3 Self-adjoint operators (unbounded)

Bounded continuous functions $f : \mathbb{R} \to \mathbb{C}$ can be applied to a (generally, unbounded) operator A, giving bounded operators $f(A)$, provided that A is self-adjoint (which amounts to three evident conditions and one inevident condition). Indicators of intervals (and some other discontinuous functions f) can be applied, too. Especially, operators $U_t = \exp(\mathrm{i}tA)$ form a unitary group whose generator is A.

3a Introduction: which operators are most useful?

The zero operator is much too good for being useful. Less good and more useful are: finite-dimensional self-adjoint operators; compact self-adjoint operators; bounded self-adjoint operators.

On the other hand, arbitrary linear operators are too bad for being useful. They do not generate groups, they cannot be diagonalized, functions of them are ill-defined.

Probably, most useful are such operators as (for example) P and Q (considered in the previous chapters); $P^2 + Q^2$ (the Hamiltonian of a harmonic one-dimensional quantum oscillator, P^2 being the kinetic energy and Q^2 the potential energy); more generally, $P^2 + v(Q)$ (the Hamiltonian of a anharmonic one-dimensional quantum oscillator) and its multidimensional counterparts.

The famous Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = \mathcal{H}\psi(t)\,, \quad \mathcal{H} = P^2 + v(Q)$$

leads to unitary operators $\exp(-\mathrm{i}t\mathcal{H})$. An important goal of functional analysis is, to define $\exp(-\mathrm{i}t\mathcal{H})$ for good operators $\mathcal{H}$ and to understand the distinction between good and bad operators.

Unitary operators are important for physics. In classical physics, many evolution operators are unitary due to conservation of energy, in quantum physics — of probability.

3b Three evident conditions

Good operators (especially, generators of unitary groups) are densely defined, symmetric, and closed.

An unbounded[1] linear operator $A : D_A \to H$, $D_A \subset H$, is basically the same as its graph

$$\mathrm{Graph}(A) = \{(x,y) : x \in D_A,\, y = Ax\}\,.$$

The phrase "B extends A" means "$\mathrm{Graph}(A) \subset \mathrm{Graph}(B)$"; the phrase "$B$ is the closure of A" means "$\mathrm{Graph}(B) = \mathrm{Closure}(\mathrm{Graph}(A))$"; the phrase "$A$ is closed" means "$\mathrm{Graph}(A)$ is closed". In addition, $\mathrm{Domain}(A) = D_A \subset H$ and $\mathrm{Range}(A) = A(\mathrm{Domain}(A)) \subset H$.

3b1 Exercise. (a) Reformulate Theorem 2c3(a,b) in the form "B is the closure of A".

(b) Prove that the operators P and Q are closed.

Further, the phrase "A is densely defined" means "$\mathrm{Domain}(A)$ is dense". Unless otherwise stated,

- ∗ all operators are assumed linear;
- ∗ all operators are assumed densely defined;
- ∗ all bounded operators are assumed everywhere defined.

Note that all bounded operators are closed.

3b2 Exercise. If A is closed and B is bounded then $A + B$ is closed.

Prove it.

[1] I mean, not necessarily bounded.

In general, Domain$(A) \cap$ Domain(B) need not be dense (and even can be $\{0\}$). Fortunately, Domain$(P) \cap$ Domain(Q) is dense.

In general, Closure(Graph(A)) need not be a graph (it may contain some $(0, y)$, $y \ne 0$); that is, not all operators are *closable.*

3b3 Definition. Operator A is *symmetric* if

$$\langle Ax, y \rangle = \langle x, Ay \rangle \quad \text{for all } x, y \in \text{Domain}(A)\,.$$

3b4 Exercise. Operator A is symmetric if and only if $\forall x \in H\ \langle Ax, x \rangle \in \mathbb{R}$.

Prove it.

Hint: the "if" part: $\langle Ax, y \rangle + \langle Ay, x \rangle = \langle A(x+y), x+y \rangle - \langle Ax, x \rangle - \langle Ay, y \rangle \in \mathbb{R}$; also $\langle Ax, \mathrm{i}y \rangle + \langle A\mathrm{i}y, x \rangle \in \mathbb{R}$.

3b5 Exercise. Prove that the operators P and Q are symmetric.

3b6 Lemma. A symmetric operator is closable, and its closure is a symmetric operator.

Proof. If $x_n \to 0$ and $Ax_n \to y$ then $\langle y, z \rangle = \lim \langle Ax_n, z \rangle = \lim \langle x_n, Az \rangle = 0$ for all $z \in$ Domain(A), therefore $y = 0$, thus, A is closable.

Given $x, y \in$ Domain(B) where $B =$ Closure(A), we take $x_n, y_n \in$ Domain(A) such that $x_n \to x$, $Ax_n \to Bx$, $y_n \to y$, $Ay_n \to By$ and get $\langle Bx, y \rangle = \lim \langle Ax_n, y_n \rangle = \lim \langle x_n, Ay_n \rangle = \langle x, By \rangle$, thus, B is symmetric. $\square$

3b7 Exercise. For every $\varphi \in L_0(\mathbb{R})$ the operators $\varphi(P)$ and $\varphi(Q)$ are closed.

Prove it.

Hint: start with $\varphi(Q)$; a sequence converging in L_2 has a subsequence converging almost everywhere.

3b8 Exercise. The following three conditions on $\varphi \in L_0(\mathbb{R})$ are equivalent:

(a) $\varphi = \overline{\varphi}$;

(b) $\varphi(P)$ is symmetric;

(c) $\varphi(Q)$ is symmetric.

Prove it.

Generator of a unitary group

3b9 Definition. A *strongly continuous one-parameter unitary group* is a family $(U_t)_{t \in \mathbb{R}}$ of unitary operators $U_t : H \to H$ such that

$$U_{s+t} = U_s U_t \quad \text{for all } s, t \in \mathbb{R}\,,$$
$$\|U_t x - x\| \to 0 \quad \text{as } t \to 0\,, \text{ for all } x \in H\,.$$

Two examples: $\big(U(a)\big)_{a\in\mathbb{R}}$ and $\big(V(b)\big)_{b\in\mathbb{R}}$ (recall 1g1).

3b10 Exercise. Let (U_t) be a unitary group[1] and $x \in H$, then the vector-function $t \mapsto U_t x$ is continuous.

Prove it.

Hint: $\|U_{t+s}x - U_t x\|$ does not depend on t.

3b11 Definition. The *generator* of a unitary group (U_t) is the operator A defined by[2]

$$\mathrm{i}Ax = y \quad \text{if and only if} \quad \frac{1}{t}(U_t x - x) \to y \text{ as } t \to 0\,.$$

3b12 Exercise. The generator of a unitary group is a densely defined operator.

Prove it.

Hint: for every $x \in H$ and every $\varepsilon > 0$ the vector $\frac{1}{\varepsilon}\int_0^\varepsilon U_t x \, \mathrm{d}t$ belongs to Domain(A).

3b13 Exercise. The generator of a unitary group is a symmetric operator.

Prove it.

Hint: $U_t^* = U_t^{-1} = U_{-t}$.

3b14 Exercise. Let (U_t) be a unitary group, A its generator, and $x \in$ Domain(A). Then the vector-function $t \mapsto U_t x$ is continuously differentiable, and $U_t x \in$ Domain(A) for all $t \in \mathbb{R}$, and

$$\frac{\mathrm{d}}{\mathrm{d}t} U_t x = \mathrm{i}AU_t x = U_t \mathrm{i}Ax \quad \text{for all } t \in \mathbb{R}\,.$$

Prove it.

Hint: $U_{t+\varepsilon} - U_t = (U_\varepsilon - 1\!\!1)U_t = U_t(U_\varepsilon - 1\!\!1)$.

Note that operators U_t leave the set Domain(A) invariant.

