Lecture Notes on Operator Theory

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Contents

Preface

In these lecture notes, we attempt to introduce a selection of topics in theory of linear operators on Hilbert spaces and its applications to non-relativistic quantum mechanics. Chapter 1 introduces basic definitions of Banach and Hilbert spaces and linear operators on them, following mostly Teschl's book (§0.2–0.6, §1.1–1.3, and §1.6) [1] and Schuller's lectures (Chapters 1–3) [2] as well as the first volume of Reed and Simon's series (Sections II.1–II.3 and Sections III.1–III.2) [4]. Chapter 2 focuses on the notions of self-adjoint and closed operators and develops spectral theorem, following mostly Teschl's book (§0.7, §2.2, §2.4, §2.6, §3.1–3.2, and §3.4 as well as §A.6) [1], Schuller's lectures (Chapters 7–8 and 10–11) [2], the first volume of Reed and Simon's series (Sections III.5 and VIII.1–VIII.2) [4], and Conway's book (§10). Chapter 3 presents applications of the developed theory, introducing axiomatic construction of non-relativistic analysis and focusing on several important classes of operators therein such as momentum operator and Schrödinger operators, following mostly Teschl's book (§6.1 and §7.1–7.3) [1] and Schuller's lectures (Chapters 9 and 18–19) [2]. For a more detailed discussion on spaces of absolutely continuous functions and Sobolev spaces used in Section 3.2, we refer to Leoni's book (Chapters 3, 7, and 10–11) [5], whereas Kato-Rellich theorem discussed in Section 3.4 can be found in Kato's book (Chapter 5, §4.1) [6] and the second volume of Reed and Simon's series (Section X.2) [7]. Chapter 4 addresses applications of nonstandard analysis as an alternative approach to operator theory, following mostly Goldblatt's book (Chapters 1–3) [8] as well as Albeverio, Fenstad, Høegh-Krohn, and Lindstrøm's book (Sections 1.1–1.2) [9] referring to the usual ultrapower construction of a hyperreal field, and the papers by Benci and Luperi Baglini referring to the Λ-limit approach and construction of space of ultrafunctions [10, 11, 12, 13]. Many thanks to Gerald Teschl (Universität Wien), Vieri Benci (Università degli Studi di Pisa), and Lorenzo Luperi Baglini (Università degli Studi di Milano) for numerous suggestions and comments that helped to improve the contents of Sections 2 and 4.

1 Banach spaces

1.1 Normed spaces and completeness

Before we start to work with operators, we have to set up the playground, which is Banach spaces. In order to develop the definition of Banach space, we start with a set V and add new structures step by step. First, we equip V with a linear structure.

Definition 1.1. *Given a non-empty set V and a field $\mathbb{K}$, a* $\mathbb{K}$***-vector (linear) space*** *is a tuple $(V, +, \cdot)$, where $+$ and $\cdot$ are binary operations dubbed summation and scalar multiplication, respectively, and defined as*

$$+: \quad V \times V \to V, \ (v, w) \mapsto v + w, \tag{1}$$

$$\cdot: \quad \mathbb{K} \times V \to V, \ (\lambda, v) \mapsto \lambda v, \tag{2}$$

satisfying the following properties.

1. *$(V, +)$ is an abelian group with identity element 0 and inverse $-v \in V$ for arbitrary $v \in V$.*
2. *$\forall \alpha, \beta \in \mathbb{K}, \ \forall v \in V : \ \alpha(\beta v) = (\alpha\beta)v$ (compatibility).*
3. *$\forall \alpha, \beta \in \mathbb{K}, \ \forall v \in V : \ (\alpha + \beta)v = \alpha v + \beta v$ (distributivity for $\mathbb{K}$)*
4. *$\forall \alpha \in \mathbb{K}, \ \forall v, g \in V : \ \alpha(v + g) = \alpha v + \alpha g$ (distributivity for V)*
5. *$\forall v \in V : \ 1v = v$, where $1 \in \mathbb{K}$ is the identity element of $\mathbb{K}$.*

In what follows, we always assume that $\mathbb{K} = \mathbb{C}$. Next step is to equip the vector space V with a certain function $\|\cdot\|_V : V \to \mathbb{R}$ known as *norm*, which satisfies certain properties highlighted the following definition.

Definition 1.2. *A $\mathbb{C}$-vector space V is called* ***normed*** *if it is equipped with a function $\|\cdot\|_V : V \to \mathbb{R}$ of properties:*

1. *$\forall v \in V, \ \|v\|_V \geq 0$ (positive definiteness),*
2. *$\forall v \in V, \forall \lambda \in \mathbb{C}, \ \|\lambda v\|_V = |\lambda| \|v\|_V$ (scaling invariance),*

3. $\forall v, w \in V,\ \|v+w\|_V \leq \|v\|_V + \|w\|_V$ *(triangular inequality),*

4. $\forall v \in V,\ \|v\|_V = 0 \Rightarrow v = 0,$

known as ***norm****. It is called* ***semi-norm*** *(with V being called respectively* ***semi-normed****) if the last property is not satisfied.*

Exercise 1.1. *Show that any semi-normed space can be made into normed by taking a subset $N = \{v \in V | \|v\|_V = 0\}$ and factorizing over it, $\tilde{V} = V/N$.*

Having equipped the vector space V with a norm, we can introduce the notion of convergence for its elements. If $\{v_n\}_{n\in\mathbb{N}}$ is a sequence of elements $v_n \in V\ \forall n \in \mathbb{N}$, we say that it converges to a certain $v \in V$ if

$$\forall \varepsilon > 0,\ \exists N \in \mathbb{N} \text{ such that } \forall n > N:\ \|v_n - v\|_V < \varepsilon, \tag{3}$$

which can be written is $v = \lim_{n\to\infty} v_n$.

Definition 1.3. *A sequence $\{v_n\}_{n\in\mathbb{N}}$ in V is* ***convergent*** *if there exists $v \in V$ such that*

$$\lim_{n\to\infty} v_n = v. \tag{4}$$

Definition 1.4. *A sequence $\{v_n\}_{n\in\mathbb{N}}$ in V is called* ***Cauchy sequence*** *if*

$$\forall \varepsilon > 0,\ \exists N \in \mathbb{N} \textit{ such that } \forall n, m > N:\ \|v_n - v_m\|_V < \varepsilon. \tag{5}$$

Every convergent sequence is Cauchy, but an arbitrary Cauchy sequence, generally speaking, does not necessarily converge to an element of V. This suggests the following definitions:

Definition 1.5. *A normed space V is called* ***complete***[1] *if every Cauchy sequence in V is convergent. A complete normed space is known as* ***Banach space****.*

1.2 Bounded operators

Having introduced normed and Banach spaces, we proceed by studying maps that preserve their linear structure.

Definition 1.6. *Let $(V, \|\cdot\|_V)$ and $(W, \|\cdot\|_W)$ be normed spaces, and $\mathcal{D}_A \subseteq V$ a linear subspace of V. We call a map $A : \mathcal{D}_A \to W$ such that*

$$A(\lambda v + h) = \lambda A v + A h \tag{6}$$

a ***linear operator*** *with* ***domain*** *$\mathcal{D}_A$.*

In what follows, we focus only on linear-structure-preserving maps and, hence, refer to Definition 1.6 as operator implying its linearity. Moreover, for the sake of simplicity, we assume $\mathcal{D}_A = V$, unless otherwise specified.

An important class of operators is bounded operators, which is defined as follows.

Definition 1.7. *An operator $A : V \to W$ is called* ***bounded*** *if*

$$\sup_{v\in V\setminus\{0\}} \frac{\|Av\|_W}{\|v\|_V} < \infty. \tag{7}$$

Importantly, for given normed spaces V and W, the set of all bounded operators $A : V \to W$ forms itself a normed space with the quantity given in (7) regarded as norm. Moreover, it is even a Banach space if W is one.

[1] In these notes, we operate with Cauchy sequences and completeness in terms of norm. However, these notions do not have to be necessarily defined via norm, but can be provided from weaker structures such as metric and topological spaces.

Theorem 1.1. *All bounded operators mapping a normed space* $(V, \|\cdot\|_V)$ *to a Banach space* $(W, \|\cdot\|_W)$ *form a Banach space* $\mathcal{L}(V, W)$ *equipped with a norm*

$$\forall A \in \mathcal{L}(V, W),\ \|A\| := \sup_{v \in V \setminus \{0\}} \frac{\|Av\|_W}{\|v\|_V}, \tag{8}$$

known as ***operator norm****.*

Proof. In order to prove the theorem, we proceed with the following steps:

1. Demonstrate that $\mathcal{L}(V, W)$ is a $\mathbb{C}$-vector space.

2. Demonstrate that $\mathcal{L}(V, W)$ is a normed space if V and W are normed.

3. Demonstrate that $\mathcal{L}(V, W)$ is a Banach space if W is Banach, i.e., prove its completeness.

Step 1. We start by considering $\mathcal{L}(V, W)$ as a set of all bounded operators from V to W and equipping it with two binary operations

$$+ : \quad \mathcal{L}(V, W) \times \mathcal{L}(V, W) \to \mathcal{L}(V, W), \tag{9}$$
$$\cdot : \quad \mathbb{C} \times \mathcal{L}(V, W) \to \mathcal{L}(V, W), \tag{10}$$

which are consistent with the corresponding linear operations in W, i.e.,

$$(A + B)v \quad := \quad Av + Bv, \tag{11}$$
$$(\lambda A)v \quad := \quad \lambda(Av), \tag{12}$$

for all $v \in V$. Linearity of operations (9) and (10) is straightforward:

$$\begin{aligned}
(A + B)(\mu v + h) &= A(\mu v + h) + B(\mu v + h) &(13)\\
&= \mu Av + Ag + \mu Bv + Bh &(14)\\
&= \mu(A + B)v + (A + B)h, &(15)\\
(\lambda A)(\mu v + h) &= \lambda A(\mu v + h) &(16)\\
&= \lambda(\mu Av + Ah) &(17)\\
&= \mu(\lambda A)v + (\lambda A)h. &(18)
\end{aligned}$$

Therefore, it remains to prove that both (9) and (10) produce a bounded operator, so that $\|A+B\| < \infty$ and $\|\lambda A\| < \infty$ for any $A, B \in \mathcal{L}(V, W)$ and $\lambda \in \mathbb{C}$. Indeed,

$$\begin{aligned}
\|A + B\| &= \sup_{v \in V \setminus \{0\}} \frac{\|(A + B)v\|_W}{\|v\|_V} &(19)\\
&= \sup_{v \in V \setminus \{0\}} \frac{\|Av + Bv\|_W}{\|v\|_V} &(20)\\
&\leq \sup_{v \in V \setminus \{0\}} \left(\frac{\|Av\|_W}{\|v\|_V} + \frac{\|Bv\|_W}{\|v\|_V} \right) &(21)\\
&= \|A\| + \|B\| &(22)\\
&< \infty, &(23)
\end{aligned}$$

where (21) follows from triangular inequality for $\|\cdot\|_W$, and

$$\begin{aligned} \|\lambda A\| &= \sup_{v\in V\setminus\{0\}} \frac{\|(\lambda A)v\|_W}{\|v\|_V} && (24)\\ &= \sup_{v\in V\setminus\{0\}} \frac{\|\lambda(Av)\|_W}{\|v\|_V} && (25)\\ &= |\lambda| \sup_{v\in V\setminus\{0\}} \left(\frac{\|Av\|_W}{\|v\|_V} + \frac{\|Bv\|_W}{\|v\|_V}\right) && (26)\\ &= |\lambda|\|A\| && (27)\\ &< \infty, && (28) \end{aligned}$$

where (26) follows from scaling invariance of $\|\cdot\|_W$. Therefore, $\mathcal{L}(V,W)$ is a $\mathbb{C}$-vector space.

Step 2. In order to prove that (8) is a norm on $\mathcal{L}(V,W)$, we recall the four properties of norm in Definition 1.2.

1. Since both $\|\cdot\|_V$ and $\|\cdot\|_W$ are norms, they are positively defined. Therefore, for every operator $A \in \mathcal{L}(V,W)$, $\|A\| \geq 0$.

2. Scaling invariance of (8) follows from (24)–(27).

3. Triangular inequality for (8) follows from (19)–(22).

4. $\frac{\|Av\|_W}{\|v\|_V} = 0$ if and only if $\|Av\|_W = 0$, which is fulfilled if $Av = 0$ $\forall v \in V$ by definition of norm. In turn, this is true if and only if $A = 0$.

Therefore, if V and W are normed with respect to certain norms $\|\cdot\|_V$ and $\|\cdot\|_W$, the space $\mathcal{L}(V,W)$ is normed with respect to operator norm (8).

