follows from the bound $\|\cdot\|_+ \geq \|\cdot\|$ that ι extends uniquely to a map from $\mathcal{H}_+$ to $\mathcal{H}$, so all that needs to be shown is that ι is injective.

Assume that $x \in \mathcal{H}_+$ is such that $\iota x = 0$. Then there exists a sequence $x_n \in \mathcal{D}(T)$ such that $\|x_n - x\|_+ \to 0$ and $\|\iota x_n\| \to 0$ (as a consequence of the boundedness of ι). One then has

$$\|x\|_+^2 = \lim_{m\to\infty}\lim_{n\to\infty} \langle x_n, x_m\rangle_+ = \lim_{m\to\infty}\lim_{n\to\infty} \bigl(\langle x_n, Tx_m\rangle + \langle x_n, x_m\rangle\bigr) = 0 \;, \quad (22)$$

so that ι is indeed injective as claimed. □

Remark 4.7 It is very important that q comes from an operator T. In the case of our favourite example, namely $q(f) = |f(0)|^2$, one can see that the inclusion $\mathcal{H}_+ \subset \mathcal{H}$ fails. The argument given above fails at the second identity in (22) which fails to makes sense. A good exercise is to give an explicit representation of $\mathcal{H}_+$ in that case and an interpretation of the operator corresponding to the closure of q.

However, even if T is the closure of an operator with a "nice" domain that we understand well, like $\mathcal{C}_0^\infty$, the Friedrichs extension of T might have a substantially larger domain. In the particular case of operators of the form $-\Delta + V$ with positive V, this tends however not to be the case. Indeed, we have the following criterion due to Katô:

Theorem 4.8 *Let $V\colon \mathbf{R}^n \to \mathbf{R}_+$ be in $L^2_{\mathrm{loc}}(\mathbf{R}^n)$ and let $T = -\Delta + V$ with domain $\mathcal{C}_0^\infty(\mathbf{R}^n)$. Then T is essentially selfadjoint in $L^2(\mathbf{R}^n)$.*

Proof. By Corollary 3.26, it is enough to verify that there cannot be any $g \in \mathcal{D}(T^*)$ such that

$$(T^* + 1)g = 0 \;.$$

Since the domain of T is given by $\mathcal{C}_0^\infty$, this precisely says that there cannot be any L^2 function g such that

$$(-\Delta + V + 1)g = 0 \;, \tag{23}$$

in the sense of distributions. (Note that all three terms appearing here make perfect sense as distributions since $V \in L^2_{\mathrm{loc}}$.) Note now that if $g \in L^2$ with Δg in L^1_{loc}, then

$$\Delta |g| \ge \mathrm{Re}\Big(\frac{\bar g}{|g|}\Delta g\Big) \;,$$

in the sense of distributions. Indeed, assuming first that g is smooth, one can set $g_\varepsilon = \sqrt{|g|^2 + \varepsilon}$ and one verifies that

$$\Delta g_\varepsilon \ge \mathrm{Re}\Big(\frac{\bar g}{g_\varepsilon}\Delta g\Big) \;.$$

The claim then follows by a standard approximation argument.

Returning to (23), we note that since $g \in L^2$ and $V \in L^2_{\mathrm{loc}}$, one has $Vg \in L^1_{\mathrm{loc}}$ and therefore $\Delta g \in L^1_{\mathrm{loc}}$. It follows that one has the distributional inequality

$$\Delta |g| \ge \mathrm{Re}\Big(\frac{\bar g}{|g|}\Delta g\Big) = \mathrm{Re}\Big(\frac{\bar g}{|g|}(V+1)g\Big) = |g|(V+1) \ge |g| \;.$$

In particular, if $g_\varepsilon = \varphi_\varepsilon \star |g|$ with φ_ε a delta-sequence consisting of positive functions, one has

$$\Delta g_\varepsilon = \varphi_\varepsilon \star \Delta |g| \ge \varphi_\varepsilon \star |g| = g_\varepsilon \;,$$

so that $\langle \Delta g_\varepsilon, g_\varepsilon\rangle \ge 0$. But for any smooth g_ε in L^2 we know that $\langle \Delta g_\varepsilon, g_\varepsilon\rangle \le 0$, so that one must have $|g| = 0$, as required. □