3b15 Exercise. Let A be the generator of a unitary group (U_t), and B the generator of a unitary group (V_t). If $A = B$ then $U_t = V_t$ for all $t \in \mathbb{R}$.

Prove it.

Hint: let $x \in$ Domain(A), then the vector-function $x(t) = U_t x - V_t x$ satisfies $\frac{\mathrm{d}}{\mathrm{d}t}x_t = \mathrm{i}Ax_t$, therefore $\frac{\mathrm{d}}{\mathrm{d}t}\|x_t\|^2 = 2\mathrm{Re}\,\langle \mathrm{i}Ax_t, x_t\rangle = 0$.

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[1] By "unitary group" I always mean "strongly continuous one-parameter unitary group".

[2] Some authors call iA (rather than A) the generator.

3b16 Exercise. Let (U_t) be a unitary group, A its generator. Then the following two conditions on $x, y \in H$ are equivalent:

(a) $x \in \text{Domain}(A)$ and $\mathrm{i}Ax = y$,

(b) for every $t \in \mathbb{R}$,

$$U_t x = x + \int_0^t U_s y \, \mathrm{d}s \, .$$

Prove it.

Hint: recall the proof of 2c3.

3b17 Exercise. The generator of a unitary group is a closed operator.

Prove it.

Hint: use 3b16.

3c The fourth, inevident condition

Strangely, the three conditions do not ensure a unique dynamics. Good operators (especially, generators of unitary groups) satisfy also the fourth condition $\text{Range}(A \pm \mathrm{i}\mathbb{1}) = H$*, and are called self-adjoint. Surprisingly, the four conditions are sufficient for all our purposes (in subsequent sections).*

Let (U_t) be a unitary group and A an operator such that $\frac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0} U_t x = \mathrm{i}Ax$ for all $x \in \text{Domain}(A)$. One may hope to construct (U_t) from A via the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t} U_t x = \mathrm{i}Ax$$

for all $x \in \text{Domain}(A)$ or, maybe, for a smaller but still dense set of "good" vectors x. However, this is a delusion! Two different generators (of two different unitary groups) can coincide on a dense set.

3c1 Example. Given $\alpha \in \mathbb{C}$, $|\alpha| = 1$, we define unitary operators $U_t^{(\alpha)}$ on $L_2(0,1)$ by

$$U_t^{(\alpha)} f : q \mapsto \alpha^k f(q + t - k) \quad \text{whenever } q + t - k \in (0,1) \, ;$$

here k runs over $\mathbb{Z}$. It is easy to see that $\big(U_t^{(\alpha)}\big)_{t \in \mathbb{R}}$ is a unitary group. Its generator $A^{(\alpha)}$ satisfies

$$A^{(\alpha)} \supset A$$

where $\mathrm{i}Af = f'$ for all $f \in \text{Domain}(A)$ and $\text{Domain}(A)$ consists of all continuously differentiable functions $(0,1) \to \mathbb{C}$ whose supports are compact subsets of the open interval $(0,1)$. (Such functions are dense in $L_2(0,1)$.)

The operator A is symmetric (integrate by parts...), and its closure satisfies all the three conditions: densely defined, symmetric, closed. Nevertheless, $\mathrm{Closure}(A) \subset A^{(\alpha)}$ for all α (since $A^{(\alpha)}$ are closed), thus, the differential equation $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = A\psi(t)$ fails to determine dynamics uniquely. Somehow, $\psi(t)$ escapes $\mathrm{Domain}(A)$. There should be a fourth condition, satisfied by all generators but violated by A.

3c2 Theorem. If $\mathrm{Closure}(A)$ is the generator of a unitary group then $\mathrm{Range}(A + \mathrm{i}1\!\!1)$ is dense.

Proof. Assuming the contrary we get $y \in H$, $y \neq 0$, such that $\langle Ax + \mathrm{i}x, y \rangle = 0$, that is, $\langle \mathrm{i}Ax, y \rangle = \langle x, y \rangle$, for all $x \in \mathrm{Domain}(A)$. It follows that $\langle \mathrm{i}Bx, y \rangle = \langle x, y \rangle$ for all $x \in \mathrm{Domain}(B)$ where $B = \mathrm{Closure}(A)$ is the generator of (U_t). For all $x \in \mathrm{Domain}(B)$ we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle U_t x, y \rangle = \langle \mathrm{i}BU_t x, y \rangle = \langle U_t x, y \rangle \quad \text{for all } t \in \mathbb{R}\,,$$

since $U_t x \in \mathrm{Domain}(B)$. We see that $\langle U_t x, y \rangle = \mathrm{const} \cdot \mathrm{e}^t$; taking into account that $|\langle U_t x, y \rangle| \le \|x\| \cdot \|y\|$ we conclude that $\langle U_t x, y \rangle = 0$. In particular, $\langle x, y \rangle = 0$ for all $x \in \mathrm{Domain}(B)$, which cannot happen for a non-zero y. $\square$

3c3 Exercise. $\mathrm{Range}(A + \mathrm{i}1\!\!1)$ is not dense for the operator A of 3c1.

Prove it.

Hint: try $y : q \mapsto \mathrm{e}^q$.

3c4 Exercise. If $\mathrm{Closure}(A)$ is the generator of a unitary group then $\mathrm{Range}(A + \mathrm{i}\lambda 1\!\!1)$ is dense for every $\lambda \in \mathbb{R}$ such that $\lambda \neq 0$.

Prove it.

Hint: $(1/\lambda)A$ is also a generator.

3c5 Exercise. If $\mathrm{Closure}(A)$ is the generator of a unitary group then $\mathrm{Range}(A + z1\!\!1)$ is dense for every $z \in \mathbb{C} \setminus \mathbb{R}$.

Prove it.

Hint: $A + \lambda 1\!\!1$ is also a generator (for $\lambda \in \mathbb{R}$).

3c6 Exercise. Every bounded symmetric operator is the generator of a unitary group.

Prove it.

Hint: the series $U_t = \sum_{k=0}^{\infty} \frac{\mathrm{i}^k}{k!} t^k A^k$ converges in the operator norm.

3c7 Corollary. $\mathrm{Range}(A + z1\!\!1)$ is dense for every bounded symmetric operator A and every $z \in \mathbb{C} \setminus \mathbb{R}$.

3c8 Exercise. Let $\operatorname{Closure}(A) = \varphi(P)$ for some $\varphi \in L_0(\mathbb{R})$, $\overline{\varphi} = \varphi$. Then $\operatorname{Range}(A + \mathrm{i}\mathbb{1})$ is dense.

Prove it.

Hint: first, replace P with Q. Second, $\frac{1}{\varphi(\cdot)+\mathrm{i}\mathbb{1}} \in L_\infty$.

3c9 Exercise. The following two conditions on $x, y \in H$ are equivalent:

(a) $\langle x, y \rangle \in \mathbb{R}$;

(b) $\|x + \mathrm{i}y\|^2 = \|x\|^2 + \|y\|^2$.

Prove it.

3c10 Lemma. The following two conditions on a symmetric operator A are equivalent:

(a) $\operatorname{Range}(A + \mathrm{i}\mathbb{1})$ is closed;

(b) A is closed.

Proof. For all $x, y \in \operatorname{Graph}(A)$ we have $\|y + \mathrm{i}x\|^2 = \|y\|^2 + \|x\|^2$ by 3c9 and 3b4. Thus, $\operatorname{Range}(A + \mathrm{i}\mathbb{1})$ and $\operatorname{Graph}(A)$ are isometric. □

3c11 Exercise. $\operatorname{Range}(A + z\mathbb{1})$ is closed for every $z \in \mathbb{C} \setminus \mathbb{R}$ and every closed symmetric operator A.

Prove it.

Hint: 3b2 can help.