Step 3. Now let us recall Definition 1.5 and assume that W is Banach, i.e., complete with respect to $\|\cdot\|_W$, so that every Cauchy sequence in W is convergent. Let $\{A_n\}_{n\in\mathbb{N}}$ be a Cauchy sequence in $\mathcal{L}(V,W)$, so that, recalling (5),

$$\forall\varepsilon > 0,\ \exists N \in \mathbb{N} \text{ such that } \forall n,m > N:\ \|A_n - A_m\| < \varepsilon. \tag{29}$$

Then, for any $v \in V \setminus \{0\}$, we can construct an associated sequence $\{A_n v\}_{n\in\mathbb{N}}$ in W, and $\forall n,m > N$ we obtain

$$\begin{aligned} \|A_n v - A_m v\|_W &= \|v\|_V \frac{\|A_n v - A_m v\|_W}{\|v\|_V} && (30)\\ &\leq \|v\|_V \sup_{v\in V\setminus\{0\}} \frac{\|A_n v - A_m v\|_W}{\|v\|_V} && (31)\\ &= \|v\|_V \sup_{v\in V\setminus\{0\}} \frac{\|(A_n - A_m)v\|_W}{\|v\|_V} && (32)\\ &= \|v\|_V \|A_n - A_m\| && (33)\\ &< \|v\|_V \varepsilon. && (34) \end{aligned}$$

Therefore, since $\varepsilon' := \|v\|_V\varepsilon$ is arbitrary, the sequence $\{A_n v\}_{n\in\mathbb{N}}$ is Cauchy for any $v \in V \setminus \{0\}$. For $v = 0$, it is a constant zero sequence, hence, trivially Cauchy. Since W is Banach, we conclude that $\{A_n v\}_{n\in\mathbb{N}}$ is even convergent, and can associate with it a new map $A : V \to W$ acting on V as follows,

$$Av := \lim_{n\to\infty} (A_n v), \tag{35}$$

for any $v \in V$. Now, it is necessary to show that map A is indeed a bounded operator and limit of $\{A_n\}_{n\in\mathbb{N}}$. Its linearity is straightforward:

$$\begin{aligned} A(\lambda v + h) &= \lim_{n\to\infty} A_n(\lambda v + h) && (36)\\ &= \lim_{n\to\infty} (\lambda A_n v + A_n h) && (37)\\ &= \lambda \lim_{n\to\infty} A_n v + \lim_{n\to\infty} A_n h && (38)\\ &= \lambda A v + A h. && (39)\end{aligned}$$

In order to show its boundedness, for any $v \in V \setminus \{0\}$, we calculate:

$$\begin{aligned} \frac{\|Av\|_W}{\|v\|_V} &= \frac{\|\lim_{n\to\infty}(A_n v)\|_W}{\|v\|_V} && (40)\\ &= \lim_{n\to\infty} \frac{\|A_n v\|_W}{\|v\|_V} && (41)\\ &\leq \lim_{n\to\infty} \sup_{v\in V\setminus\{0\}} \frac{\|A_n v\|_W}{\|v\|_V} && (42)\\ &= \lim_{n\to\infty} \|A_n\|. && (43)\end{aligned}$$

Recalling triangular inequality and scaling invariance from Definition 1.2 for norm, we can show that

$$\begin{aligned} \|C\| &= \|C - D + D\| && (44)\\ &\leq \|C - D\| + \|D\|, && (45)\\ \|D\| &= \|C - D - C\| && (46)\\ &\leq \|C - D\| + \|C\|, && (47)\end{aligned}$$

for any $C, D \in \mathcal{L}(V, W)$. Combining both inequalities, we find:

$$\|C - D\| \geq \Big| \|C\| - \|D\| \Big|, \quad (48)$$

for any $C, D \in \mathcal{L}(V, W)$. Since we assumed that $\{A_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence, we combine (29) and (48) with $C = A_n$ and $D = A_m$ and obtain

$$\Big| \|A_n\| - \|A_m\| \Big| < \varepsilon. \quad (49)$$

Therefore, $\{\|A_n\|\}_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathbb{R}$. Since the former is complete, $\{\|A_n\|\}_{n\in\mathbb{N}}$ is also convergent, and (43) is finite,

$$\frac{\|Av\|_W}{\|v\|_V} < \infty. \quad (50)$$

Since it is valid for any $v \in V \setminus \{0\}$, it remains valid if supremum of the left-hand side of (50) over $V \setminus \{0\}$ is taken, so that

$$\|A\| < \infty, \quad (51)$$

hence, proving that $A \in \mathcal{L}(V, W)$. In order to prove that it is a limit of $\{A_n\}_{n\in\mathbb{N}}$, we fix some $n \in \mathbb{N}$ and, in order to exploit (3), for any $v \in V \setminus \{0\}$, we calculate:

$$\begin{aligned} \frac{\|(A_n - A)v\|_W}{\|v\|_V} &= \frac{\|A_n v - \lim_{m\to\infty} A_m v\|_W}{\|v\|_V} && (52)\\ &= \lim_{m\to\infty} \frac{\|(A_n - A_m)v\|_W}{\|v\|_V} && (53)\\ &\leq \lim_{m\to\infty} \sup_{v\in V\setminus\{0\}} \frac{\|(A_n - A_m)v\|_W}{\|v\|_V} && (54)\\ &= \lim_{m\to\infty} \|A_n - A_m\|. && (55)\end{aligned}$$

Since $\{A_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence, we recall (29) and obtain

$$\frac{\|(A_n - A)v\|_W}{\|v\|_V} < \varepsilon, \tag{56}$$

if $n > N$. Since it is valid for any $v \in V \setminus \{0\}$, it remains valid if supremum of the left-hand side of (56) over $V \setminus \{0\}$ is taken, so that

$$\|A_n - A\| < \varepsilon, \tag{57}$$

Recalling (3) we find that $\lim_{n\to\infty} A_n = A$, hence, concluding the proof. □

We highlight a particular class of bounded operators that will be important in the following chapters, namely, bounded operators that map elements of the normed space V to $\mathbb{C}$, and provide the following definition.

Definition 1.8. *Given a normed space $(V, \|\cdot\|_V)$, a bounded operator $A : V \to \mathbb{C}$ is called* ***(bounded) linear functional*** *on V, and the corresponding Banach space $\mathcal{L}(V, \mathbb{C})$ is known as* ***dual space*** *of V and is denoted as V^*.*

Existence of the dual space for a given normed space allows one to introduce an extended notion of convergence as proposed in the following definition

Definition 1.9. *Given a normed space $(V, \|\cdot\|_V)$ and $v \in V$, a sequence $\{v_n\}_{n\in\mathbb{N}}$* ***converges weakly*** *to v if*

$$\forall v^* \in V^* : \lim_{n\to\infty} v^*(v_n) = v^*(v). \tag{58}$$

In this case, v is called ***weak limit*** *of $\{v_n\}_{n\in\mathbb{N}}$ and is denoted as $\text{w-lim}_{n\to\infty} v_n = v$ and $v_n \rightharpoonup v$.*

Exercise 1.2. *Show that $\text{w-lim}_{n\to\infty} v_n = v$ is necessary but not sufficient for $\lim_{n\to\infty} v_n = v$.*

We conclude with a particularly important result for bounded operators, which allows one to define one only on a dense subset of a given normed space. Before to proceed with it, we provide the following definition.

Definition 1.10. *Given normed spaces $(V, \|\cdot\|_V)$ and $(W, \|\cdot\|_W)$ and an operator $A : \mathcal{D}_A \to W$ with domain $\mathcal{D}_A \subset V$, an operator $\hat{A} : V \to W$ such that*

$$\forall d \in \mathcal{D}_A : \hat{A}d = Ad, \tag{59}$$

is called ***extension*** *of A.*

Theorem 1.2 (Bounded linear transformation (BLT))**.** *Let $(V, \|\cdot\|_V)$ be a normed space, $(W, \|\cdot\|_W)$ be a Banach space, and $A \in \mathcal{L}(\mathcal{D}_A, W)$ be a bounded operator with a domain $\mathcal{D}_A$ being a dense subset of V, i.e., $\overline{\mathcal{D}_A} = V$. Then there exists a unique extension of A to a bounded operator $\hat{A} \in \mathcal{L}(V, W)$, with $\|\hat{A}\| = \|A\|$.*

Proof. In order to prove the theorem, we proceed with the following steps:

1. Construction of a well-defined extension $\hat{A} : V \to W$ of A.
2. Proof of linearity and boundedness of $\hat{A}$, i.e., $\hat{A} \in \mathcal{L}(V, W)$.
3. Proof of uniqueness of $\hat{A}$ and $\|\hat{A}\| = \|A\|$.

Step 1. Since $\mathcal{D}_A$ is a dense subset of V, for any element $v \in V$, there can be constructed a sequence $\{d_n\}_{n\in\mathbb{N}}$ in $\mathcal{D}_A$ that converges to v,

$$\lim_{n\to\infty} d_n = v. \tag{60}$$

In turn, $\forall n, m \in \mathbb{N}$ and $d_n \neq d_m$,

$$\begin{aligned} \|Ad_n - Ad_m\|_W &= \|d_n - d_m\|_V \frac{\|A(d_n - d_m)\|_W}{\|d_n - d_m\|_V} \\ &\leq \|d_n - d_m\|_V \sup_{(d_n - d_m)\in\mathcal{D}_A\setminus\{0\}} \frac{\|A(d_n - d_m)\|_W}{\|d_n - d_m\|_V} \qquad (61) \\ &= \|d_n - d_m\|_V \|A\|. \qquad (62) \end{aligned}$$

For $d_n = d_m$, trivially $\|Ad_n - Ad_m\|_W \leq \|d_n - d_m\|_V\|A\|$, therefore, (62) remains valid. On the other hand, since $\{d_n\}_{n\in\mathbb{N}}$ is convergent in V, it is also a Cauchy sequence. Hence, recalling (5), there exists $N \in \mathbb{N}$ such that $\forall n, m > N$ and $\forall \varepsilon > 0$

$$\|d_n - d_m\|_V < \varepsilon. \tag{63}$$

Therefore, inequality (62) can be developed further,

$$\|Ad_n - Ad_m\|_W < \varepsilon\|A\|.$$

Since A is bounded, $\|A\| < \infty$, and $\varepsilon' := \varepsilon\|A\|$ is arbitrary. This means that $\{Ad_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence in W, which is convergent due to the completeness of W as a Banach space. Therefore, we can define an operator $\hat{A} : V \to W$ such that

$$\hat{A}v = \lim_{n\to\infty} Ad_n, \tag{64}$$

$\forall v = \lim_{n\to\infty} d_n \in V$ with $d_n \in \mathcal{D}_A$ $\forall n \in \mathbb{N}$. In order to show that it is indeed an extension of A in accordance with Definition 1.10, it is enough to notice that $\forall d \in \mathcal{D}_A$ we can construct a trivial constant sequence $\{d_n\}_{n\in\mathbb{N}}$ with $d_n = d\ \forall n \in \mathbb{N}$. In this case, $\lim_{n\to\infty} d_n = d$, and

$$\forall d \in \mathcal{D}_A : \ \hat{A}d = Ad. \tag{65}$$

Therefore, it remains to show that $\hat{A}$ is well-defined, i.e., for $\{d_n\}_{n\in\mathbb{N}}$ and $\{\tilde{d}_n\}_{n\in\mathbb{N}}$ both converging to $v \in V$, $\{Ad_n\}_{n\in\mathbb{N}}$ and $\{A\tilde{d}_n\}_{n\in\mathbb{N}}$ have to converge to the same element $\hat{A}v \in W$. Recalling (3), there exists $N \in \mathbb{N}$ and $\tilde{N} \in \mathbb{N}$ such that $\forall n > N$, $\forall \tilde{n} > \tilde{N}$, and $\forall \varepsilon > 0$

$$\begin{aligned} \|d_n - v\|_V &< \frac{\varepsilon}{2}, \qquad (66) \\ \|\tilde{d}_{\tilde{n}} - v\|_V &< \frac{\varepsilon}{2}. \qquad (67) \end{aligned}$$

In turn, $\forall n > \max\{N, \tilde{N}\}$ and $d_n \neq \tilde{d}_n$,

$$\begin{aligned} \|Ad_n - A\tilde{d}_n\|_W &= \|d_n - \tilde{d}_n\|_V \frac{\|A(d_n - \tilde{d}_n)\|_W}{\|d_n - \tilde{d}_n\|_V} \\ &\leq \|d_n - \tilde{d}_n\|_V \sup_{(d_n - \tilde{d}_n)\in\mathcal{D}_A\setminus\{0\}} \frac{\|A(d_n - \tilde{d}_n)\|_W}{\|d_n - \tilde{d}_n\|_V} \qquad (68) \\ &= \|d_n - \tilde{d}_n\|_V \|A\| \qquad (69) \\ &\leq \Big(\|d_n - v\|_V + \|\tilde{d}_n - v\|_V\Big)\|A\| \qquad (70) \\ &< \varepsilon\|A\|, \qquad (71) \end{aligned}$$

where (70) follows from the triangular inequality for norm. In turn, for $d_n = \tilde{d}_n$, trivially $\|Ad_n - A\tilde{d}_n\|_W < \varepsilon\|A\|$, and, hence, (71) remains valid. Since A is bounded, $\|A\| < \infty$, and $\varepsilon' := \varepsilon\|A\|$ is arbitrary. Therefore, recalling (3), we obtain

$$\lim_{n\to\infty}(Ad_n - A\tilde{d}_n) = 0, \tag{72}$$

or, taking into account continuity of linear operations on W,

$$\lim_{n\to\infty}(Ad_n) = \lim_{n\to\infty}(A\tilde{d}_n), \tag{73}$$

and $\hat{A}$ is well-defined.

Step 2. In order to prove that $\hat{A} \in \mathcal{L}(V, W)$, it is necessary to demonstrate that $\hat{A}$ is linear and bounded. Proof of linearity of $\hat{A}$ is similar to one provided in the proof of Theorem 1.1 and is left as an *exercise*. Boundedness of $\hat{A}$ can be proven by calculating its norm,

$$\begin{aligned}
\|\hat{A}\| &= \sup_{v\in V\setminus\{0\}} \frac{\|\hat{A}v\|_W}{\|v\|_V} && (74)\\
&= \sup_{\substack{v\in V\setminus\{0\}\\ d_n\in\mathcal{D}_A\forall n\in\mathbb{N}\\ \lim_{n\to\infty} d_n=v}} \frac{\|\lim_{n\to\infty} Ad_n\|_W}{\|v\|_V} && (75)\\
&= \sup_{\substack{v\in V\setminus\{0\}\\ d_n\in\mathcal{D}_A\forall n\in\mathbb{N}\\ \lim_{n\to\infty} d_n=v}} \frac{\lim_{n\to\infty}\|Ad_n\|_W}{\|v\|_V} && (76)\\
&\le \sup_{\substack{v\in V\setminus\{0\}\\ d_n\in\mathcal{D}_A\forall n\in\mathbb{N}\\ \lim_{n\to\infty} d_n=v}} \frac{\|A\|\lim_{n\to\infty}\|d_n\|_V}{\|v\|_V} && (77)\\
&\le \sup_{\substack{v\in V\setminus\{0\}\\ d_n\in\mathcal{D}_A\forall n\in\mathbb{N}\\ \lim_{n\to\infty} d_n=v}} \frac{\|A\|\|\lim_{n\to\infty} d_n\|_V}{\|v\|_V} && (78)\\
&= \|A\| && (79)\\
&< \infty, && (80)
\end{aligned}$$

where (75) uses the fact that every $v \in V$ can be written as a limit of a sequence $\{d_n\}_{n\in\mathbb{N}}$ in $\mathcal{D}_A$, and (76) and (78) exploit continuity of norms $\|\cdot\|_W$ and $\|\cdot\|_V$, respectively.