Exercise 4.9 *Consider the case where $V \ge 0$ as above and $V \in L^1_{\mathrm{loc}}$. Show then that if $T = -\Delta + V$ is the Friedrich's extension of the operator defined on $\mathcal{C}_0^\infty$, then*

$$\mathcal{D}(T) = \{f \in L^2 \,:\, Vf \in L^1_{\mathrm{loc}} \;\&\; -\Delta f + Vf \in L^2\} \;.$$

Here, the expression $-\Delta f + Vf$ should be interpreted in the sense of distributions, which makes sense since $Vf \in L^1_{\mathrm{loc}}$ by assumption.

5 Compactness of the resolvent

In this section, we give conditions for the resolvent of a Schrödinger operator to be compact. For a normal operator, being compact is equivalent to being bounded and having purely discrete spectrum, except at 0. As a consequence, the resolvent of a selfadjoint operator T is compact if and only if $\sigma(T) = \sigma_{\text{disc}}(T)$ or, in other words, if $\sigma_{\text{ess}}(T) = \emptyset$. We also have:

Proposition 5.1 *A positive selfadjoint operator T has compact resolvent if and only if the set*

$$\mathbf{1}_T = \{x \in \mathcal{Q}(q) \,:\, \|x\|^2 + q(x,x) \le 1\}\;,$$

is compact, where q is the quadratic form associated to T.

Proof. As a consequence of the spectral theorem, T has compact resolvent if and only if $\sqrt{T}$ has compact resolvent. The set $\mathbf{1}_T$ is nothing but the unit ball of $\mathcal{D}(\sqrt{T})$ equipped with the graph norm of $\sqrt{T}$, which on the other hand is precisely the image of the unit ball under $(\sqrt{T}+i)^{-1}$. □

Remark 5.2 The set $\mathbf{1}_T$ is automatically closed as a consequence of the spectral decomposition theorem. Therefore, it actually suffices to show that $\mathbf{1}_T$ is precompact to conclude that T has compact resolvent.

One also has the following alternative characterisation:

Proposition 5.3 *In the same setting, let μ_m be defined as*

$$\mu_m = \sup_{V_m \subset \mathcal{H}} \inf_{x \in V_m^\perp} \frac{\langle x, Tx\rangle}{\|x\|^2}\;,$$

where the supremum runs over all m-dimensional subspaces V_m of $\mathcal{H}$. Then

$$\lim_{m\to\infty} \mu_m = \inf \sigma_{\text{ess}}(T) \in [0,\infty]\;.$$

In particular, T has compact resolvent if and only if $\mu_m \to \infty$.

Proof. The proof is a rather straightforward consequence of the spectral representation theorem, so we leave it as an exercise. □

Since the set $\mathbf{1}_T$ is closed for every selfadjoint operator T, this implies in particular that if T and U are two selfadjoint operators with associated forms q and r such that $\mathcal{Q}(r) \subset \mathcal{Q}(q)$ and

$$q(x,x) \le r(x,x) ,$$

then U has compact resolvent as soon as T has. Indeed, it suffices to remark that any closed subset of a compact set is again compact.

This suggests that an important tool in the derivation of criteria for the compactness of the resolvent of T should be given by the stability of the essential spectrum under relatively compact perturbations. Recall also that the set of compact operators is closed in the topology of operator norm convergence and that any integral operator of the type

$$\mathcal{K}f(x) = \int K(x,y)\, f(y)\, dy ,$$

is compact on L^2 if the kernel K is itself in L^2, whatever the underlying measure space is. (Actually $\mathcal{K}$ is even Hilbert-Schmidt in this case as can easily be checked, at least formally.)