3c12 Definition. [1] A *self-adjoint operator* is a densely defined, closed symmetric operator A such that $\operatorname{Range}(A - \mathrm{i}\mathbb{1}) = H$ and $\operatorname{Range}(A + \mathrm{i}\mathbb{1}) = H$.

Note that "symmetric" and "self-adjoint" mean the same for bounded operators (recall 3c7) but differ for closed unbounded operators.

3c13 Proposition. The generator of a unitary group is self-adjoint.

Proof. We combine 3b12, 3b13, 3b17, 3c2 and 3c10. □

3c14 Exercise. If A is self-adjoint then $(A - \mathrm{i}\mathbb{1})^{-1}$ and $(A + \mathrm{i}\mathbb{1})^{-1}$ are well-defined bounded operators of norm ≤ 1.

Prove it.

3c15 Exercise. If A is self-adjoint, B is symmetric and B extends A, then $A = B$.

Prove it.

Hint: otherwise $(B + \mathrm{i}\mathbb{1})y = (A + \mathrm{i}\mathbb{1})x = (B + \mathrm{i}\mathbb{1})x$ for some $y \in \operatorname{Domain}(B)$ and $x \in \operatorname{Domain}(A)$, $x \ne y$.

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[1] Not the standard definition, but equivalent. Another equivalent definition will be given in 3i3.

3c16 Exercise. If Range$(A - \mathrm{i}1\!\!1)$ and Range$(A + \mathrm{i}1\!\!1)$ are dense and (U_t), (V_t) are unitary groups such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} U_t x = Ax = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} V_t x \quad \text{for all } x \in \mathrm{Domain}(A)\,,$$

then $U_t = V_t$ for all t.

Prove it.

Hint: 3c15 and 3b15.

The dense range condition is essential! (Do not forget Example 3c1.)

3d Application to the Schrödinger equation

The Schrödinger operator is self-adjoint, which ensures uniqueness (recall 3c16) and existence (wait for Sect. 3i) of the corresponding dynamics.

Given a continuous $v : \mathbb{R} \to \mathbb{R}$, we consider the operator

$$\mathcal{H} = P^2 + v(Q) : \psi \mapsto -\psi'' + v \cdot \psi$$

on the set Domain$(\mathcal{H})$ of all twice continuously differentiable, compactly supported functions $\psi : \mathbb{R} \to \mathbb{C}$.

3d1 Theorem. If $v(\cdot)$ is bounded from below then Closure$(\mathcal{H})$ is self-adjoint.[1]

We assume that $v(\cdot) > 0$ (otherwise add a constant and use 3i5). Clearly, $\mathcal{H}$ is symmetric. If Closure$(\mathcal{H})$ is not self-adjoint then either Range$(\mathcal{H} - \mathrm{i}1\!\!1)$ or Range$(\mathcal{H} + \mathrm{i}1\!\!1)$ is not closed. Consider the former case (the latter is similar): there exists $f \in L_2(\mathbb{R})$ such that $\|f\| \ne 0$ and $\langle (\mathcal{H} - \mathrm{i}1\!\!1)\psi, f\rangle = 0$ for all $\psi \in \mathrm{Domain}(\mathcal{H})$. That is,

$$\text{(3d2)} \quad \int \big(-\psi''(q) + v(q)\psi(q) - \mathrm{i}\psi(q) \big) \bar{f}(q)\,\mathrm{d}q = 0 \quad \text{for all } \psi \in \mathrm{Domain}(\mathcal{H})\,.$$

Clearly, (3d2) holds whenever f is twice continuously differentiable and

$$\text{(3d3)} \qquad -f''(q) + v(q)f(q) + \mathrm{i}f(q) = 0 \quad \text{for all } q\,,$$

but we need the converse: (3d3) follows from (3d2). Proving it we restrict ourselves to the interval $(0,1)$ and functions ψ with compact support within $(0,1)$. Clearly, $\int_0^1 \psi''(q)\,\mathrm{d}q = 0$ and $\int_0^1 q\psi''(q)\,\mathrm{d}q = 0$, but the converse is also

[1] In fact, $v(q) \ge -\mathrm{const} \cdot q^2$ (for large $|q|$) is still good, but $v(q) \sim -\mathrm{const} \cdot |q|^{2+\varepsilon}$ is bad.

true: every continuous $g : (0,1) \to \mathbb{C}$ with a compact support within $(0,1)$, satisfying

$$\int_0^1 g(q)\,\mathrm{d}q = 0 \quad \text{and} \quad \int_0^1 qg(q)\,\mathrm{d}q = 0 \tag{3d4}$$

is of the form $g = \psi''$. We have

$$\psi(a) = \int_0^1 K(a,b)\psi''(b)\mathrm{d}b = \int_0^1 K(a,b)g(b)\,\mathrm{d}b$$

where

$$K(a,b) = -\min(a,b)\min(1-a,1-b)\,.$$

Thus,

$$\begin{aligned} 0 = \int \big(-\psi''(q) + (v(q)-\mathrm{i})\psi(q)\big)\bar f(q)\,\mathrm{d}q = \\ = \int \bar f(q)\Big(- g(q) + (v(q)-\mathrm{i})\int K(q,r)g(r)\,\mathrm{d}r\Big)\,\mathrm{d}q = \\ = -\int \bar f(a)g(a)\,\mathrm{d}a + \iint \bar f(q)(v(q)-\mathrm{i})K(q,r)g(r)\,\mathrm{d}q\mathrm{d}r = \\ = \int \mathrm{d}r\, g(r)\Big(- \bar f(r) + \int \bar f(q)(v(q)-\mathrm{i})K(q,r)\,\mathrm{d}q\Big) \end{aligned}$$

for all g satisfying (3d4) (not only continuous). It follows that

$$\bar f(r) = \int \bar f(q)(v(q)-\mathrm{i})K(q,r)\,\mathrm{d}q \quad \text{for almost all } r\,;$$

this integral is a smooth function of r. Now (3d3) follows easily.

The function $|f(\cdot)|$ has (at least one) local maximum at some q_0. Multiplying f by a constant we ensure $f(q_0) = 1$. Then $\frac{\mathrm{d}^2}{\mathrm{d}q^2}|_{q=q_0}\operatorname{Re} f(q) \le 0$. However, $\operatorname{Re} f''(q_0) = \operatorname{Re}\big(v(q_0)f(q_0) - \mathrm{i}f(q_0)\big) = v(q_0) > 0$; the contradiction completes the proof of the theorem.

3e Cayley transform

Every self-adjoint operator results from some unitary operator by $A = (\mathbb{1} + U)(\mathbb{1} - U)^{-1}$.

3e1 Theorem. For every self-adjoint operator A there exists a unique unitary operator U such that

(a) $U(A + \mathrm{i}\mathbb{1})x = (A - \mathrm{i}\mathbb{1})x$ for all $x \in \operatorname{Domain}(A)$;

(b) $\operatorname{Range}(\mathbb{1} - U) = \operatorname{Domain}(A)$, and $A(\mathbb{1} - U)x = \mathrm{i}(\mathbb{1} + U)x$ for all $x \in H$.

Proof. Uniqueness of U follows from (a); indeed, $U = (A - \mathrm{i}\mathbb{1})(A + \mathrm{i}\mathbb{1})^{-1}$. In order to prove existence we consider the set G of all pairs (x, y) such that $x - y \in \operatorname{Domain}(A)$ and

$$2\mathrm{i}x = (A + \mathrm{i}\mathbb{1})(x - y)\,,$$
$$2\mathrm{i}y = (A - \mathrm{i}\mathbb{1})(x - y)\,.$$

We have $\|x\| = \|y\|$ for all $(x, y) \in G$ by 3c9.

For every $x \in H$ there exists $y \in H$ such that $(x, y) \in G$. Indeed, $x = (A + \mathrm{i}\mathbb{1})z$ for some $z \in \operatorname{Domain}(A)$; taking $y = (A - \mathrm{i}\mathbb{1})z$ we get $x - y = 2\mathrm{i}z$.