Step 3. For demonstration of uniqueness of $\hat{A}$, we assume that there exists another extension $\hat{B}$ of A, so that

$$\forall d \in \mathcal{D}_A: \ \hat{B}d = Ad. \tag{81}$$

Let $v \in V$. Recalling (3), there exists $N \in \mathbb{N}$ such that $\forall n > N$ and $\forall \varepsilon > 0$

$$\|d_n - v\|_V < \varepsilon. \tag{82}$$

Therefore, if $d_n \neq v$,

$$\begin{aligned}
\|\hat{B}v - Ad_n\|_W &= \|\hat{B}(v - d_n)\|_W && (83)\\
&= \|v - d_n\|_V \frac{\|\hat{B}(v - d_n)\|_W}{\|v - d_n\|_V} && (84)\\
&\le \|v - d_n\|_V \sup_{\substack{(d_n - v)\in V\setminus\{0\}\\ d_n\in\mathcal{D}_A\forall n\in\mathbb{N}\\ \lim_{n\to\infty} d_n=v}} \frac{\|\hat{B}(v - d_n)\|_W}{\|v - d_n\|_V} && (85)\\
&= \|v - d_n\|_V\|\hat{B}\| && (86)\\
&< \varepsilon\|\hat{B}\|, && (87)
\end{aligned}$$

where (83) follows from (81). In turn, for $d_n = v$, trivially $\|\hat{B}v - \hat{B}d_n\|_W < \varepsilon\|\hat{B}\|$, and, hence, (87) remains valid. Since $\hat{B}$ is an extension of A, it is bounded, as proven in Step 2 of this proof, so that $\|\hat{B}\| < \infty$, and $\varepsilon'' := \varepsilon\|\hat{B}\|$ is arbitrary. Therefore, recalling (3),

$$\lim_{n\to\infty} (\hat{B}v - A_n v) = 0, \tag{88}$$

or, equivalently,

$$\hat{B}v = \lim_{n\to\infty} (A_n v). \tag{89}$$

However, recalling the definition (64) of the extension $\hat{A}$, we find

$$\hat{B}v = \hat{A}v. \tag{90}$$

Since it is valid for any $v \in V$, we find that $\hat{B} = \hat{A}$. Finally, we check the norm of A,

$$\begin{aligned}
\|A\| &= \sup_{v\in\mathcal{D}_A\setminus\{0\}} \frac{\|Av\|_W}{\|v\|_V} && (91)\\
&= \sup_{v\in\mathcal{D}_A\setminus\{0\}} \frac{\|\hat{A}v\|_W}{\|v\|_V} && (92)\\
&\leq \sup_{v\in V\setminus\{0\}} \frac{\|\hat{A}v\|_W}{\|v\|_V} && (93)\\
&= \|\hat{A}\|, && (94)
\end{aligned}$$

where (92) follows from the definition of extension, and (93) follows from enlarging the set, on which the supremum is calculated. On the other hand, (79) suggests that $\|A\| \geq \|\hat{A}\|$. Therefore, $\|A\| = \|\hat{A}\|$, and this concludes the proof. □

1.3 Hilbert spaces

In this subchapter, we discuss Hilbert spaces, a particular class of Banach spaces, which is highly important for applications of operator theory, e.g., in quantum mechanics. Similarly to introduction of Banach spaces in subchapter 1.1, we introduce Hilbert spaces via several steps, starting with a $\mathbb{C}$-vector space $\mathcal{H}$ and equipping it with a particular kind of binary map on it.

Definition 1.11. *Given a $\mathbb{C}$-vector space $\mathcal{H}$, a map $\langle\cdot,\cdot\rangle_\mathcal{H} : \mathcal{H}\times\mathcal{H} \to \mathbb{C}$ is called a* ***sesquilinear form*** *on $\mathcal{H}$ if it is antilinear on first argument and linear on the second argument, i.e.,*

$$\begin{aligned}
\langle \lambda h + g, v\rangle_\mathcal{H} &= \overline{\lambda}\langle h, v\rangle_\mathcal{H} + \langle h, v\rangle_\mathcal{H}, && (95)\\
\langle v, \lambda h + g\rangle_\mathcal{H} &= \lambda\langle v, h\rangle_\mathcal{H} + \langle v, g\rangle_\mathcal{H}, && (96)
\end{aligned}$$

for any $h, g, v \in \mathcal{H}$ and $\lambda \in \mathbb{C}$, where $\overline{\lambda}$ is the complex conjugate of λ.

Definition 1.12. *A $\mathbb{C}$-vector space $\mathcal{H}$ is called* ***inner product space*** *if it is equipped with a sesquilinear form denoted $\langle\cdot|\cdot\rangle_\mathcal{H}$[2] of properties:*

1. *$\forall h \in \mathcal{H}\setminus\{0\}$, $\langle h|h\rangle_\mathcal{H} > 0$ (positive definiteness),*
2. *$\forall h, g \in \mathcal{H}$, $\langle h|g\rangle_\mathcal{H} = \overline{\langle g|h\rangle}_\mathcal{H}$ (symmetry),*

known as ***inner product****.*

[2] We stick to the notation $\langle\cdot|\cdot\rangle_\mathcal{H}$, which is typical for literature on quantum mechanics and roots from the so-called Dirac bra-ket notation, which is discussed later. In mathematical literature, another convention $(\cdot,\cdot)_\mathcal{H}$ with linearity in first argument and antilinearity in second argument can be found.

Inner product has an important property, which is frequently used in proofs of results for Hilbert spaces and is stated in the following lemma.

Lemma 1.1 (Cauchy-Schwarz inequality)**.** *Given an inner product space* $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$*, its inner product satisfies:*

$$\forall h, g \in \mathcal{H}: \ |\langle h|g\rangle|^2 \leq \langle h|h\rangle\langle g|g\rangle. \tag{97}$$

Proof. We leave it to the reader as an exercise. □

Interestingly, inner product induces a norm on the corresponding vector space, as is shown in the following theorem, guaranteeing, hence, that any inner product space is a normed space.

Theorem 1.3. *An inner product space* $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ *is a normed space with a norm* $\|\cdot\|_{\mathcal{H}}$ *defined as*

$$\forall h \in \mathcal{H}: \ \|h\|_{\mathcal{H}} := \sqrt{\langle h|h\rangle_{\mathcal{H}}}. \tag{98}$$

Proof. In order to prove that (98) is a norm, we recall the four properties of norm in Definition 1.2.

1. Since the inner product $\langle\cdot|\cdot\rangle_{\mathcal{H}}$ is positively defined by Definition 1.12, we have $\|\cdot\|_{\mathcal{H}} \geq 0$.
2. For scaling invariance, let $\lambda \in \mathbb{C}$ and $h \in \mathcal{H}$. Then

$$\begin{aligned} \|\lambda h\|_{\mathcal{H}} &= \sqrt{\langle \lambda h|\lambda h\rangle_{\mathcal{H}}} && (99)\\ &= |\lambda|\sqrt{\langle h|h\rangle_{\mathcal{H}}} && (100)\\ &= |\lambda|\|h\|_{\mathcal{H}}. && (101)\end{aligned}$$

3. Triangular inequality is obtained as follows:

$$\begin{aligned} \|h+g\|_{\mathcal{H}} &= \sqrt{\langle h+g|h+g\rangle_{\mathcal{H}}} && (102)\\ &= \sqrt{\langle h|h\rangle_{\mathcal{H}} + \langle h|g\rangle_{\mathcal{H}} + \langle g|h\rangle_{\mathcal{H}} + \langle g|g\rangle_{\mathcal{H}}} && (103)\\ &= \sqrt{\langle h|h\rangle_{\mathcal{H}} + \langle h|g\rangle_{\mathcal{H}} + \overline{\langle h|g\rangle}_{\mathcal{H}} + \langle g|g\rangle_{\mathcal{H}}} && (104)\\ &= \sqrt{\langle h|h\rangle_{\mathcal{H}} + 2\mathrm{Re}[\langle h|g\rangle_{\mathcal{H}}] + \langle g|g\rangle_{\mathcal{H}}} && (105)\\ &\leq \sqrt{\langle h|h\rangle_{\mathcal{H}} + 2|\langle h|g\rangle_{\mathcal{H}}| + \langle g|g\rangle_{\mathcal{H}}} && (106)\\ &\leq \sqrt{\langle h|h\rangle_{\mathcal{H}} + 2\langle h|h\rangle_{\mathcal{H}}\langle g|g\rangle_{\mathcal{H}} + \langle g|g\rangle_{\mathcal{H}}} && (107)\\ &= \sqrt{\left(\sqrt{\langle h|h\rangle_{\mathcal{H}}} + \sqrt{\langle g|g\rangle_{\mathcal{H}}}\right)^2} && (108)\\ &= \left|\sqrt{\langle h|h\rangle_{\mathcal{H}}} + \sqrt{\langle g|g\rangle_{\mathcal{H}}}\right| && (109)\\ &= \left|\|h\|_{\mathcal{H}} + \|g\|_{\mathcal{H}}\right| && (110)\\ &= \|h\|_{\mathcal{H}} + \|g\|_{\mathcal{H}}, && (111)\end{aligned}$$

   where (104) follows from the symmetry of inner product in Definition 1.12, (107) follows from Lemma 1.1, and (111) follows from already proven positive definiteness of norm.

4. $\|h\|_{\mathcal{H}} = 0$ if and only if $\langle h|h\rangle_{\mathcal{H}} = 0$. In turn, this implies $h = 0$ due to the positive definiteness in Definition 1.12.

□

The converse, however, is not true, and the following theorem provides a condition on norm inducing an inner product.

Theorem 1.4 (Jordan, von Neumann). *Given a normed space $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$, the norm $\|\cdot\|_{\mathcal{H}}$ induces an inner product $\langle\cdot|\cdot\rangle_{\mathcal{H}}$ on it if and only if*

$$\forall h, g \in \mathcal{H}: \ \|h+g\|_{\mathcal{H}}^2 + \|h-g\|_{\mathcal{H}}^2 = 2(\|h\|_{\mathcal{H}}^2 + \|g\|^2) \quad (\textit{parallelogram identity}), \tag{112}$$

with

$$\forall h, g \in \mathcal{H}: \ \langle h|g\rangle_{\mathcal{H}} := \frac{1}{4}\Big(\|h+g\|_{\mathcal{H}}^2 - \|h-g\|_{\mathcal{H}}^2 + i\|h-ig\|_{\mathcal{H}}^2 - i\|h+ig\|_{\mathcal{H}}^2\Big) \quad (\textit{polarization identity}). \tag{113}$$

Proof. We proceed with proof of the theorem in both directions.

Step 1 (⇒). Let us assume that the norm $\|\cdot\|_{\mathcal{H}}$ induces an inner product $\langle\cdot|\cdot\rangle_{\mathcal{H}}$ defined by (98). Then both (112) and (113) can be recovered by direct calculation which we leave to the reader as an exercise.

Step 2 (⇐). Let us assume that the norm $\|\cdot\|_{\mathcal{H}}$ fulfills (112). Then we consider a binary map $\langle\cdot|\cdot\rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ defined by (113) and verify the properties of inner product as given in Definition 1.11 and 1.12. First, let us show that symmetry and linearity on second argument of inner product imply its anti-linearity:

$$\begin{aligned}
\langle \lambda h + g|v\rangle_{\mathcal{H}} &= \overline{\langle v|\lambda h + g\rangle}_{\mathcal{H}} && (114)\\
&= \overline{\lambda}\overline{\langle v|h\rangle}_{\mathcal{H}} + \overline{\langle v|g\rangle}_{\mathcal{H}} && (115)\\
&= \overline{\lambda}\langle h|v\rangle_{\mathcal{H}} + \langle g|v\rangle_{\mathcal{H}}. && (116)
\end{aligned}$$

Therefore, in order to show that $\langle\cdot|\cdot\rangle_{\mathcal{H}}$ is an inner product, it is enough to verify (96) and two properties of Definition 1.12. For linearity in first argument, we first prove additivity:

$$\begin{aligned}
\langle v|h+g\rangle_{\mathcal{H}} &= \frac{1}{4}\Big(\|v+h+g\|_{\mathcal{H}}^2 - \|v-h-g\|_{\mathcal{H}}^2 + i\|v-ih-ig\|_{\mathcal{H}}^2 - i\|v+ih+ig\|_{\mathcal{H}}^2\Big) && (117)\\
&= \frac{1}{4}\Big(\|v+h+g\|_{\mathcal{H}}^2 + \|v+h-g\|_{\mathcal{H}}^2 - \|v+h-g\|_{\mathcal{H}}^2 - \|v-h-g\|_{\mathcal{H}}^2\\
&\quad + i\|v-ih-ig\|_{\mathcal{H}}^2 + \|v-ih+ig\|_{\mathcal{H}}^2 - \|v-ih+ig\|_{\mathcal{H}}^2 - i\|v+ih+ig\|_{\mathcal{H}}^2\Big) && (118)\\
&= \frac{1}{4}\Big(2(\|v+h\|_{\mathcal{H}}^2 + \|g\|^2) - 2(\|v-g\|_{\mathcal{H}}^2 + \|h\|^2)\\
&\quad + 2i(\|v-ih\|_{\mathcal{H}}^2 + \|g\|^2) - 2i(\|v+ig\|_{\mathcal{H}}^2 + \|h\|^2)\Big) && (119)\\
&= \frac{1}{4}\Big(2(\|v+h\|_{\mathcal{H}}^2 + \|v\|_{\mathcal{H}}^2 + \|g\|^2) - 2(\|v-g\|_{\mathcal{H}}^2 + \|v\|_{\mathcal{H}}^2 + \|h\|^2)\\
&\quad + 2i(\|v-ih\|_{\mathcal{H}}^2 + \|v\|_{\mathcal{H}}^2 + \|ig\|^2) - 2i(\|v+ig\|_{\mathcal{H}}^2 + \|v\|_{\mathcal{H}}^2 + \|ih\|^2)\Big) && (120)\\
&= \frac{1}{4}\Big(2\|v+h\|_{\mathcal{H}}^2 + \|v+g\|_{\mathcal{H}}^2 + \|v-g\|_{\mathcal{H}}^2 - 2\|v-g\|_{\mathcal{H}}^2 - \|v+h\|_{\mathcal{H}}^2 - \|v-h\|^2)\\
&\quad + i(2\|v-ih\|_{\mathcal{H}}^2 + \|v+ig\|_{\mathcal{H}}^2 + \|v-ig\|_{\mathcal{H}}^2\\
&\quad - 2\|v+ig\|_{\mathcal{H}}^2 - \|v+ih\|_{\mathcal{H}}^2 - \|v-ih\|^2)\Big) && (121)\\
&= \frac{1}{4}\Big(\|v+h\|_{\mathcal{H}}^2 - \|v-h\|_{\mathcal{H}}^2 + i\|v-ih\|_{\mathcal{H}}^2 - i\|v+ih\|_{\mathcal{H}}^2\Big)\\
&\quad + \frac{1}{4}\Big(\|v+g\|_{\mathcal{H}}^2 - \|v-g\|_{\mathcal{H}}^2 + i\|v-ig\|_{\mathcal{H}}^2 - i\|v+ig\|_{\mathcal{H}}^2\Big) && (122)\\
&= \langle v|h\rangle_{\mathcal{H}} + \langle v|g\rangle_{\mathcal{H}}, && (123)
\end{aligned}$$