In this section, we will always take $\mathcal{H} = L^2(\mathbf{R}^n)$. We then make the following abuse of notation. For a function $W\colon \mathbf{R}^n \to \mathbf{R}$, we denote by V the multiplication operator given by

$$(Wf)(x) = W(x)f(x) ,$$

and by $\hat{W}$ the operator

$$(\mathcal{F}\hat{W}f)(k) = W(k)(\mathcal{F}f)(k) ,$$

where $\mathcal{F}$ denotes the Fourier transform, viewed as an isometry on $\mathcal{H}$. Given any two *positive* functions $V, W\colon \mathbf{R}^n \to \mathbf{R}_+$, we then consider the operator

$$T = \hat{W} + V ,$$

defined as a sum of quadratic forms. We will always assume that V and W are such that T is densely defined, which is true as soon as they belong to L^1_{loc} with some growth condition at infinity. We then have:

Theorem 5.4 (Rellich) *If both V and W grow at infinity in the sense that $\{x : V(x) \le K\}$ is bounded for every K (and similarly for W), then T defined as above has compact resolvent.*

Proof. Note first that we can assume without loss of generality that one has $V(x) \leq |x|^2$ and similarly for W. Indeed, increasing V or W decreases the set $\mathbf{1}_T$, so that compactness of T for one pair (V, W) implies precompactness (and therefore compactness by Remark 5.2) of T for any larger pair.

Note now that if $\bar{V} \leq V$ and we denote by $\bar{\mu}_m$ the sequence associated to $\bar{T} = \hat{W} + \bar{V}$, then $\bar{\mu}_m \leq \mu_m$. As a consequence it remains to show that for every $K > 0$, it is possible to find such a $\bar{V}$ such that $\lim_{m\to\infty} \bar{\mu}_m \geq K$. We claim that a possible choice of $\bar{V}$ is given by

$$\bar{V}(x) = V(x) \wedge K \;.$$

Note that $\bar{V}$ can be written as $\bar{V}(x) = K + U(x)$, where the function U is bounded with compact support. We claim that the operator of multiplication by U is relatively compact with respect to $\hat{W}$. Assuming that this is true, we know that $\sigma_{\text{ess}}(\hat{W} + U) = \sigma_{\text{ess}}(\hat{W}) \subset \mathbf{R}_+$. As a consequence, $\sigma_{\text{ess}}(\bar{T}) \subset [K, \infty)$, so that one does indeed have $\lim_{m\to\infty} \bar{\mu}_m \geq K$ by Proposition 5.3.

It remains to show that $X := U(1 + \hat{W})^{-1}$ is compact. For this, recall that if (E, μ) is a measure space and $\mathcal{K}\colon E \times E \to \mathbf{R}$ is a kernel in $L^2(E \times E, \mu \otimes \mu)$, then the integral operator $\mathcal{K}\psi(x) = \int \mathcal{K}(x,y)\psi(y)\,\mu(dy)$ is Hilbert-Schmidt on $L^2(E, \mu)$. As a consequence, since U belongs to $L^2(\mathbf{R}^n)$ and $p \mapsto (1 + W(p) + \varepsilon|p|^{2n})^{-1}$ is in L^2 for every $\varepsilon > 0$, the operator

$$X_\varepsilon := U(1 + \hat{W} + \varepsilon(-\Delta)^n)^{-1}$$

is Hilbert-Schmidt for every $\varepsilon \to 0$. Furthermore, since $W \to \infty$, the function $(1 + W(p) + \varepsilon|p|^{2n})^{-1}$ converges to $(1 + W(p))^{-1}$ in $L^\infty(\mathbf{R}^n)$, so that $X_\varepsilon \to X$ in operator norm. Since the set of compact operators is closed under operator norm convergence, this shows that X is indeed compact, as required. □

6 Bloch wave decomposition

7 Announcements

Students should register with `gradstud@maths.ox.ac.uk`

Deadline: 8th of June for Warwick. 2 weeks before exam board meetings for others.

Possible subjects:

- Work out details for functional calculus for commuting operators.
- Explain Bloch wave decomposition
- Work out conditions for $-\Delta + V$ to have compact resolvent even if V does not grow to infinity at infinity.
- Characterise selfadjoint extensions of symmetric operators and work out an example.
- Work out boundary conditions / selfadjoint extensions for $-\partial_x^2 + V$ in 1-D.