Similarly, for every $y \in H$ there exists $x \in H$ such that $(x, y) \in G$. Thus, $G = \operatorname{Graph}(U)$ for a unitary operator U satisfying (a). It remains to prove (b).

For every $z \in \operatorname{Domain}(A)$ there exists a pair $(x, y) \in G$ such that $x - y = 2\mathrm{i}z$. Thus, $x - Ux = 2\mathrm{i}z$, which shows that $\operatorname{Domain}(A) \subset \operatorname{Range}(\mathbb{1} - U)$.

For every $x \in H$ there exists $y \in H$ and $z \in \operatorname{Domain}(A)$ such that $y = Ux$, $x = (A + \mathrm{i}\mathbb{1})z$ and $y = (A - \mathrm{i}\mathbb{1})z$. Thus, $2\mathrm{i}z = x - y = (\mathbb{1} - U)x$; we see that $\operatorname{Range}(\mathbb{1} - U) \subset \operatorname{Domain}(A)$ and so, $\operatorname{Range}(\mathbb{1} - U) = \operatorname{Domain}(A)$. Further, $x + y = Az + \mathrm{i}z + Az - \mathrm{i}z = 2Az = -\mathrm{i}A(x - y)$, that is, $x + Ux = -\mathrm{i}A(x - Ux)$, which shows that $(\mathbb{1} + U)x = -\mathrm{i}A(\mathbb{1} - U)x$. □

This operator U is called the *Cayley transformed* of A.

3e2 Exercise. Let U be the Cayley transformed of A, then $(\mathbb{1} - U)x \neq 0$ for all $x \neq 0$.

Prove it.

Thus, $A = \mathrm{i}(\mathbb{1} + U)(\mathbb{1} - U)^{-1}$.

3e3 Exercise. Let U be the Cayley transformed of A, then $\operatorname{Domain}(A)$ is invariant under U and U^{-1}, and $UAx = AUx$ for all $x \in \operatorname{Domain}(A)$.

Prove it.

Hint: $UAx = Ax - \mathrm{i}Ux - \mathrm{i}x = AUx$.

3e4 Exercise. Let $\varphi \in L_0(\mathbb{R} \to \mathbb{R})$, then

(a) the Cayley transformed of $\varphi(Q)$ is $\frac{\varphi(\cdot) - \mathrm{i}}{\varphi(\cdot) + \mathrm{i}}(Q)$;

(b) the same for P instead of Q.

Prove it.

3f Continuous functions of unitary operators

Continuous functions of unitary operators are defined. In combination with the Cayley transform they provide some functions of self-adjoint operators.

The Banach space $C^2(\mathbb{T})$ of all twice continuously differentiable complex-valued functions on the circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$ is closed under (pointwise) multiplication: $f, g \in C^2(T)$ implies $f \cdot g \in C^2(\mathbb{T})$. Also, $f_n \to f$ and $g_n \to g$ imply $f_n \cdot g_n \to f \cdot g$ (since $\|f \cdot g\| \le \text{const} \cdot \|f\| \cdot \|g\|$ and $f_n \cdot g_n - f \cdot g = f_n \cdot (g_n - g) + (f_n - f) \cdot g$); convergence in $\|\cdot\|_{C^2(\mathbb{T})}$ is meant.[1]

Fourier coefficients $c_k = \int_0^1 f(\mathrm{e}^{2\pi \mathrm{i} x}) \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}x$ of $f \in C^2(\mathbb{T})$ satisfy $|c_k| \le \text{const} \cdot \|f\|/k^2$ (since $c_k = \frac{-\mathrm{i}}{2\pi k} \int \bigl(\frac{\mathrm{d}}{\mathrm{d}x} f(\mathrm{e}^{2\pi \mathrm{i} x}) \bigr) \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}x = \frac{-1}{4\pi^2 k^2} \int \bigl(\frac{\mathrm{d}^2}{\mathrm{d}^2 x} f(\mathrm{e}^{2\pi \mathrm{i} x}) \bigr) \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}x$), therefore $\sum_{k \in \mathbb{Z}} |c_k| \le \text{const} \cdot \|f\|_{C^2(\mathbb{T})}$.[2]

Given a unitary operator U, we define $f(U)$ for $f \in C^2(\mathbb{T})$ by

$$f(U) = \sum_{k \in \mathbb{Z}} c_k U^k \, ;$$

the series converges in the operator norm, and $\|f(U)\| \le \sum_{k \in \mathbb{Z}} |c_k| \le \text{const} \cdot \|f\|_{C^2(\mathbb{T})}$.

Here is a simple special case: $U : l_2 \to l_2$,

$$U = \operatorname{diag}(u_1, u_2, \dots) : (z_1, z_2, \dots) \mapsto (u_1 z_1, u_2 z_2, \dots)$$

for given $u_1, u_2, \dots \in \mathbb{T}$.

3f1 Exercise. In this case

(a) $f(U) = \operatorname{diag}\bigl(f(u_1), f(u_2), \dots \bigr)$ for all $f \in C^2(\mathbb{T})$;

(b) the map $f \mapsto f(U)$ is a $*$-homomorphism (recall Sect. 2a) from $C^2(\mathbb{T})$ to bounded operators; it is positive, and $\|f(U)\| \le \|f\|_{C(\mathbb{T})}$.[3]

(c) Is it true that $\|f(U)\| = \|f\|_{C(\mathbb{T})}$?

Prove (a) and (b); decide (c).

Hint: (a): first consider $f(z) = z^k$; second, linear combinations (trigonometric polynomials); and finally, limits.

The same holds whenever $U : H \to H$ is diagonal in some orthonormal basis.

Another simple case: $U = \varphi(Q) : L_2(\mathbb{R}) \to L_2(\mathbb{R})$, $U : f \mapsto \varphi \cdot f$ for a given $\varphi \in L_\infty(\mathbb{R})$, $|\varphi(\cdot)| = 1$.

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[1] Thus, $C^2(\mathbb{T})$ is a commutative Banach algebra.

[2] In fact, the same holds also for $C^1(\mathbb{T})$ and even for $\mathrm{Lip}_\alpha(\mathbb{T})$, $\alpha > 1/2$; however, $C^2(\mathbb{T})$ is quite enough here.

[3] Note the norm in $C(\mathbb{T})$ rather than $C^2(\mathbb{T})$.

3f2 Exercise. In this case

(a) $f(\varphi(Q)) = f(\varphi(\cdot))(Q)$ for all $f \in C^2(\mathbb{T})$;

(b) the map $f \mapsto f(U)$ is a $*$-homomorphism from $C^2(\mathbb{T})$ to bounded operators; it is positive, and $\|f(U)\| \le \|f\|_{C(\mathbb{T})}$.

(c) Is it true that $\|f(U)\| = \|f\|_{C(\mathbb{T})}$?

Prove (a) and (b); decide (c).

We return to the general case.

3f3 Exercise. $(f \cdot g)(U) = f(U)g(U)$ for all $f, g \in C^2(\mathbb{T})$.

Prove it.

Hint: first consider $f(z) = z^k$ and $g(z) = z^l$; second, linear combinations (trigonometric polynomials); and finally, limits.

3f4 Exercise. $\overline{f}(U) = \big(f(U)\big)^*$ for all $f \in C^2(\mathbb{T})$.

Prove it.

We have a $*$-homomorphism. What about positivity, and the supremal norm?

3f5 Lemma. If $f \in C^2(\mathbb{T})$ is such that $f(x) \in [0, \infty)$ for all $x \in \mathbb{T}$ then $f(U) \ge 0$.