where (119) and (121) follow from the parallelogram identity (112). Scaling invariance can be proven by induction, starting with the trivial case of $\lambda = 0$:

$$\begin{aligned}
\langle h|0g\rangle_{\mathcal{H}} &= \langle h|0\rangle_{\mathcal{H}} && (124)\\
&= \frac{1}{4}\Big(\|h\|_{\mathcal{H}}^2 - \|h\|_{\mathcal{H}}^2 + i\|h\|_{\mathcal{H}}^2 - i\|h\|_{\mathcal{H}}^2\Big) && (125)\\
&= 0 && (126)\\
&= 0\langle h|g\rangle_{\mathcal{H}}, && (127)
\end{aligned}$$

and having by additivity

$$\begin{aligned}
\langle h|-g\rangle_{\mathcal{H}} &= \frac{1}{4}\Big(\|h-g\|^2_{\mathcal{H}} - \|h+g\|^2_{\mathcal{H}} + i\|h+ig\|^2_{\mathcal{H}} - i\|h-ig\|^2_{\mathcal{H}}\Big) &(128)\\
&= -\frac{1}{4}\Big(\|h+g\|^2_{\mathcal{H}} - \|h-g\|^2_{\mathcal{H}} + i\|h-ig\|^2_{\mathcal{H}} - i\|h+ig\|^2_{\mathcal{H}}\Big) &(129)\\
&= -\langle h|g\rangle_{\mathcal{H}}. &(130)
\end{aligned}$$

Therefore, supposing $\langle h|\pm ng\rangle_{\mathcal{H}} = \pm n\langle h|g\rangle_{\mathcal{H}}$ for some $n\in\mathbb{N}$, we calculate:

$$\begin{aligned}
\langle h|\pm(n+1)g\rangle_{\mathcal{H}} &= \pm\langle h|(n+1)g\rangle_{\mathcal{H}} &(131)\\
&= \pm\langle h|ng+g\rangle_{\mathcal{H}} &(132)\\
&= \pm(\langle h|ng\rangle_{\mathcal{H}} + \langle h|g\rangle_{\mathcal{H}}) &(133)\\
&= \pm(n+1)\langle h|g\rangle_{\mathcal{H}}, &(134)
\end{aligned}$$

proving, hence, scaling invariance in $\mathbb{Z}$. In turn, for any $n\in\mathbb{Z}$ and $m\in\mathbb{Z}\setminus\{0\}$,

$$\begin{aligned}
m\Big\langle h\Big|\frac{n}{m}g\Big\rangle_{\mathcal{H}} &= \langle h|ng\rangle_{\mathcal{H}} &(135)\\
&= n\langle h|g\rangle_{\mathcal{H}}. &(136)
\end{aligned}$$

Therefore, $\langle h|\frac{n}{m}g\rangle_{\mathcal{H}} = \frac{n}{m}\langle h|g\rangle_{\mathcal{H}}$, proving scaling invariance in $\mathbb{Q}$. In order to prove scaling invariance for $\lambda\in\mathbb{R}$, we take into account that $\mathbb{Q}$ is a dense set of $\mathbb{R}$, so that any $\lambda\in\mathbb{R}$ is a limit of some sequence $(\lambda_n)_n$ in $\mathbb{Q}$. Therefore, $\forall\varepsilon>0$ there exists $N\in\mathbb{N}$ such that $\forall n>N$ we have $|\lambda_n-\lambda|<\varepsilon$ and can calculate

$$\begin{aligned}
|\lambda_n\langle h|g\rangle_{\mathcal{H}} - \langle h|\lambda g\rangle_{\mathcal{H}}| &= |\langle h|(\lambda_n-\lambda)g\rangle_{\mathcal{H}}| &(137)\\
&= \frac{1}{4}\Big|\|h+(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - \|h-(\lambda_n-\lambda)g\|^2_{\mathcal{H}}\\
&\quad + i\|h-i(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - i\|h+i(\lambda_n-\lambda)g\|^2_{\mathcal{H}}\Big| &(138)\\
&= \frac{1}{4}\Big|2\|h+(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - \|h+(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - \|h-(\lambda_n-\lambda)g\|^2_{\mathcal{H}}\\
&\quad + 2i\|h-i(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - i\|h-i(\lambda_n-\lambda)g\|^2_{\mathcal{H}}\\
&\quad - i\|h+i(\lambda_n-\lambda)g\|^2_{\mathcal{H}}\Big| &(139)\\
&= \frac{1}{4}\Big|2\|h+(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - \|h\|^2_{\mathcal{H}} - |\lambda_n-\lambda|\|g\|^2_{\mathcal{H}}\\
&\quad + 2i\|h-i(\lambda_n-\lambda)g\|^2_{\mathcal{H}} - i\|h\|^2_{\mathcal{H}} - i|\lambda_n-\lambda|\|g\|^2_{\mathcal{H}}\Big| &(140)\\
&\le \frac{1}{4}\Big|2(\|h\|_{\mathcal{H}} + |\lambda_n-\lambda|\|g\|_{\mathcal{H}})^2 - \|h\|^2_{\mathcal{H}} - |\lambda_n-\lambda|\|g\|^2_{\mathcal{H}}\\
&\quad + 2i(\|h\|_{\mathcal{H}} + |\lambda_n-\lambda|\|g\|_{\mathcal{H}})^2 - i\|h\|^2_{\mathcal{H}} - i|\lambda_n-\lambda|\|g\|^2_{\mathcal{H}}\Big| &(141)\\
&= \Big||\lambda_n-\lambda|\|h\|_{\mathcal{H}}\|g\|_{\mathcal{H}} + i|\lambda_n-\lambda|\|h\|_{\mathcal{H}}\|g\|_{\mathcal{H}}\Big| &(142)\\
&= \sqrt{2}|\lambda_n-\lambda|\|h\|_{\mathcal{H}}\|g\|_{\mathcal{H}} &(143)\\
&< \sqrt{2}\varepsilon\|h\|_{\mathcal{H}}\|g\|_{\mathcal{H}}, &(144)
\end{aligned}$$

where (140) follows from parallelogram identity (112), while (141) exploits triangular inequality and scaling invariance of the norm. Therefore, $\lim_{n\to\infty}\lambda_n\langle h|g\rangle_{\mathcal{H}} = \langle h|\lambda g\rangle_{\mathcal{H}}$. In turn, we have

$$\begin{aligned}
\lambda\langle h|g\rangle_{\mathcal{H}} &= \lim_{n\to\infty}\lambda_n\langle h|g\rangle_{\mathcal{H}} &(145)\\
&= \langle h|\lambda g\rangle_{\mathcal{H}}, &(146)
\end{aligned}$$

hence, proving scaling invariance in $\mathbb{R}$. Finally, in order to prove it for any complex $\lambda \in \mathbb{C}$, we calculate:

$$\begin{aligned}
\langle h|\lambda g\rangle_{\mathcal{H}} &= \langle h|(\mathrm{Re}[\lambda] + i\mathrm{Im}[\lambda])g\rangle_{\mathcal{H}} &(147)\\
&= \mathrm{Re}[\lambda]\langle h|g\rangle_{\mathcal{H}} + \mathrm{Im}[\lambda]\langle h|ig\rangle_{\mathcal{H}} &(148)\\
&= \mathrm{Re}[\lambda]\langle h|g\rangle_{\mathcal{H}} + \frac{\mathrm{Im}[\lambda]}{4}\Big(\|h+ig\|_{\mathcal{H}}^2 - \|h-ig\|_{\mathcal{H}}^2 + i\|h+g\|_{\mathcal{H}}^2 - i\|h-g\|_{\mathcal{H}}^2\Big) &(149)\\
&= \mathrm{Re}[\lambda]\langle h|g\rangle_{\mathcal{H}} + i\frac{\mathrm{Im}[\lambda]}{4}\Big(\|h+g\|_{\mathcal{H}}^2 - \|h-g\|_{\mathcal{H}}^2 + i\|h-ig\|_{\mathcal{H}}^2 - i\|h+ig\|_{\mathcal{H}}^2\Big) &(150)\\
&= \mathrm{Re}[\lambda]\langle h|g\rangle_{\mathcal{H}} + i\mathrm{Im}[\lambda]\langle h|g\rangle_{\mathcal{H}} &(151)\\
&= \lambda\langle h|g\rangle_{\mathcal{H}}. &(152)
\end{aligned}$$

In order to verify the properties of Definition 1.12, we prove positive definiteness of $\langle\cdot|\cdot\rangle_{\mathcal{H}}$:

$$\begin{aligned}
\langle h|h\rangle_{\mathcal{H}} &= \frac{1}{4}\Big(\|h+h\|_{\mathcal{H}}^2 - \|h-h\|_{\mathcal{H}}^2 + i\|h-ih\|_{\mathcal{H}}^2 - i\|h+ih\|_{\mathcal{H}}^2\Big) &(153)\\
&= \|h\|_{\mathcal{H}}^2, &(154)
\end{aligned}$$

using the positive definiteness of norm, and symmetry:

$$\begin{aligned}
\overline{\langle g|h\rangle}_{\mathcal{H}} &= \frac{1}{4}\Big(\|g+h\|_{\mathcal{H}}^2 - \|g-h\|_{\mathcal{H}}^2 - i\|g-ih\|_{\mathcal{H}}^2 + i\|g+ih\|_{\mathcal{H}}^2\Big) &(155)\\
&= \frac{1}{4}\Big(\|h+g\|_{\mathcal{H}}^2 - \|h-g\|_{\mathcal{H}}^2 + i\|h-ig\|_{\mathcal{H}}^2 - i\|h+ig\|_{\mathcal{H}}^2\Big) &(156)\\
&= \langle h|g\rangle_{\mathcal{H}}, &(157)
\end{aligned}$$

and concluding that $\langle\cdot|\cdot\rangle_{\mathcal{H}}$ is indeed an inner product on $\mathcal{H}$. □

Let us check several important examples of Banach and Hilbert spaces.

Exercise 1.3. *A normed space $(\ell^p(\mathbb{N}), \|\cdot\|_p)$ is a space of all sequences $a = (a_i)_i$, for which the corresponding so-called p-norm is finite, i.e.,*

$$\begin{aligned}
\|a\|_{\ell^p(\mathbb{N}),\,1\leq p<\infty} &= \Big(\sum_{i=1}^{\infty}|a_i|^p\Big)^{\frac{1}{p}} < \infty, &(158)\\
\|a\|_{\ell^p(\mathbb{N}),\,p=\infty} &= \sup_{i\in\mathbb{N}}|a_i| < \infty. &(159)
\end{aligned}$$

With respect to $\|\cdot\|_p$, $\ell^p(\mathbb{N})$ are Banach spaces. However, only $\ell^2(\mathbb{N})$ induces an inner product

$$\forall a = (a_i)_i, b = (b_i)_i \in \ell^2(\mathbb{N}):\ \langle a|b\rangle_{\ell^2(\mathbb{N})} = \sum_{i=1}^{\infty}\overline{a_i}b_i, \tag{160}$$

and, hence, is a Hilbert space. Prove this.

Exercise 1.4. *Let (X,Σ,μ) be a σ-finite measure space and $\mathcal{L}^p(X,d\mu)$ be the set of all measurable functions $f: X \to \mathbb{C}$ equipped with functions $\|\cdot\|_p : \mathcal{L}^p(X,d\mu) \to \mathbb{R}$ such that*

$$\begin{aligned}
\|f\|_{1\leq p<\infty} &= \Big(\int_X |f|^p d\mu\Big)^{\frac{1}{p}} < \infty, &(161)\\
\|f\|_{p=\infty} &= \inf\{C|\mu(\{x||f(x)| > C\}) = 0\} < \infty. &(162)
\end{aligned}$$

Normed spaces $L^p(X,d\mu) = \mathcal{L}^p(X,d\mu)/\mathcal{N}(X,d\mu)$ are quotient spaces of $\mathcal{L}^p(X,d\mu)$ with respect to all functions that are zero almost everywhere, $\mathcal{N}(X,d\mu) = \{f|f(x) = 0$ a.e.$\}$. The functions $\|\cdot\|_p := \|\cdot\|_{L^2(X,d\mu)}$ are norms in these spaces, and, with respect to them, $L^p(X,d\mu)$ are Banach spaces. However, only $L^2(X,d\mu)$ induces an inner product

$$\forall f,g \in L^2(X,d\mu):\ \langle f|g\rangle_{L^2(X,d\mu)} = \int_X \overline{f}g\,d\mu, \tag{163}$$

and, hence, is a Hilbert space. Prove this.

Now, we proceed with introduction of the notion of basis. We start with vector spaces that are not necessarily equipped with a norm, and then proceed with Banach spaces.