Proof. We assume that $f(x) > 0$ for all $x \in \mathbb{T}$ (otherwise consider $f(\cdot) + \varepsilon$). The function

$$\sqrt{f} : x \mapsto \sqrt{f(x)}$$

belongs to $C^2(\mathbb{T})$. Thus,

$$f(U) = (\sqrt{f} \cdot \sqrt{f})(U) = \big(\sqrt{f}(U)\big)^* \big(\sqrt{f}(U)\big) \ge 0\,.$$

□

3f6 Lemma. $\|f(U)\| \le \|f\|_{C(\mathbb{T})}$ for all $f \in C^2(\mathbb{T})$.

Proof. For every $\varepsilon > 0$ there exists $g \in C^2(\mathbb{T})$ such that $|f(\cdot)|^2 + |g(\cdot)|^2 = \|f\|^2_{C(\mathbb{T})} + \varepsilon$, which implies $\|f(U)x\|^2 \le \|f(U)x\|^2 + \|g(U)x\|^2 = \big(\|f\|^2_{C(\mathbb{T})} + \varepsilon\big)\|x\|^2$. □

3f7 Theorem. For every unitary operator U there exists a unique positive $*$-homomorphism $f \mapsto f(U)$ from $C(\mathbb{T})$ to bounded operators, such that $\|f(U)\| \le \|f\|$ for all f, and if $\forall z \in \mathbb{T}\ f(z) = z$ then $f(U) = U$.

Proof. Uniqueness: first consider monomials, then polynomials, then limits. Existence: we just extend the map $f \mapsto f(U)$ from $C^2(\mathbb{T})$ to $C(\mathbb{T})$ by continuity. □

Such a map $f \mapsto f(U)$ (as well as $f \mapsto f(A)$ defined below, and their extensions to wider classes of functions) is well-known as "function calculus" or "functional calculus"; the corresponding existence theorems are closely related to "spectral mapping theorems".

Application to self-adjoint operators

Consider the Banach algebra $C(\mathbb{R} \cup \{\infty\})$ of all continuous functions $f : \mathbb{R} \to \mathbb{C}$ having a (finite) limit $f(\infty) = f(-\infty) = f(+\infty)$.

3f8 Theorem. For every self-adjoint operator A there exists a unique positive $*$-homomorphism $f \mapsto f(A)$ from $C(\mathbb{R} \cup \{\infty\})$ to bounded operators, such that $\|f(A)\| \le \|f\|$ for all f, and if $\forall a \in \mathbb{R}\ f(a) = \frac{a-\mathrm{i}}{a+\mathrm{i}}$ then $f(A)$ is the Cayley transformed of A.

Proof. The homeomorphism

$$\mathbb{R} \cup \{\infty\} \ni a \mapsto \frac{a - \mathrm{i}}{a + \mathrm{i}} \in \mathbb{T} \tag{3f9}$$

between $\mathbb{R} \cup \{\infty\}$ and $\mathbb{T}$ induced an isomorphism between $C(\mathbb{R} \cup \{\infty\})$ and $C(\mathbb{T})$,

$$C(\mathbb{R} \cup \{\infty\}) \ni f \mapsto g \in C(\mathbb{T}) \quad \text{when } \forall a\ f(a) = g\Big(\frac{a - \mathrm{i}}{a + \mathrm{i}}\Big) ;$$

it remains to let

$$f(A) = g(U)$$

where U is the Cayley transformed of A. □

3f10 Exercise. (a) Let $\varphi \in L_0(\mathbb{R} \to \mathbb{R})$ and $A = \varphi(Q)$, then $f(A) = f(\varphi(\cdot))(Q)$ for all $f \in C(\mathbb{R} \cup \{\infty\})$;

(b) the same for P instead of Q.

Prove it.

Hint: 3e4 and 3f2(a).

Note however that $\mathrm{e}^{\mathrm{i}\lambda A}$ is still not defined, since the function $a \mapsto \mathrm{e}^{\mathrm{i}\lambda a}$ does not belong to $C(\mathbb{R} \cup \{\infty\})$ (unless $\lambda = 0$). Also, indicators of intervals do not belong to $C(\mathbb{R} \cup \{\infty\})$. And of course the unbounded function $\mathrm{id}_{\mathbb{R}} : a \mapsto a$ does not.

3g Some discontinuous functions of unitary operators

Monotone sequences of continuous functions lead to semicontinuous functions by a limiting procedure.

3g1 Definition. For an operator A we write $A \ge 0$ if A is symmetric and

$$\forall x \in \operatorname{Domain}(A) \quad \langle Ax, x \rangle \ge 0 \,.$$

We need some general operator-related inequalities. Recall that $\forall x \in H$ $\|x\|^2 \ge 0$; applying it to $ax - by$ we get $2\operatorname{Re}\,(a\bar{b}\langle x, y\rangle) \le |a|^2\|x\|^2 + |b|^2\|y\|^2$ for all $a, b \in \mathbb{C}$, and therefore $|\langle x, y\rangle| \le \|x\|\|y\|$ for all $x, y \in H$, — the Cauchy-Schwartz inequality.

Similarly, the generalized Cauchy-Schwartz inequality

$$\forall x, y \in \operatorname{Domain}(A) \quad |\langle Ax, y\rangle| \le \sqrt{\langle Ax, x\rangle}\sqrt{\langle Ay, y\rangle}$$

holds for every operator $A \ge 0$. In particular, for a bounded $A \ge 0$

$$\forall x \in H \quad \|Ax\|^2 \le \|A\|^{3/2}\|x\|\sqrt{\langle Ax, x\rangle}\,. \tag{3g2}$$

(Take $y = Ax$ and note that $\langle A^2x, Ax\rangle \le \|A\|^3\|x\|^2$.)

3g3 Lemma. If $\mathbb{1} + A \ge 0$ and $\mathbb{1} - A \ge 0$ then $\|A\| \le 1$.

Proof. $2\operatorname{Re}\langle Ax, y\rangle = \langle A(x+y), x+y\rangle - \langle A(x-y), x-y\rangle \le \|x+y\|^2 + \|x-y\|^2 = 2\|x\|^2 + 2\|y\|^2$; the same holds for ax, by and therefore $|\langle Ax, y\rangle| \le \|x\|\|y\|$ (not only for $x, y \in \operatorname{Domain}(A)$). □

Another important general relation:

$$\|A\|^2 = \|A^*A\| \quad \text{for every bounded operator } A\,.$$

Proof: On one hand, $\|A^*A\| \le \|A^*\|\|A\| = \|A\|^2$; on the other hand, $\|Ax\|^2 = \langle Ax, Ax\rangle = \langle A^*Ax, x\rangle \le \|A^*A\|\|x\|^2$.

3g4 Lemma. A bounded increasing sequence of symmetric bounded operators is strongly convergent. In other words: let symmetric bounded operators $A_1, A_2, \dots$ on H satisfy $A_1 \le A_2 \le \dots$ and $\sup_n \|A_n\| < \infty$; then there exists a symmetric bounded operator A such that

$$\forall x \in H \quad \|A_n x - Ax\| \to 0 \quad \text{as } n \to \infty\,.$$

Proof. For $n > m$ we have

$$\|(A_n - A_m)x\|^2 \le \|A_n - A_m\|^{3/2}\|x\|\sqrt{\langle (A_n - A_m)x, x\rangle} \to 0 \text{ as } m \to \infty$$

uniformly in n. □

Can we define $f(U) = \lim f_n(U)$ whenever $f_n \uparrow f$, $f_n \in C(\mathbb{T} \to \mathbb{R})$, $f : \mathbb{T} \to \mathbb{R}$ is bounded, but $f \notin C(\mathbb{T})$? Yes, but not just now.

3g5 Lemma. Let $f_1, f_2, \dots \in C(\mathbb{T} \to \mathbb{R})$, $g_1, g_2, \dots \in C(\mathbb{T} \to \mathbb{R})$, $f_n \uparrow f$, $g_n \uparrow g$ (pointwise) for some bounded $f, g : \mathbb{T} \to \mathbb{R}$. If $f(\cdot) \le g(\cdot)$ on $\mathbb{T}$ then $\lim_n f_n(U) \le \lim_n g_n(U)$.

Proof. We may assume that $f(\cdot) < g(\cdot)$ (otherwise take $g(\cdot) + \varepsilon$). Open sets $\{z \in \mathbb{T} : f_1(z) < g_n(z)\}$ cover $\mathbb{T}$. By compactness, $\exists n \; f_1(\cdot) < g_n(\cdot)$. Therefore $f_1(U) \le \lim_n g_n(U)$. Similarly, $f_m(U) \le \lim_n g_n(U)$ for each m. □

Thus, $f_n \uparrow f$ and $g_n \uparrow f$ imply $\lim_n f_n(U) = \lim_n g_n(U)$, and we define

$$f(U)x = \lim_n f_n(U)x \quad \text{for all } x \in H$$
$$\text{whenever } f_n \uparrow f,\ f_n \in C(\mathbb{T} \to \mathbb{R}), \text{ and } f : \mathbb{T} \to \mathbb{R} \text{ is bounded.}$$

Note that it extends (not redefines) $f(U)$ for $f \in C(\mathbb{T} \to \mathbb{R})$.

The class $K(\mathbb{T})$ of all functions $f : \mathbb{T} \to [0, \infty)$ obtainable in this way is well-known as the class of all bounded lower semicontinuous functions.[1] Indicators of open sets belong to $K(\mathbb{T})$ (open intervals are enough for us).

3g6 Exercise. If $f, g \in K(\mathbb{T})$ and $c \in [0, \infty)$ then $cf \in K(\mathbb{T})$, $f + g \in K(\mathbb{T})$, $f \cdot g \in K(\mathbb{T})$, and

$$(cf)(U) = cf(U)\,, \quad (f+g)(U) = f(U) + g(U)\,, \quad (f \cdot g)(U) = f(U)g(U)\,.$$

Prove it.

Hint: $f_n \uparrow f$, $g_n \uparrow f$ imply $f_n + g_n \uparrow f + g$, etc.

However, $(-f) \notin K(\mathbb{T})$. Can we define $(f - g)(U)$ as $f(U) - g(U)$?

If $f - g = f_1 - g_1$ then $f + g_1 = g + f_1$, therefore $f(U) + g_1(U) = g(U) + f_1(U)$ and so, $f(U) - g(U) = f_1(U) - g_1(U)$. Thus, we define

$$(f - g)(U) = f(U) - g(U)$$

for all $f, g \in K(\mathbb{T})$.

3g7 Exercise. If $f_1, f_2, \dots \in K(\mathbb{T})$, $f_n \uparrow f$ and f is bounded, then $f \in K(\mathbb{T})$ and $f_n(U)x \to f(U)x$ for all $x \in H$.

Prove it.

Hint: given $f_{n,k} \uparrow f_n$ (as $k \to \infty$), introduce $g_n = \max(f_{1,n}, \dots, f_{n,n})$, prove that $g_n \uparrow f$, note that $g_n \le f_n \le f$ implies $g_n(U) \le f_n(U) \le f(U)$, and use (3g2) (similarly to the proof of 3g4).

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[1] "Lower semicontinuous" means: $\liminf_{s \to t} f(s) \ge f(t)$.

3g8 Lemma. The class $L(\mathbb{T} \to \mathbb{R}) = \{f - g : f, g \in K(\mathbb{T})\}$ is an algebra (over $\mathbb{R}$). The map $f \mapsto f(U)$ is a homomorphism from $L(\mathbb{T} \to \mathbb{R})$ to bounded operators; it is positive, and $\|f(U)\| \le \sup |f(\cdot)|$.

Proof. First, $c(f - g) = cf - cg$ for $c \ge 0$, and $-(f - g) = (g - f)$; further, $(f_1 - g_1) + (f_2 - g_2) = (f_1 + f_2) - (g_1 + g_2)$ and $(f_1 - g_1) \cdot (f_2 - g_2) = (f_1 \cdot f_2 + g_1 \cdot g_2) - (f_1 \cdot g_2 + g_1 \cdot f_2)$, which shows that $K - K$ is an algebra. Second, $\big((f_1 - g_1) + (f_2 - g_2)\big)(U) = (f_1 - g_1)(U) + (f_2 - g_2)(U)$, since both are equal to $f_1(U) + f_2(U) - g_1(U) - g_2(U)$; treating $c(f - g)(U)$ and $\big((f_1 - g_1) \cdot (f_2 - g_2)\big)(U)$ in the same way we conclude that $f \mapsto f(U)$ is a homomorphism.

Positivity: if $f - g \ge 0$ then $(f - g)(U) \ge 0$, since $f(U) \ge g(U)$ by 3g5.

Finally, $-C \le f(\cdot) \le C$ implies $-C \cdot \mathbb{1} \le f(U) \le C \cdot \mathbb{1}$ by positivity (and linearity), and then $\|f(U)\| \le C$ by 3g3.[1] □

Now, for $f \in L(\mathbb{T}) = L(\mathbb{T} \to \mathbb{C}) = \{g + \mathrm{i}h : g, h \in L(\mathbb{T} \to \mathbb{R})\}$ we define

$$f(U) = (\operatorname{Re} f)(U) + \mathrm{i}(\operatorname{Im} f)(U)$$

and get a $*$-homomorphism. Note that

$$\|f(U)\| \le \sup_{\mathbb{T}} |f(\cdot)| \,,$$

since $\|f(U)\|^2 = \|(f(U))^*(f(U))\| = \|(|f|^2)(U)\| \le \sup |f(\cdot)|^2$.

3g9 Exercise. (a) Let $\varphi \in L_\infty(\mathbb{R})$, $|\varphi(\cdot)| = 1$, and $U = \varphi(Q)$, then $f(U) = f(\varphi(\cdot))(Q)$ for all $f \in L(\mathbb{T})$;

(b) the same for P instead of Q.

Prove it.

Hint: 3f2.

3h Bounded functions of (unbounded) self-adjoint operators

Semicontinuous functions of a self-adjoint operator are defined via semicontinuous functions of the corresponding unitary operator.

The homeomorphism (3f9) between $\mathbb{R} \cup \{\infty\}$ and $\mathbb{T}$ transforms the classes $K(\mathbb{T})$, $L(\mathbb{T} \to \mathbb{R})$ and $L(\mathbb{T} \to \mathbb{C})$ of functions on $\mathbb{T}$ into the corresponding classes $K(\mathbb{R} \cup \{\infty\})$, $L(\mathbb{R} \cup \{\infty\} \to \mathbb{R})$ and $L(\mathbb{R} \cup \{\infty\}) = L(\mathbb{R} \cup \{\infty\} \to \mathbb{C})$

[1] It is clear that the approach to $\|f(U)\|$ used here can be used also in the proof of 3f6. It is not clear, whether the approach of 3f6 can be used here, or not. (Try it.)

of functions on $\mathbb{R} \cup \{\infty\}$. Namely, $K(\mathbb{R} \cup \{\infty\})$ consists of all bounded $f : \mathbb{R} \cup \{\infty\} \to [0, \infty)$ such that $f_n \uparrow f$ for some $f_n \in C(\mathbb{R} \cup \{\infty\})$; $L(\mathbb{R} \cup \{\infty\} \to \mathbb{R}) = \{f - g : f, g \in K(\mathbb{R} \cup \{\infty\})$; and $L(\mathbb{R} \cup \{\infty\} \to \mathbb{C}) = \{f + \mathrm{i}g : f, g \in L(\mathbb{R} \cup \{\infty\} \to \mathbb{R})\}$. A function $f \in L(\mathbb{R} \cup \{\infty\} \to \mathbb{C})$ corresponds to $g \in L(\mathbb{T} \to \mathbb{C})$,

$$f(a) = g\Big(\frac{a - \mathrm{i}}{a + \mathrm{i}}\Big), \quad g(z) = f\Big(\mathrm{i}\frac{1+z}{1-z}\Big),$$

and we define $f(A)$ by

$$f(A) = g(U)$$

where the unitary operator $U = (A - \mathrm{i}\mathbb{1})(A + \mathrm{i}\mathbb{1})^{-1}$ is the Cayley transformed of A. However, $g(1) = f(\infty)$; is this value essential? No, it is not.