Definition 1.13. *Given a vector space V, a subset $B \subseteq V$ is called* ***Hamel basis*** *if any finite subset $\{e_i\}_{i=1}^n \subseteq B$ is linearly independent, and $V = \text{span}(B)$, where*

$$\text{span}(B) = \Big\{\sum_{i=1}^n \lambda_i e_i | \lambda_i \in \mathbb{C}\ \forall 1 \le i \le n,\ e_i \in B\ \forall 1 \le i \le n,\ n \ge 1\Big\}. \tag{164}$$

V is called finite-dimensional if it admits a final Hamel basis, and $\dim(V) = |B|$, otherwise it is called infinite-dimensional.

Definition 1.14. *Given a Banach space $(V, \|\cdot\|_V)$, a sequence $\{e_i\}_{i\in\mathbb{N}}$ in V is called* ***Schauder basis*** *if $\forall f \in V$ there exists a unique sequence $\{\lambda_i\}_{i\in\mathbb{N}}$ such that*

$$f = \lim_{n\to\infty} \sum_{i=1}^n \lambda_i e_i. \tag{165}$$

In what follows, we denote this as $f = \sum_{i=1}^\infty \lambda_i e_i$. If $\|e_i\|_V = 1$ for all $i \in \mathbb{N}$, the Schauder basis is called ***normalized****.*

Definition 1.15. *A Hilbert space $\mathcal{H}$ is called* ***separable*** *if it admits an orthonormal Schauder basis, i.e., a normalized Schauder basis $\{e_i\}_{i\in\mathbb{N}}$ such that*

$$\forall i \neq j :\ \langle e_i | e_j \rangle_{\mathcal{H}} = 0. \tag{166}$$

Exercise 1.5. *Show that, given a Hilbert space $\mathcal{H}$ that admits a Schauder basis $\{e_i\}_{i\in\mathbb{N}}$, for any $h \in \mathcal{H}$, which by Definition 1.14 has a unique expansion $h = \sum_{i=1}^\infty a_i e_i$ with respect to $\{e_i\}_{i\in\mathbb{N}}$, we have $a_i = \langle e_i | h \rangle_{\mathcal{H}}$.*

Exercise 1.6. *Prove that the Hilbert spaces $\ell^2(\mathbb{N})$ and $L^2(X, d\mu)$ are separable.*

In what follows, we focus only on **separable Hilbert spaces**, hence, assuming that there always exists an orthonormal Schauder basis.

Definition 1.16. *Vectors $h, g \in \mathcal{H}$ are called* ***orthogonal*** *if*

$$\langle h | g \rangle_{\mathcal{H}} = 0. \tag{167}$$

Let $\mathcal{M} \subset \mathcal{H}$ be a linear subspace. Its ***orthogonal complement*** *$\mathcal{M}^\perp$ is called a set of vectors in $\mathcal{H}$, which are orthogonal to any vector of $\mathcal{M}$, i.e.,*

$$\mathcal{M}^\perp = \{h \in \mathcal{H} | \forall g \in \mathcal{M} :\ \langle h | g \rangle_{\mathcal{H}} = 0\}. \tag{168}$$

Lemma 1.2 (Pythagorean theorem)**.** *Let $\{h_i\}_{i=1}^n \subset \mathcal{H}$ be a set of pairwise orthogonal vectors. Then*

$$\Big\|\sum_{i=1}^n h_i\Big\|_{\mathcal{H}}^2 = \sum_{i=1}^n \|h_i\|_{\mathcal{H}}^2. \tag{169}$$

Proof. Let $\{h_i\}_{i=1}^n \subset \mathcal{H}$ such that $\forall i \neq j :\ \langle h_i | h_j \rangle_{\mathcal{H}} = 0$. Then we calculate:

$$\Big\|\sum_{i=1}^n h_i\Big\|_{\mathcal{H}}^2 = \Big\langle \sum_{i=1}^n h_i \Big| \sum_{j=1}^n h_j \Big\rangle_{\mathcal{H}} \tag{170}$$

$$= \sum_{i=1}^n \langle h_i | h_i \rangle_{\mathcal{H}} + \sum_{i\neq j} \langle h_i | h_j \rangle_{\mathcal{H}} \tag{171}$$

$$= \sum_{i=1}^n \langle h_i | h_i \rangle_{\mathcal{H}} \tag{172}$$

$$= \sum_{i=1}^n \|h_i\|_{\mathcal{H}}^2. \tag{173}$$

□

Definition 1.17. *Given Hilbert spaces V and W, a bijective map $U : V \to W$ is called* ***unitary operator*** *if it preserves inner product:*

$$\forall h, g \in V : \langle Uh|Ug\rangle_W = \langle h|g\rangle_V. \tag{174}$$

If such an operator exists, V and W are called ***unitarily equivalent****.*

Exercise 1.7. *Prove that any surjective map $U : V \to W$ that preserves inner product is a unitary operator.*

Theorem 1.5. *Any infinite-dimensional separable Hilbert space is unitarily equivalent to $\ell^2(\mathbb{N})$.*

Proof. Let us consider a separable Hilbert space $\mathcal{H}$. By Definition 1.15, it admits an orthonormal Schauder basis $\{e_i\}_{i\in\mathbb{N}}$. Let us consider a map $U : \mathcal{H} \to \ell^2(\mathbb{N})$ which maps any $h \in \mathcal{H}$ to a sequence $(\langle e_i|h\rangle)_{i\in\mathbb{N}}$ that indeed exists due to Definition 1.15 and Exercise 1.5. First, we have to verify that $(\langle e_i|h\rangle)_{i\in\mathbb{N}} \in \ell^2(\mathbb{N})$. Let us calculate its norm,

$$\begin{aligned}
\|(\langle e_i|h\rangle)_{i\in\mathbb{N}}\|^2_{\ell^2(\mathbb{N})} &= \sum_{i=1}^{\infty} |\langle e_i|h\rangle|^2 && (175)\\
&= \lim_{n\to\infty} \sum_{i=1}^{n} |\langle e_i|h\rangle|^2 && (176)\\
&= \lim_{n\to\infty} \sum_{i=1}^{n} |\langle e_i|h\rangle|^2 \|e_i\|^2_{\mathcal{H}} && (177)\\
&= \lim_{n\to\infty} \sum_{i=1}^{n} \|\langle e_i|h\rangle e_i\|^2_{\mathcal{H}} && (178)\\
&= \lim_{n\to\infty} \left\|\sum_{i=1}^{n} \langle e_i|h\rangle e_i\right\|^2_{\mathcal{H}} && (179)\\
&= \left\|\lim_{n\to\infty} \sum_{i=1}^{n} \langle e_i|h\rangle e_i\right\|^2_{\mathcal{H}} && (180)\\
&= \left\|\sum_{i=1}^{\infty} \langle e_i|h\rangle e_i\right\|^2_{\mathcal{H}} && (181)\\
&= \|h\|^2 && (182)\\
&< \infty, && (183)
\end{aligned}$$

where (177) uses orthonormality of the Schauder basis $\{e_i\}_{i\in\mathbb{N}}$, (178) follows from scale invariance of the norm, (179) follows from Lemma 1.2, and (179) exploits continuity of the norm. Therefore, indeed, $(\langle e_i|h\rangle)_{i\in\mathbb{N}} \in \ell^2(\mathbb{N})$. In order to prove that U is unitary, due to the result of Exercise 1.7, we have to proceed with two steps and demonstrate that it is surjective and preserves inner product.

Step 1. In order to prove surjectivity of U, it is necessary to show that for any element of $\ell^2(\mathbb{N})$, there exists the corresponding element of $\mathcal{H}$. Let $(a_i)_{i\in\mathbb{N}} \in \ell^2(\mathbb{N})$. Therefore, there exists $\lim_{n\to\infty} \sum_{i=1}^{n} |a_i|^2$, i.e., the sequence $(\sum_{i=1}^{n} |a_i|^2)_{n\in\mathbb{N}}$ is convergent in $\mathbb{R}$ and, hence, is a Cauchy sequence. Therefore, for any $\varepsilon > 0$, there exists $N \in \mathbb{N}$ such that $\forall n, m > N$,

$$\begin{aligned}
\left|\sum_{i=1}^{n} |a_i|^2 - \sum_{i=1}^{m} |a_i|^2\right| &= \sum_{i=\min(n,m)+1}^{\max(n,m)} |a_i|^2 && (184)\\
&< \varepsilon. && (185)
\end{aligned}$$

In turn,

$$\Big\|\sum_{i=1}^{n} a_i e_i - \sum_{i=1}^{m} a_i e_i\Big\|_{\mathcal{H}}^2 = \Big\|\sum_{i=\min(n,m)+1}^{\max(n,m)} a_i e_i\Big\|_{\mathcal{H}}^2 \tag{186}$$

$$= \sum_{i=\min(n,m)+1}^{\max(n,m)} |a_i|^2 \|e_i\|_{\mathcal{H}}^2 \tag{187}$$

$$= \sum_{i=\min(n,m)+1}^{\max(n,m)} |a_i|^2 \tag{188}$$

$$< \varepsilon, \tag{189}$$

where (187) follows from Lemma 1.2, and (188) follows from orthonormality of the Schauder basis $\{e_i\}_{i\in\mathbb{N}}$. Hence, $(\sum_{i=1}^{n} a_i e_i)_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathcal{H}$. Since a Hilbert space is a Banach space, every Cauchy sequence in it is convergent, and there exists a vector $h \in \mathcal{H}$ such that

$$h = \sum_{i=1}^{\infty} a_i e_i. \tag{190}$$

On the other hand, $Uh = (a_i)_{i\in\mathbb{N}}$, hence, for any sequence in $\ell^2(\mathbb{N})$ there exists an associated vector $h \in \mathcal{H}$.

Step 2. In order to prove that U preserves the inner product, we calculate:

$$\langle h|g\rangle_{\mathcal{H}} = \Big\langle \sum_{i=1}^{\infty} \langle e_i|h\rangle_{\mathcal{H}} e_i \Big| \sum_{j=1}^{\infty} \langle e_j|g\rangle_{\mathcal{H}} e_j \Big\rangle_{\mathcal{H}} \tag{191}$$

$$= \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \overline{\langle e_i|h\rangle_{\mathcal{H}}} \langle e_j|g\rangle_{\mathcal{H}} \langle e_i|e_j\rangle_{\mathcal{H}} \tag{192}$$

$$= \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \overline{\langle e_i|h\rangle_{\mathcal{H}}} \langle e_i|g\rangle_{\mathcal{H}} \tag{193}$$

$$= \Big\langle (\langle e_i|h\rangle_{\mathcal{H}})_{i\in\mathbb{N}} \Big| (\langle e_j|g\rangle_{\mathcal{H}})_{j\in\mathbb{N}} \Big\rangle_{\ell^2(\mathbb{N})} \tag{194}$$

$$= \langle Uh|Ug\rangle_{\ell^2(\mathbb{N})}, \tag{195}$$

where (192) follows from continuity and sesquilinearity of inner product. □

Lemma 1.3. *Let $\mathcal{M} \subseteq \mathcal{H}$ be a linear subspace. Then $\mathcal{M}^\perp$ is a closed linear subspace of $\mathcal{H}$.*

Proof. First, let us prove linearity of $\mathcal{M}^\perp$. Indeed, let $f, g \in \mathcal{M}^\perp$ and $\lambda \in \mathbb{C}$. Then, for any $h \in \mathcal{M}$,

$$\langle h|\lambda f + g\rangle_{\mathcal{H}} = \lambda\langle h|f\rangle + \langle h|g\rangle_{\mathcal{H}} \tag{196}$$

$$= 0, \tag{197}$$

Hence, $\mathcal{H}^\perp$ is a linear subspace of $\mathcal{H}$. In order to show that it is closed, let us define maps $\mathtt{f}_h : \mathcal{H} \to \mathbb{C}$, which, for a certain fixed $H \in \mathcal{H}$, maps any vector $g \in \mathcal{H}$ into its inner product with h, $g \mapsto \langle g|h\rangle_{\mathcal{H}}$. Then, since $\mathcal{M}^\perp$ consists of vectors orthogonal to all elements of $\mathcal{M}$, we can write it as

$$\mathcal{M}^\perp = \bigcap_{h\in\mathcal{M}} \mathrm{preim}_{\mathtt{f}_h}(\{0\}), \tag{198}$$

where $\mathrm{preim}_{\mathtt{f}_h}(\{0\})$ denotes the preimage of zero with respect to $\mathtt{f}_h$. The inner product is continuous, therefore, the preimage of a closed set with respect to $\mathtt{f}_h$ is a closed set. If we assume standard topology on $\mathbb{C}$, $\{0\}$ is a closed set, hence, its preimage is closed as well. Since any intersection of closed sets is again a closed set, we conclude that $\mathcal{M}^\perp$ is closed. □

Lemma 1.4. *Let* $\{e_1, \ldots, e_n\} \subset \mathcal{H}$ *be an orthonormal subset of Hilbert space* $\mathcal{H}$*, i.e., a subset of normalized pairwise orthogonal vectors. Then every* $h \in \mathcal{H}$ *can be written as:*

$$h = h_{\parallel} + h_{\perp}, \tag{199}$$

where $h_{\parallel} = \sum_{i=1}^{n} \langle e_i | h \rangle_{\mathcal{H}} e_i$*, and* $\langle e_i | h_{\perp} \rangle_{\mathcal{H}} = 0$ *for any* $i \in \{1, \ldots, n\}$*, and*

$$\|h\|_{\mathcal{H}}^2 = \|h_{\parallel}\|_{\mathcal{H}}^2 + \|h_{\perp}\|_{\mathcal{H}}^2. \tag{200}$$

Moreover, for any $\tilde{h} \in \operatorname{span}\{e_1, \ldots, e_n\}$*,*

$$\|h - \tilde{h}\|_{\mathcal{H}} \geq \|h_{\perp}\|_{\mathcal{H}}, \tag{201}$$

where the equality holds if and only if $\tilde{h} = h_{\parallel}$*, so that* $h_{\parallel}$ *is uniquely characterized as the closest to* h *vector in* $\operatorname{span}\{e_1, \ldots, e_n\}$*.*

Proof. In order to prove the theorem, we prove first (199) and (200) and proceed with proving (201).