3h1 Lemma. $\mathbb{1}_{\{1\}}(U) = 0$ whenever U is the Cayley transformed (of some A).

Proof. First, the number 1 is not an eigenvalue of U, that is, $Ux = x$ implies $x = 0$. Indeed, $A(\mathbb{1} - U)x = \mathrm{i}(\mathbb{1} + U)x$ by 3e1(b), thus $Ux = x$ implies $(\mathbb{1} + U)x = 0$, $Ux = -x$ and so, $x = 0$.

Second, the relation $\forall z \in \mathbb{T}\ (1 - z)\mathbb{1}_{\{1\}}(z) = 0$ between functions implies the relation $(\mathbb{1} - U)\mathbb{1}_{\{1\}}(U) = 0$ between operators. □

Thus, $f(A)$ is well-defined for $f \in L(\mathbb{R})$. Here $L(\mathbb{R}) = L(\mathbb{R} \to \mathbb{C}) = \{f|_{\mathbb{R}} : f \in L(\mathbb{R} \cup \{\infty\} \to \mathbb{C})\}$ is an algebra of bounded functions that contains all bounded semicontinuous functions. In particular it contains all bounded continuous functions, especially, $a \mapsto \mathrm{e}^{\mathrm{i}ta}$. Now (at last!) operators $\exp(\mathrm{i}tA)$ for $t \in \mathbb{R}$ are well-defined. Also spectral projections $\mathbb{1}_{(a,b)}(A)$, $\mathbb{1}_{[a,b)}(A)$, $\mathbb{1}_{(a,b]}(A)$, $\mathbb{1}_{[a,b]}(A)$ are well-defined.

3h2 Exercise. (a) Let $\varphi \in L_0(\mathbb{R} \to \mathbb{R})$ and $A = \varphi(Q)$, then $f(A) = f(\varphi(\cdot))(Q)$ for all $f \in L(\mathbb{R})$;

(b) the same for P instead of Q.

Prove it.

Hint: 3g9 and 3e4.

3h3 Exercise. $\mathbb{1}_{(-n,n)}(A)x \to x$ as $n \to \infty$, for every $x \in H$.

Prove it.

Hint: 3g7 and 3h1.

3h4 Lemma. Let $f_n : a \mapsto a\mathbb{1}_{(-n,n)}(a)$, then $f_n(A)x \to Ax$ as $n \to \infty$, for every $x \in \mathrm{Domain}(A)$.

Proof. By 3e1, $x = (\mathbb{1} - U)y$ and $Ax = \mathrm{i}(\mathbb{1} + U)y$ for some $y \in H$. We have $f_n(A)x = f_n(A)(\mathbb{1} - U)y = g_n(A)y$ where

$$g_n(a) = f_n(a)\Big(1 - \frac{a - \mathrm{i}}{a + \mathrm{i}}\Big) = f_n(a) \cdot \frac{2\mathrm{i}}{a + \mathrm{i}} = \\ = 2\mathrm{i}\frac{a}{a + \mathrm{i}}\mathbb{1}_{(-n,n)}(a) = \mathrm{i}\Big(1 + \frac{a - \mathrm{i}}{a + \mathrm{i}}\Big)\mathbb{1}_{(-n,n)}(a)\,.$$

Thus, $f_n(A)x = \mathrm{i}\mathbb{1}_{(-n,n)}(A)(\mathbb{1} + U)y \to \mathrm{i}(\mathbb{1} + U)y = Ax$. □

3h5 Exercise. The following three conditions on $\lambda \in \mathbb{R}$ are equivalent (for every given self-adjoint operator A):

(a) $\mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(A) = 0$ for some $\varepsilon > 0$;

(b) $\exists \varepsilon > 0 \;\; \forall x \in \mathrm{Domain}(A) \;\; \|(A - \lambda\mathbb{1})x\| \ge \varepsilon\|x\|$;

(c) there exists a bounded operator $(A - \lambda\mathbb{1})^{-1}$ inverse to $A - \lambda\mathbb{1}$.

Prove it.

The set $\sigma(A)$ of all numbers $\lambda \in \mathbb{R}$ that *violate* these conditions is called the *spectrum* of A. It is a closed set, the smallest closed set such that $\mathbb{1}_{\mathbb{R}\setminus\sigma(A)}(A) = 0$.

3h6 Exercise. $\sigma(A) \subset [0, \infty)$ if and only if $A \ge 0$.

Prove it.

Hint: on one hand, if $A \ge 0$ then $\|(A + \varepsilon\mathbb{1})x\|^2 \ge \varepsilon^2\|x\|^2$; on the other hand, if $\sigma(A) \subset [0, \infty)$ then $f_n(A) = (g_n(A))^2 \ge 0$ where $f_n : a \mapsto \mathbb{1}_{(-n,n)}(a)$ and $g_n : a \mapsto \sqrt{a}\mathbb{1}_{(0,n)}(a)$.

3h7 Exercise. $\sigma(\mathcal{H}) \subset [\inf v(\cdot), \infty)$ for the Schrödinger operator (recall 3d).

Prove it.

Hint: $\langle -\psi'', \psi\rangle = \langle \psi', \psi'\rangle \ge 0$.

3h8 Exercise. $\sigma(A) \subset [-1, +1]$ if and only if $\|A\| \le 1$.

Prove it.

It is easy to see that the function $f_n : a \mapsto a\mathbb{1}_{(-n,n)}(a)$ may be written as

$$f_n = \int_{-n}^{n} a \,\mathrm{d}\mathbb{1}_{(-\infty,a]}$$

(Riemann-Stieltjes integral in the space of functions with the supremal norm), which implies

$$f_n(A) = \int_{-n}^{n} a \,\mathrm{d}E_A(a)\,, \quad E_A(a) = \mathbb{1}_{(-\infty,a]}(A)$$

(Riemann-Stieltjes integral in the space of operators with the operator norm), and finally, by 3h4,

$$Ax = \int_{-\infty}^{\infty} a \, \mathrm{d}E_A(a)x$$

(improper Riemann-Stieltjes integral in the Hilbert space).

In fact, using measure theory one can extend the map $f \mapsto f(A)$ to all Borel functions f and even all functions measurable w.r.t. a finite Borel measure (that depends on A). Pointwise convergence (and even convergence almost everywhere w.r.t. that measure) of functions, in combination with uniform boundedness, implies strong convergence of operators. Moreover, every self-adjoint operator A is unitarily equivalent to $\varphi(Q)$ for some $\varphi \in L_0(\mathbb{R} \to \mathbb{R})$. (Think, why the "moreover".)

3i Generating a unitary group

Every self-adjoint operator is the generator of a unitary group.

3i1 Theorem. Let A be a self-adjoint operator. Then operators

$$U_t = \exp(\mathrm{i}tA)$$

are a (strongly continuous one-parameter) unitary group, and A is its generator.

First of all, $U_s U_t = U_{s+t}$ since $\mathrm{e}^{\mathrm{i}sa}\mathrm{e}^{\mathrm{i}ta} = \mathrm{e}^{\mathrm{i}(s+t)a}$, and $U_0 = 1\!\!1$, and $U_{-t} = U_t^{-1}$. On the other hand, $U_{-t} = U_t^*$ since $\mathrm{e}^{-\mathrm{i}ta} = \overline{\mathrm{e}^{\mathrm{i}ta}}$. Thus, $U_t^{-1} = U_t^*$, which means that U_t is unitary.