Step 1. Let $h_{\parallel} := \sum_{i=1}^{n} \langle e_i | h \rangle_{\mathcal{H}} e_i$, and $h_{\perp} := h - h_{\parallel}$. Then trivially $h = h_{\parallel} + h_{\perp}$. In turn, for any $j \in \{1, \ldots, n\}$:

$$\begin{aligned}
\langle e_j | h_{\perp} \rangle_{\mathcal{H}} &= \left\langle e_j \middle| h - \sum_{i=1}^{n} \langle e_i | h \rangle_{\mathcal{H}} e_i \right\rangle_{\mathcal{H}} && (202) \\
&= \langle e_j | h \rangle_{\mathcal{H}} - \sum_{i=1}^{n} \langle e_i | h \rangle_{\mathcal{H}} \langle e_j | e_i \rangle_{\mathcal{H}} && (203) \\
&= \langle e_j | h \rangle_{\mathcal{H}} - \langle e_j | h \rangle_{\mathcal{H}} && (204) \\
&= 0. && (205)
\end{aligned}$$

Therefore, by sesquilinearity of inner product, $\langle h_{\perp} | h_{\parallel} \rangle_{\mathcal{H}} = 0$, and $h_{\perp}$ and $h_{\parallel}$ are orthogonal. Hence, applying Lemma 1.2, we verify (200).

Step 2. Let $\tilde{h} \in \operatorname{span}\{e_1, \ldots, e_n\}$, so that

$$\tilde{h} = \sum_{i=1}^{n} c_i e_i, \tag{206}$$

where $c_i \in \mathbb{C}$ for any $i \in \{1, \ldots, n\}$. In turn,

$$\begin{aligned}
\|h - \tilde{h}\|_{\mathcal{H}}^2 &= \|h_{\parallel} + h_{\perp} - \tilde{h}\|_{\mathcal{H}}^2 && (207) \\
&= \left\| \sum_{i=1}^{n} \langle e_i | h \rangle_{\mathcal{H}}^2 e_i + h_{\perp} - \sum_{i=1}^{n} c_i e_i \right\|_{\mathcal{H}}^2 && (208) \\
&= \left\| \sum_{i=1}^{n} \Big(\langle e_i | h \rangle_{\mathcal{H}}^2 - c_i \Big) e_i + h_{\perp} \right\|_{\mathcal{H}}^2 && (209) \\
&= \left\| \sum_{i=1}^{n} \Big(\langle e_i | h \rangle_{\mathcal{H}}^2 - c_i \Big) e_i \right\|_{\mathcal{H}} + \|h_{\perp}\|_{\mathcal{H}}^2 && (210) \\
&= \sum_{i=1}^{n} |\langle e_i | h \rangle_{\mathcal{H}} - c_i|^2 + \|h_{\perp}\|_{\mathcal{H}}^2, && (211)
\end{aligned}$$

where (209) follows from Lemma 1.2, while (210) uses Lemma 1.2 and the fact that vectors e_i are normalized. Therefore, due to positive definiteness of norm, $\|h - \tilde{h}\|_{\mathcal{H}} \geq \|h_{\perp}\|_{\mathcal{H}}$. In turn, equality holds if and only if $\sum_{i=1}^{n} |\langle e_i | h \rangle_{\mathcal{H}} - c_i|^2 = 0$, i.e., $|\langle e_i | h \rangle_{\mathcal{H}} - c_i| = 0$ for every $i \in \{1, \ldots, n\}$. Hence, we conclude that equality holds of and only if $\tilde{h} = h_{\parallel}$. ∎

Theorem 1.6 (Projection theorem)**.** *Let $\mathcal{M} \subseteq \mathcal{H}$ be a closed linear subset of a Hilbert space $\mathcal{H}$. Then every $h \in \mathcal{H}$ can be written as*

$$h = h_{\|} + h_{\perp}, \tag{212}$$

where $h_{\|} \in \mathcal{M}$ and $h_{\perp} \in \mathcal{M}^{\perp}$.

Proof. First, let us show that $\mathcal{M}$ itself is a Hilbert space. Obviously, $\mathcal{M}$ is an inner product space due its linear structure and inner product induced by $\mathcal{H}$. Therefore, it is enough to prove its completeness. Let $\{m_i\}_{i\in\mathbb{N}}$ be a Cauchy sequence in $\mathcal{M}$. Since $\mathcal{H}$ is complete, there exists

$$\mathcal{H} \ni h = \lim_{i\to\infty} m_i. \tag{213}$$

Let us assume that $h \notin \mathcal{M}$, i.e., $h \in \mathcal{H} \setminus \mathcal{M}$, which is an open subset of $\mathcal{H}$ due to closedness of $\mathcal{M}$. Then for any $m \in \mathcal{H} \setminus \mathcal{M}$ there exists $\varepsilon_m > 0$ such that any $h \in \mathcal{H}$ is an element of $\mathcal{H} \setminus \mathcal{M} \ni h$ if $\|m - h\|_{\mathcal{H}} < \varepsilon_m$. On the other hand, due to (213) and (3), there exists $N \in \mathbb{N}$ such that for all $i > N$,

$$\|m_i - h\|_{\mathcal{H}} < \varepsilon_m, \tag{214}$$

meaning that $m_i \in \mathcal{H} \setminus \mathcal{M}$ for all $i > N$, leading to a contradiction. Therefore, any Cauchy sequence in $\mathcal{M}$ converges to an element of $\mathcal{M}$, so that $\mathcal{M}$ is complete and, hence, a Hilbert space. Moreover, if $\mathcal{H}$ is separable, so is $\mathcal{M}$, and there exists an orthonormal basis $\{e_i\}_{i\in\mathbb{N}}$: we leave the proof of this fact to the reader as an *exercise*.

Given $h \in \mathcal{H}$, we define $h_{\|} = \sum_{i=1}^{\infty} h_i e_i \in \mathcal{M}$ and $h_{\perp} = h - h_{\|}$. Calculating

$$\begin{aligned} \langle e_j | h_{\perp} \rangle_{\mathcal{H}} &= \left\langle e_j \middle| h - \sum_{i=1}^{\infty} \langle e_i | h \rangle_{\mathcal{H}} e_i \right\rangle_{\mathcal{H}} & (215) \\ &= \lim_{n\to\infty} \left\langle e_j \middle| h - \sum_{i=1}^{n} \langle e_i | h \rangle_{\mathcal{H}} e_i \right\rangle_{\mathcal{H}} & (216) \\ &= 0, & (217) \end{aligned}$$

where the (216) follows from continuity of inner product, and (217) follows from Lemma 1.4. Therefore, using sesquilinearity and continuity of inner product, we obtain $\langle h_{\|} | h_{\perp} \rangle_{\mathcal{H}}$, so that $h_{\perp} \in \mathcal{M}^{\perp}$. □

Lemma 1.5. *Let $\mathcal{M} \subseteq \mathcal{H}$ be a linear subspace. Then $\mathcal{M}^{\perp\perp} = \overline{\mathcal{M}}$.*

Proof. We proceed with the proof in several steps.

Step 1. Let $h \in \overline{\mathcal{M}}^{\perp}$. Then

$$\forall g \in \overline{\mathcal{M}} : \ \langle g | h \rangle = 0. \tag{218}$$

Since $\mathcal{M} \subseteq \overline{\mathcal{M}}$, we have that

$$\forall g \in \mathcal{M} : \ \langle g | h \rangle = 0. \tag{219}$$

Therefore, $\overline{\mathcal{M}}^{\perp} \subseteq \mathcal{M}^{\perp}$.

Step 2. Let $h \in \mathcal{M}^{\perp\perp}$. Then

$$\forall g \in \mathcal{M}^{\perp} : \ \langle g | h \rangle = 0. \tag{220}$$

Due to Step 1, $\overline{\mathcal{M}}^{\perp} \subseteq \mathcal{M}^{\perp}$, we have that

$$\forall g \in \overline{\mathcal{M}}^{\perp} : \ \langle g | h \rangle = 0. \tag{221}$$

Hence, $\mathcal{M}^{\perp\perp} \subseteq \overline{\mathcal{M}}^{\perp\perp}$.

Step 3. Let $h \in \overline{\mathcal{M}}$. Then

$$\forall g \in \overline{\mathcal{M}}^{\perp} : \ \langle g | h \rangle = 0. \tag{222}$$

Hence, $\overline{\mathcal{M}} \subseteq \overline{\mathcal{M}}^{\perp\perp}$.

Step 4. Let $h \in \overline{\mathcal{M}}^{\perp\perp}$. Due to Theorem 1.6, there exists a decomposition $h = m + n$ with $m \in \overline{\mathcal{M}}$ and $n \in \overline{\mathcal{M}}^{\perp}$. Therefore, calculating

$$\begin{aligned} \langle n|h\rangle_{\mathcal{H}} &= \langle n|m+n\rangle_{\mathcal{H}} && (223)\\ &= \langle n|m\rangle_{\mathcal{H}} + \langle n|n\rangle_{\mathcal{H}} && (224)\\ &= \|n\|^2_{\mathcal{H}} && (225)\\ &\equiv 0, && (226) \end{aligned}$$

where (225) follows from the Definition 1.16 and (98), we obtain that $n = 0$. Therefore, $\overline{\mathcal{M}}^{\perp\perp} \subseteq \overline{\mathcal{M}}$ and, due to Step 3, $\overline{\mathcal{M}}^{\perp\perp} = \overline{\mathcal{M}}$. Therefore, due to Step 2, we conclude that $\mathcal{M}^{\perp\perp} \subseteq \overline{\mathcal{M}}$. On the other hand, Lemma 1.3 suggests that $\mathcal{M}^{\perp\perp}$ is a closed subspace of $\mathcal{H}$. Therefore, since $\mathcal{M} \subseteq \mathcal{M}^{\perp\perp}$, we have $\overline{\mathcal{M}} \subseteq \mathcal{M}^{\perp\perp}$ and conclude that $\mathcal{M}^{\perp\perp} = \overline{\mathcal{M}}$. □

Definition 1.18. *Let $\mathcal{H}$ be a separable Hilbert space, and $\mathcal{M} \subseteq \mathcal{H}$ be its closed linear subspace. An **orthogonal projector** onto $\mathcal{M}$ is called a map $P_{\mathcal{M}} : \mathcal{H} \to \mathcal{M}$ such that for any $h \in \mathcal{H}$,*

$$P_{\mathcal{M}} h = h_{\parallel}. \qquad (227)$$

Lemma 1.6. *Let $P_{\mathcal{M}}$ be an orthogonal projector onto a closed linear subset $\mathcal{M} \subseteq \mathcal{H}$. Then $P_{\mathcal{M}}$ is a bounded idempotent (i.e., $P_{\mathcal{M}} \circ P_{\mathcal{M}} = P_{\mathcal{M}}$) operator such that $\forall h, g \in \mathcal{H}$:*

$$\langle h|P_{\mathcal{M}} g\rangle_{\mathcal{H}} = \langle P_{\mathcal{M}} h|g\rangle_{\mathcal{H}}. \qquad (228)$$

Proof. First, let us prove boundedness of $P_{\mathcal{M}}$ by calculating its norm:

$$\begin{aligned} \|P_{\mathcal{M}}\| &= \sup_{h\in\mathcal{H}\setminus\{0\}} \frac{\|P_{\mathcal{M}} h\|_{\mathcal{H}}}{\|h\|_{\mathcal{H}}} && (229)\\ &= \sup_{h\in\mathcal{H}\setminus\{0\}} \frac{\|h_{\parallel}\|_{\mathcal{H}}}{\|h\|_{\mathcal{H}}} && (230)\\ &= \sup_{h\in\mathcal{H}\setminus\{0\}} \frac{\sqrt{\|h\|^2_{\mathcal{H}} - \|h_{\perp}\|^2_{\mathcal{H}}}}{\|h\|_{\mathcal{H}}} && (231)\\ &= \sup_{h\in\mathcal{H}\setminus\{0\}} \sqrt{1 - \frac{\|h_{\perp}\|^2_{\mathcal{H}}}{\|h\|^2_{\mathcal{H}}}} && (232)\\ &\leq 1 && (233)\\ &< \infty, && (234) \end{aligned}$$

where 231 follows from continuity of norm and Lemma 1.4. In turn, calculating the composition of two operators $P_{\mathcal{M}}$ we obtain:

$$\begin{aligned} (P_{\mathcal{M}} \circ P_{\mathcal{M}})h &= P_{\mathcal{M}}(P_{\mathcal{M}} h) && (235)\\ &= P_{\mathcal{M}}\Big(\sum_{i=1}^{\infty} \langle e_i|h\rangle_{\mathcal{H}} e_i\Big) && (236)\\ &= \sum_{j=1}^{\infty} \Big\langle e_j \Big| \sum_{i=1}^{\infty} \langle e_i|h\rangle_{\mathcal{H}} e_i \Big\rangle_{\mathcal{H}} e_j && (237)\\ &= \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \langle e_i|h\rangle_{\mathcal{H}} \langle e_j|e_i\rangle_{\mathcal{H}} e_j && (238)\\ &= \sum_{i=1}^{\infty} \langle e_i|h\rangle_{\mathcal{H}} e_i && (239)\\ &= P_{\mathcal{M}} h, && (240) \end{aligned}$$

where (238) follows from continuity of inner product, and (239) follows from the fact that e_i are pairwise orthogonal and normalized, proving hence idempotence of $P_{\mathcal{M}}$. Finally, we calculate:

$$\begin{aligned}
\langle h|P_{\mathcal{M}} g\rangle_{\mathcal{H}} &= \Big\langle h\Big|\sum_{i=1}^{\infty}\langle e_i|g\rangle_{\mathcal{H}} e_i\Big\rangle_{\mathcal{H}} && (241)\\
&= \sum_{i=1}^{\infty}\langle e_i|g\rangle_{\mathcal{H}}\langle h|e_i\rangle_{\mathcal{H}} && (242)\\
&= \sum_{i=1}^{\infty}\overline{\langle e_i|h\rangle_{\mathcal{H}}}\langle e_i|g\rangle_{\mathcal{H}} && (243)\\
&= \Big\langle \sum_{i=1}^{\infty}\langle e_i|h\rangle_{\mathcal{H}} e_i\Big| g\Big\rangle_{\mathcal{H}} && (244)\\
&= \langle P_{\mathcal{M}} h|g\rangle_{\mathcal{H}}, && (245)
\end{aligned}$$

where (242) and (244) follows from continuity of inner product, concluding the proof. □

Theorem 1.7 (Riesz representation theorem)**.** *Let $\mathcal{H}$ be a Hilbert space. Then its dual space is equivalent to it*[3]*, $\mathcal{H}^* = \mathcal{H}$, so that for every $\mathtt{f} \in \mathcal{H}^*$ there exists a unique $h \in \mathcal{H}$ such that*

$$\forall g \in \mathcal{H}: \ \mathtt{f}(g) = \langle h|g\rangle_{\mathcal{H}}. \tag{246}$$

Proof. In order to prove the theorem, we prove first that an element of $\mathcal{H}^*$ can be given in the form (246) and proceed with proving its uniqueness.

Step 1. If $f = 0$ is a zero functional in $\mathcal{H}^*$, we can trivially choose $h = 0$. Therefore, let us assume that $\mathtt{f} \neq 0$ and consider a subset $\ker(\mathtt{f}) = \mathrm{preim}_{\mathtt{f}}(\{0\})$. Since $\mathtt{f}$ is linear, for all $\lambda \in \mathbb{C}$ and $m, n \in \ker(\mathtt{f})$, we have:

$$\begin{aligned}
\mathtt{f}(\lambda m + n) &= \lambda \mathtt{f}(m) + \mathtt{f}(n) && (247)\\
&= 0, && (248)
\end{aligned}$$

so that $\ker(\mathtt{f})$ is a linear subspace of $\mathcal{H}$. Since $\mathtt{f} \in \mathcal{L}(\mathcal{H}, \mathbb{C})$, it is a bounded operator, so that $\|\mathtt{f}\| = C < \infty$. In turn, for any $h \in \mathcal{H}$

$$\begin{aligned}
|\mathtt{f}(h)| &\leq \|\mathtt{f}\|\|h\|_{\mathcal{H}} && (249)\\
&= C\|\mathtt{f}\|_{\mathcal{H}}. && (250)
\end{aligned}$$

Hence, $\mathtt{f}$ is Lipschitz continuous and, in turn, continuous. Since $\{0\}$ is a closed set in standard topology on $\mathbb{C}$, we conclude that $\ker(\mathtt{f})$ is a closed linear subspace and, due to Theorem 1.6, we can expand any $h \in \mathcal{H}$ as

$$h = h_{\|} + h_{\perp}, \tag{251}$$

where $h_{\|} \in \ker(\mathtt{f})$ and $h_{\perp} \in \ker(\mathtt{f})^{\perp}$.

If $\mathtt{f} \neq 0$, $\ker(\mathtt{f})^{\perp}$ is a proper subspace of $\mathcal{H}$, and it is possible to find a normalized vector $\tilde{h} \in \ker(\mathtt{f})^{\perp}$, so that $\|\tilde{h}\|_{\mathcal{H}} = 1$. Let $h = \overline{\mathtt{f}(\tilde{h})}\tilde{h} \in \ker(\mathtt{f})^{\perp}$ and define $\mathtt{f}_h := \langle h|\cdot\rangle_{\mathcal{H}}$. Then, for any $g \in \mathcal{H}$,

$$\begin{aligned}
\mathtt{f}\Big(\mathtt{f}(\tilde{h})g - \mathtt{f}(g)\tilde{h}\Big) &= \mathtt{f}(\tilde{h})\mathtt{f}(g) - \mathtt{f}(g)\mathtt{f}(\tilde{h}) && (252)\\
&= 0, && (253)
\end{aligned}$$

[3] This result is widely used in quantum physics and its applications in the form of so-called *bra-ket notation*, where a vector $g \in \mathcal{H}$ is denoted by $|g\rangle$ (dubbed *ket-vector*), while an element $\mathtt{f}_h \in \mathcal{H}^*$ of the dual space is denoted by $\langle h|$ (dubbed *bra-vector*) and associated with the vector $h \in \mathcal{H}$. The inner product $\langle h|g\rangle$ is interpreted then as "action" of bra-vector $\langle h|$ on ket-vector $|g\rangle$.

so that $\mathtt{f}(\tilde{h})g - \mathtt{f}(g)\tilde{h} \in \ker(\mathtt{f})$. Therefore, for any $g \in \mathcal{H}$,

$$\begin{aligned}
\mathtt{f}_h(g) - \mathtt{f}(g) &= \langle h|g\rangle_{\mathcal{H}} - \mathtt{f}(g) && (254)\\
&= \langle \overline{\mathtt{f}(\tilde{h})}\tilde{h}|g\rangle_{\mathcal{H}} - \mathtt{f}(g) && (255)\\
&= \langle \tilde{h}|\mathtt{f}(\tilde{h})g\rangle_{\mathcal{H}} - \mathtt{f}(g) && (256)\\
&= \langle \tilde{h}|\mathtt{f}(\tilde{h})g\rangle_{\mathcal{H}} - \mathtt{f}(g)\langle \tilde{h}|\tilde{h}\rangle_{\mathcal{H}} && (257)\\
&= \langle \tilde{h}|\mathtt{f}(\tilde{h})g\rangle_{\mathcal{H}} - \langle \tilde{h}|\mathtt{f}(g)\tilde{h}\rangle_{\mathcal{H}} && (258)\\
&= \langle \tilde{h}|\mathtt{f}(\tilde{h})g - \mathtt{f}(g)\tilde{h}\rangle_{\mathcal{H}} && (259)\\
&= 0. && (260)
\end{aligned}$$

where (260) takes into account that $\tilde{h} \in \ker(\mathtt{f})^{\perp}$. Hence, we conclude that $\mathtt{f}_h = \mathtt{f}$.

Step 2. In order to prove that, for every $\mathtt{f} \in \mathcal{H}^*$, there is a unique associated $h \in \mathcal{H}$, let us assume that there exist $h, h' \in \mathcal{H}$ such that $\mathtt{f}_h = \mathtt{f}_{h'} = \mathtt{f}$. Then, for any $g \in \mathcal{H}$, we have $\mathtt{f}_h(g) - \mathtt{f}_{h'}(g)$. On the other hand,

$$\begin{aligned}
\mathtt{f}_h(g) - \mathtt{f}_{h'}(g) &= \langle h|g\rangle_{\mathcal{H}} - \langle h'|g\rangle_{\mathcal{H}} && (261)\\
&= \langle h - h'|g\rangle_{\mathcal{H}} && (262)\\
&\equiv 0. && (263)
\end{aligned}$$

Therefore, we conclude that $h = h'$. □

2 Self-adjoint and closed operators

In this chapter, if other is not highlighted, we will study *densely defined* operators on separable Hilbert space $\mathcal{H}$, i.e., operators with a domain $\mathcal{D}_A \subseteq \mathcal{H}$ being a dense subset of $\mathcal{H}$, i.e., $\overline{\mathcal{D}_A} = \mathcal{H}$ (see, for example, Theorem 1.2).

2.1 Adjoint, symmetric, and self-adjoint operators

Definition 2.1. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator on $\mathcal{H}$. The* ***adjoint operator*** *$A^* : \mathcal{D}_{A^*} \to \mathcal{H}$ of A is defined as follows:*

$$\begin{aligned}
\mathcal{D}_{A^*} &= \{h \in \mathcal{H} | \exists \tilde{h} \in \mathcal{H} : \ \langle h|Ag\rangle_{\mathcal{H}} = \langle \tilde{h}|g\rangle_{\mathcal{H}} \ \forall g \in \mathcal{D}_A\}, && (264)\\
A^*h &= \tilde{h}. && (265)
\end{aligned}$$

Lemma 2.1. *Let $\ker(A) = \{h \in \mathcal{D}_A | Ah = 0\}$ and $\mathrm{ran}(A) = \{Ah | h \in \mathcal{D}_A\}$ be the kernel and range of a densely defined operator $A : \mathcal{D}_A \to \mathcal{H}$, respectively. Then we have:*

$$\ker(A^*) = \mathrm{ran}(A)^{\perp}. \tag{266}$$

Proof. Let $h \in \ker(A^*)$, i.e., $A^*h = 0$. Then, recalling (264), this is true if and only if

$$\langle h|Ag\rangle_{\mathcal{H}} = 0, \tag{267}$$

for any $g \in \mathcal{D}_A$. This means that h is orthogonal to Ag for any vector g in the domain of A. In other words, h is orthogonal to any vector in the range of A, hence, $h \in \mathrm{ran}(A)^{\perp}$, and this proves the lemma. □

In Definition 1.10, we have defined an extension of a densely defined operator to the entire Banach space. Now, we extend this definition to extension between arbitrary domains.

Definition 2.2. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator defined on some domain $\mathcal{D}_A$. An operator $B : \mathcal{D}_B \to \mathcal{H}$ is called* ***extension*** *of A if $\mathcal{D}_A \subseteq \mathcal{D}_B$ and $Ah = Bh$ for any $h \in \mathcal{D}_A$. We denote it as $A \subseteq B$.*

Lemma 2.2. *Let A and B be densely defined operators in $\mathcal{H}$, and $A \subseteq B$. Then $B^* \subseteq A^*$.*

Proof. Let $h \in \mathcal{D}_{B^*}$. Then, recalling (264), the exists $\tilde{h} \in \mathcal{H}$ such that

$$\forall g \in \mathcal{D}_B : \ \langle h|Bg\rangle_{\mathcal{H}} = \langle \tilde{h}|g\rangle_{\mathcal{H}}. \tag{268}$$

Since B is an extension of A, we have $\mathcal{D}_A \subseteq \mathcal{D}_B$, hence,

$$\forall g \in \mathcal{D}_A : \ \langle h|Bg\rangle_{\mathcal{H}} = \langle h|Ag\rangle_{\mathcal{H}} = \langle \tilde{h}|g\rangle_{\mathcal{H}}. \tag{269}$$

Therefore, $\mathcal{D}_{B^*} \subseteq \mathcal{D}_{A^*}$, and $A^*h = B^*h = \tilde{h}$ for any $h \in \mathcal{D}_{B^*}$, hence, proving that A^* is an extension of B^*. □

Definition 2.3. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. It is called **symmetric** or **Hermitian**[4] if for any $h, g \in \mathcal{D}_A$:*

$$\langle h|Ag\rangle_{\mathcal{H}} = \langle Ah|g\rangle_{\mathcal{H}}. \tag{270}$$

Lemma 2.3. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. Then $A \subseteq A^*$.*

Proof. Let $h \in \mathcal{D}_A$, and $\tilde{h} = Ah$. Then, by Definition 2.3, for any $g \in \mathcal{D}_A$:

$$\langle h|Ag\rangle_{\mathcal{H}} = \langle \tilde{h}|g\rangle_{\mathcal{H}}, \tag{271}$$

so that $h \in \mathcal{D}_{A^*}$. Therefore, $\mathcal{D}_A \subseteq \mathcal{D}_{A^*}$. Since $A^*h = Ah = \tilde{h}$, we have $A \subseteq A^*$. □

Next definition provides a crucial class of operators, which is stronger than one of symmetric operators.

Definition 2.4. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. It is called **self-adjoint** if $A^* = A$.*

Lemma 2.4. *A self-adjoint operator is maximal with respect to symmetric and self-adjoint extensions.*

Proof. Let A be a self-adjoint operator, and B its symmetric extension, so that $A \subseteq B$. Due to Lemma 2.3, $B \subseteq B^*$. In turn, Lemma 2.2 suggests that $B^* \subseteq A^*$, i.e., $B \subseteq A^* = A$ due to Definition 2.4. Therefore, A is maximal with respect to symmetric extension and, since any self-adjoint operator is symmetric, self-adjoint extension as well. □

Theorem 2.1. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. If there exists $z \in \mathbb{C}$ such that* $\mathrm{ran}(A+\mathsf{z}) = \mathrm{ran}(A+\overline{\mathsf{z}}) = \mathcal{H}$, *where $\mathsf{z} := z\mathrm{id}$ and $\overline{\mathsf{z}} := \overline{z}\mathrm{id}$, with $\mathrm{id} : d \mapsto d$ for any $d \in \mathcal{D}_A$, then A is self-adjoint.*

Proof. Let $h \in \mathcal{D}_{A^*}$, so that $A^*h = \tilde{h} \in \mathcal{H}$, and $z \in \mathbb{C}$. Since $\mathrm{ran}(A+\overline{\mathsf{z}}) = \mathcal{H}$, we can find an element $g \in \mathcal{D}_A$ such that

$$(A+\overline{\mathsf{z}})g = \tilde{h} + \overline{z}h \tag{272}$$
$$= (A^* + \overline{\mathsf{z}})h. \tag{273}$$

Therefore, for any $d \in \mathcal{D}_A$, we can calculate

$$\langle h|(A+\mathsf{z})d\rangle_{\mathcal{H}} = \langle (A+\mathsf{z})^*h|d\rangle_{\mathcal{H}} \tag{274}$$
$$= \langle A^*h + \overline{z}h|d\rangle_{\mathcal{H}} \tag{275}$$
$$= \langle (A+\overline{\mathsf{z}})g|d\rangle_{\mathcal{H}} \tag{276}$$
$$= \langle Ag|d\rangle_{\mathcal{H}} + z\langle g|d\rangle_{\mathcal{H}} \tag{277}$$
$$= \langle g|Ad\rangle_{\mathcal{H}} + z\langle g|d\rangle_{\mathcal{H}} \tag{278}$$
$$= \langle g|(A+\mathsf{z})d\rangle_{\mathcal{H}}. \tag{279}$$

Hence, we conclude that $h = g$, so that $\mathcal{D}_{A^*} \subseteq \mathcal{D}_A$ and, in turn, $A^* \subseteq A$. However, A is assumed to be symmetric, so that $A \subseteq A^*$ due to Lemma 2.2. Hence, $A = A^*$, i.e., A is self-adjoint. □

[4]The term "symmetric" is usually used in mathematical literature, whereas "Hermitian" can be usually found in physical literature, first of all on quantum mechanics. In what follows, we stick to the term "symmetric".