In order to check that $\|U_t x - x\| \to 0$ as $t \to 0$ (which is sufficient to check on a dense set) we introduce subspaces

$$H_n \subset H\,, \quad H_n = 1\!\!1_{(-n,n)}(A)H\,;$$
$$H_1 \cup H_2 \cup \dots \text{ is dense}$$

(by 3h3) and observe that

$$\|U_t x - x\| \le n|t|\|x\| \quad \text{for all } x \in H_n$$

since $|\mathrm{e}^{\mathrm{i}ta} - 1| 1\!\!1_{(-n,n)}(a) \le n|t|$.

It remains to prove that A is the generator of (U_t).

3i2 Exercise. For every n the subspace H_n is invariant under all U_t, and the restricted operators

$$U_t^{(n)} = U_t|_{H_n}$$

are a unitary group on H_n, whose generator is the bounded operator

$$A_n = f_n(A)|_{H_n} , \quad f_n : a \mapsto a1\!\!1_{(-n,n)}(a) .$$

Prove it.

Hint: consider the functions $a \mapsto \mathrm{e}^{\mathrm{i}ta} 1\!\!1_{(-n,n)}(a)$.

The unitary group (U_t) has a generator, — a self-adjoint operator B (recall Sect. 3b); we have to prove that $A = B$. By 3i2,

$$H_n \subset \mathrm{Domain}(B) \quad \text{and} \quad B|_{H_n} = A_n .$$

On the other hand,

$$H_n \subset \mathrm{Domain}(A) \quad \text{and} \quad A|_{H_n} = A_n ,$$

since $f_n(A)x = f_{n+k}(A)x \to Ax$ (as $k \to \infty$) for $x \in H_n$ (recall 3h4). Thus, the self-adjoint operators A and B coincide on the dense set $H_1 \cup H_2 \cup \dots$

Does it mean that $A = B$? No, it does not! Recall Example 3c1. There, self-adjoint operators $A^{(\alpha)}$, different for different α, coincide on a dense set. Continuing that example we may consider subspaces $G_n = L_2\big(\frac1n, \frac{n-1}{n}\big) \subset L_2(0,1)$ and observe that $\mathrm{Domain}(A^{(\alpha)}) \cap G_n$ is dense in G_n, and $A^{(\alpha)}x \in G_n$ for all $x \in \mathrm{Domain}(A^{(\alpha)}) \cap G_n$. Nevertheless G_n is not invariant under the Cayley transformed $U^{(\alpha)}$ of $A^{(\alpha)}$.[1]

Returning to our situation we see that it is much better. The Cayley transformed operators U (of A) and V (of B) coincide on H_n for the following reason. The restricted operator A_n, being bounded (and symmetric) is a self-adjoint operator on H_n. For every $x \in H_n$ there exists $z \in H_n$ such that $x = (A_n + \mathrm{i}1\!\!1)z$. It means both $x = (A + \mathrm{i}1\!\!1)z$ and $x = (B + \mathrm{i}1\!\!1)z$. Thus, $Ux = (A - \mathrm{i}1\!\!1)z = (A_n - \mathrm{i}1\!\!1)z$ as well as $Vx = (B - \mathrm{i}1\!\!1)z = (A_n - \mathrm{i}1\!\!1)z$.

We see that $U = V$ on a dense set, therefore on the whole H. Thus, $A = B$, which completes the proof of Theorem 3i1.

Combining 3i1 with 3c13 we get three corollaries.

3i3 Corollary. An operator generates a unitary group if and only if it is self-adjoint.

3i4 Corollary. If A is self-adjoint then $\mathrm{Range}(A + z1\!\!1) = H$ for every $z \in \mathbb{C} \setminus \mathbb{R}$.

3i5 Corollary. If A is self-adjoint then $\lambda A + c1\!\!1$ is self-adjoint for all $\lambda, c \in \mathbb{R}$.

Combining 3i1, 3c13 and 3b15 we get Stone's theorem: every unitary group (U_t) is of the form $U_t = \exp(\mathrm{i}tA)$ for a self-adjoint A.

[1] In fact, $U^{(\alpha)}x : q \mapsto x(q) - \frac{2\alpha}{\mathrm{e}-\alpha} \int_0^q \mathrm{e}^{q-r} x(r)\,\mathrm{d}r - \frac{2\mathrm{e}}{\mathrm{e}-\alpha} \int_q^1 \mathrm{e}^{q-r} x(r)\,\mathrm{d}r$.

3j List of results

3j1 Theorem. For every self-adjoint operator A there exists a unique unitary operator U (so-called Cayley transformed of A) such that

(a) $U(A + \mathrm{i}\mathbb{1})x = (A - \mathrm{i}\mathbb{1})x$ for all $x \in \mathrm{Domain}(A)$;

(b) $\mathrm{Range}(\mathbb{1} - U) = \mathrm{Domain}(A)$, and $A(\mathbb{1} - U)x = \mathrm{i}(\mathbb{1} + U)x$ for all $x \in H$.

3j2 Theorem. For every unitary operator U there exists a unique positive $*$-homomorphism $f \mapsto f(U)$ from $C(\mathbb{T})$ to bounded operators, such that $\|f(U)\| \le \|f\|$ for all f, and if $\forall z \in \mathbb{T}\ \ f(z) = z$ then $f(U) = U$.

3j3 Theorem. For every self-adjoint operator A there exists a unique positive $*$-homomorphism $f \mapsto f(A)$ from $C(\mathbb{R} \cup \{\infty\})$ to bounded operators, such that $\|f(A)\| \le \|f\|$ for all f, and if $\forall a \in \mathbb{R}\ f(a) = \frac{a-\mathrm{i}}{a+\mathrm{i}}$ then $f(A)$ is the Cayley transformed of A.

3j4 Theorem. The $*$-homomorphism of 3j2 has a unique extension from $C(\mathbb{T})$ to the $*$-algebra $L(\mathbb{T})$ (spanned by all bounded semicontinuous functions) satisfying

$\|f(U)\| \le \sup |f(\cdot)|$ for all $f \in L(\mathbb{T})$;

$C(\mathbb{T} \to \mathbb{R}) \ni f_n \uparrow f \in L(\mathbb{T} \to \mathbb{R})$ implies $\forall x \in H\ \ f_n(U)x \to f(U)x$.

3j5 Theorem. The $*$-homomorphism of 3j3 has a unique extension from $C(\mathbb{R} \cup \{\infty\})$ to the $*$-algebra $L(\mathbb{R})$ (spanned by all bounded semicontinuous functions) satisfying

$\|f(A)\| \le \sup |f(\cdot)|$ for all $f \in L(\mathbb{R})$;

$C(\mathbb{R} \cup \{\infty\} \to \mathbb{R}) \ni f_n \uparrow f \in L(\mathbb{R} \to \mathbb{R})$ implies $\forall x \in H\ \ f_n(A)x \to f(A)x$;

if $\forall n, a\ \ f_n(a) = a\mathbb{1}_{(-n,n)}(a)$ then $\forall x \in \mathrm{Domain}(A)\ \ f_n(A)x \to Ax$.

3j6 Theorem. The formulas

$$U_t = \exp(\mathrm{i}tA)\,,$$
$$Ax = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} U_t x$$

establish a one-to-one correspondence between all strongly continuous one-parameter unitary groups (U_t) and all self-adjoint operators A.

3j7 Theorem. For every continuous function $v : \mathbb{R} \to \mathbb{R}$ bounded from below there exists one and only one strongly continuous one-parameter unitary group (U_t) on $L_2(\mathbb{R})$ such that

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} U_t \psi = -\psi'' + v \cdot \psi$$

for all twice continuously differentiable, compactly supported functions $\psi : \mathbb{R} \to \mathbb{C}$.

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