2.2 Closable, closed, and essentially self-adjoint operators

While densely defined bounded operators can be always straightforwardly extended to the entire Hilbert space by virtue of Theorem 1.2, generally speaking, this is not true in the case of unbounded operators. Relaxing requirements on the extension of an operator $A : \mathcal{D}_A \to \mathcal{H}$, instead of demanding convergence of $(Ah_n)_{n\in\mathbb{N}}$ for any convergent sequence $(h_n)_{n\in\mathbb{N}}$ in $\mathcal{D}_A$, we can request only that A is well-defined if the corresponding limits exist, i.e., for $\lim_{n\to\infty} h_n = \lim_{n\to\infty} \tilde{h}_n$, we demand $\lim_{n\to\infty} Ah_n = \lim_{n\to\infty} A\tilde{h}_n$ if these limits exist. For this aim, we introduce new classes of operators.

Definition 2.5. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator. A subset $\Gamma(A) \subset \mathcal{H} \times \mathcal{H}$ is called a **graph** of A if*

$$\Gamma(A) = \{(h, Ah) | h \in \mathcal{D}_A\}, \tag{280}$$

*and it is equipped with the **graph norm***

$$\forall (h, Ah) \in \Gamma(A) : \ \|(h, Ah)\|_{\Gamma(A)} = \sqrt{\|h\|^2_{\mathcal{H}} + \|Ah\|^2_{\mathcal{H}}}. \tag{281}$$

Exercise 2.1. *Prove that $\|\cdot\|_{\Gamma(A)}$ is induced by the inner product*

$$\forall h, \tilde{h}, g, \tilde{g} \in \mathcal{H} : \ \langle (h, \tilde{h}) | (g, \tilde{g}) \rangle_{\mathcal{H}\times\mathcal{H}} := \langle h|g\rangle_{\mathcal{H}} + \langle \tilde{h}|\tilde{g}\rangle_{\mathcal{H}} \tag{282}$$

on $\mathcal{H} \times \mathcal{H}$.

Definition 2.6. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator. It is called **closed** if $\Gamma(A)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.*

Exercise 2.2. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator. It is closed if and only if $(\Gamma(A), \|\cdot\|_{\Gamma(A)})$ is complete.*

Definition 2.7. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator. It is called **closable** if there exists a unique operator $\overline{A} : \mathcal{D}_{\overline{A}} \to \mathcal{H}$ such that $\Gamma(\overline{A}) = \overline{\Gamma(A)}$. In this case, $\overline{A}$ is called **closure** if A.*

Exercise 2.3. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator. It is closable if and only if, for any sequence h_n in $\mathcal{D}_A$ such that $\lim_{n\to\infty} h_n = 0$ and $\lim_{n\to\infty} Ah_n = g$, it follows $g = 0$.*

Theorem 2.2. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. Then its adjoint A^* is a closed operator. Furthermore, A is closable if and only if A^* is densely defined and $\overline{A} = A^{**}$.*

Proof. We proceed in two steps.

Step 1. Let us define a unitary operator $U : \mathcal{H} \times \mathcal{H} \to \mathcal{H} \times \mathcal{H}$ such that $\forall h, g \in \mathcal{H}$:

$$U(h, g) = (g, -h). \tag{283}$$

From Definition 2.5, the graph of A^* is given by

$$\begin{aligned} \Gamma(A^*) &= \{(h, A^*h) | h \in \mathcal{D}_{A^*}\} && (284)\\ &= \{(h, \tilde{h}) | \langle h|Ag\rangle_{\mathcal{H}} = \langle \tilde{h}|g\rangle_{\mathcal{H}} \ \forall g \in \mathcal{D}_A\}, && (285) \end{aligned}$$

where (285) follows from (264). Now let us consider $(g, \tilde{g}) \in \Gamma(A)$ and $(h, \tilde{h}) \in \Gamma(A^*)$ and calculate

$$\begin{aligned} \langle (h, \tilde{h}) | U(g, \tilde{g}) \rangle_{\mathcal{H}\times\mathcal{H}} &= \langle (h, \tilde{h}) | (\tilde{g}, -g) \rangle_{\mathcal{H}\times\mathcal{H}} && (286)\\ &= \langle h|\tilde{g}\rangle_{\mathcal{H}} - \langle \tilde{h}|g\rangle_{\mathcal{H}} && (287)\\ &= \langle h|Ag\rangle_{\mathcal{H}} - \langle h|Ag\rangle_{\mathcal{H}} && (288)\\ &= 0, && (289) \end{aligned}$$

where (288) follows from (285) and the fact that $\tilde{g} = Ag$ for any $(g, \tilde{g}) \in \Gamma(A)$. Therefore,

$$\Gamma(A^*) = \{(h, \tilde{h}) | \langle (h, \tilde{h}) | U(g, \tilde{g}) \rangle_{\mathcal{H}\times\mathcal{H}} = 0 \ \forall (g, \tilde{g}) \in \Gamma(A)\}. \tag{290}$$

Therefore, we conclude that the graph

$$\Gamma(A^*) = (U\Gamma(A))^\perp, \tag{291}$$

which, due to Lemma 1.3, is a closed subspace of $\mathcal{H}\times\mathcal{H}$. Hence, by Definition 2.6, A^* is a closed operator.

Step 2. Due to Definition 2.7, we have to construct an operator $\overline{A}$, whose graph is a closure of the graph of A, so that $\Gamma(\overline{A}) = \overline{\Gamma(A)}$. First, we notice that $\overline{\Gamma(A)} = \Gamma(A)^{\perp\perp}$ due to Lemma 1.5. On the other hand,

$$\begin{aligned}
\Gamma(A)^\perp &= \{(h,\tilde{h})|\langle(h,\tilde{h})|(g,\tilde{g})\rangle_{\mathcal{H}\times\mathcal{H}} = 0\ \forall (g,\tilde{g})\in\Gamma(A)\} && (292)\\
&= \{(h,\tilde{h})|\langle(h,\tilde{h})|(g,Ag)\rangle_{\mathcal{H}\times\mathcal{H}} = 0\ \forall g\in\mathcal{D}_A\} && (293)\\
&= \{(h,\tilde{h})|\langle\tilde{h}|Ag\rangle_{\mathcal{H}} = -\langle h|g\rangle_{\mathcal{H}}\ \forall g\in\mathcal{D}_A\} && (294)\\
&= \{U(h,\tilde{h})|\langle h|g\rangle_{\mathcal{H}} = \langle\tilde{h}|Ag\rangle_{\mathcal{H}}\ \forall g\in\mathcal{D}_A\} && (295)\\
&= U\Gamma(A^*). && (296)
\end{aligned}$$

Therefore, $\overline{\Gamma(A)} = (U\Gamma(A^*))^\perp$. Now, we notice that for any linear subset $\mathcal{M}\subseteq\mathcal{H}$ and any $h\in\mathcal{M}^\perp$,

$$\begin{aligned}
\langle Uh|Ug\rangle_{\mathcal{H}} &= \langle h|g\rangle_{\mathcal{H}} && (297)\\
&= 0\ \forall g\in\mathcal{M}, && (298)
\end{aligned}$$

since U is a unitary operator, so that $U\mathcal{M}^\perp\subseteq(U\mathcal{M})^\perp$. On the other hand, let $\tilde{h}\in(U\mathcal{M})^\perp$ and $h\in\mathcal{H}$ such that $\tilde{h} = Uh$. Then:

$$\begin{aligned}
\langle h|g\rangle_{\mathcal{H}} &= \langle Uh|Ug\rangle_{\mathcal{H}} && (299)\\
&= \langle\tilde{h}|Ug\rangle_{\mathcal{H}} && (300)\\
&= 0\ \forall g\in\mathcal{M}, && (301)
\end{aligned}$$

so that $h\in\mathcal{M}^\perp$ and $(U\mathcal{M})^\perp\subseteq U\mathcal{M}^\perp$. Therefore, $(U\mathcal{M})^\perp = U\mathcal{M}^\perp$, and we have $(U\Gamma(A^*))^\perp = U\Gamma(A^*)^\perp$, so that:

$$\begin{aligned}
U\Gamma(A^*)^\perp &= \{U(h,\tilde{h})|\langle(h,\tilde{h})|(g,\tilde{g})\rangle_{\mathcal{H}\times\mathcal{H}} = 0\ \forall (g,\tilde{g})\in\Gamma(A^*)\}, && (302)\\
&= \{U(h,\tilde{h})|\langle(h,\tilde{h})|(g,A^*g)\rangle_{\mathcal{H}\times\mathcal{H}} = 0\ \forall g\in\mathcal{D}_{A^*}\} && (303)\\
&= \{U(h,\tilde{h})|\langle\tilde{h}|A^*g\rangle_{\mathcal{H}} = -\langle h|g\rangle_{\mathcal{H}}\ \forall g\in\mathcal{D}_{A^*}\} && (304)\\
&= \{(h,\tilde{h})|\langle h|A^*g\rangle_{\mathcal{H}} = \langle\tilde{h}|g\rangle_{\mathcal{H}}\ \forall g\in\mathcal{D}_{A^*}\} && (305)\\
&= \Gamma(A^{**}). && (306)
\end{aligned}$$

Therefore, we conclude that $\overline{A} = A^{**}$. In turn, (305) suggests that $(0,\tilde{h})\in\Gamma(A^{**})$ if and only if $\langle\tilde{h}|g\rangle_{\mathcal{H}} = 0$ for any $g\in\mathcal{D}_{A^*}$, i.e., $\tilde{h}\in\mathcal{D}_{A^*}^\perp$. On the other hand, from Exercise 2.3 it follows that A is closable if and only if $\tilde{h} = 0$, i.e., $\mathcal{D}_{A^*}^\perp = \{0\}$. In turn, by Step 1 of the proof of Lemma 1.5, $\overline{\mathcal{D}_{A^*}}^\perp = \{0\}$, so that $\overline{\mathcal{D}_{A^*}} = \mathcal{H}$ due to Theorem 1.6, i.e., A^* is densely defined. On the other hand, if $\mathcal{D}_{A^*}$ is dense, for any $h\in\mathcal{D}_{A^*}^\perp$ we can find a sequence $(d_n)_{n\in\mathbb{N}}$ in $\mathcal{D}_{A^*}$ such that $\lim_{n\to\infty} d_n = h$. In turn,

$$\langle d_n|h\rangle_{\mathcal{H}} = 0\ \forall n\in\mathbb{N}. \tag{307}$$

Therefore, using the continuity of inner product, we find that

$$\begin{aligned}
\|h\|_{\mathcal{H}} &= \sqrt{\langle h|h\rangle_{\mathcal{H}}} && (308)\\
&= 0, && (309)
\end{aligned}$$

and $h = 0$ by the definition of norm. Therefore, we conclude that $\overline{\mathcal{D}_{A^*}}^\perp = \{0\}$ if and only if $\mathcal{D}_{A^*}$ is dense, and, in turn, A is closable if and only if A^* is densely defined. □

Corollary 2.1. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a closable operator. Then $A \subseteq A^{**}$.*

Proof. The proof follows straightforwardly from Theorem 2.2 that claims $A^{**} = \overline{A}$. □

Theorem 2.3. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. Then it is closable.*

Proof. Since A is symmetric, by Lemma 2.3, $\mathcal{D}_A \subseteq \mathcal{D}_{A^*}$. In turn, $\overline{\mathcal{D}_A} \subseteq \overline{\mathcal{D}_{A^*}}$. Since symmetric operators are densely defined, we have $\overline{\mathcal{D}_A} = \mathcal{H}$, so that $\mathcal{H} \subseteq \overline{\mathcal{D}_{A^*}}$, which is true only if $\overline{\mathcal{D}_{A^*}} = \mathcal{H}$, i.e., A^* is densely defined. Therefore, by Theorem 2.2, A is closable. □

Lemma 2.5. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. Then $A \subseteq A^{**} \subseteq A^*$.*

Proof. Since A is symmetric, by Lemma 2.3, $A \subseteq A^*$ and, by Lemma 2.2, $A^{**} \subseteq A^*$. On the other hand, by Theorem 2.3, it is closable, so that $A \subseteq A^{**}$. Therefore, $A \subseteq A^{**} \subseteq A^*$. □

Definition 2.8. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. It is called **essentially self-adjoint** if its closure $\overline{A}$ is a self-adjoint operator, and $\mathcal{D}_A$ is called **core** of $\overline{A}$.*

Corollary 2.2. *If A is an essentially self-adjoint operator, $\overline{A}$ is its unique self-adjoint extension.*

Lemma 2.6. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. If A is injective and $\overline{\operatorname{ran}(A)} = \mathcal{H}$, then $(A^*)^{-1} = (A^{-1})^*$. If A is closable and $\overline{A}$ is injective, then $\overline{A}^{-1} = \overline{A^{-1}}$.*

Proof. We proceed in two steps in order to prove both statements of the Lemma.

Step 1. Let us define two unitary operators $U : \mathcal{H} \times \mathcal{H} \to \mathcal{H} \times \mathcal{H}$ and $V : \mathcal{H} \times \mathcal{H} \to \mathcal{H} \times \mathcal{H}$ such that $\forall h, g \in \mathcal{H}$:

$$U(h,g) = (g,-h) \tag{310}$$
$$V(h,g) = (g,h). \tag{311}$$

Then, if A is injective,

$$\Gamma(A^{-1}) = V\Gamma(A). \tag{312}$$

Therefore, if $\operatorname{ran}(A)$ is dense in $\mathcal{H}$, we have $\operatorname{ran}(A)^\perp = \{0\}$. In turn, due to Lemma 2.1, this means that $\ker(A^*) = \{0\}$. Therefore, A^* is injective, and we obtain

$$\begin{aligned}
\Gamma((A^*)^{-1}) &= V\Gamma(A^*) &(313)\\
&= V(U\Gamma(A))^\perp &(314)\\
&= VU\Gamma(A)^\perp &(315)\\
&= UV\Gamma(A)^\perp &(316)\\
&= U(V\Gamma(A))^\perp &(317)\\
&= U(\Gamma(A^{-1}))^\perp &(318)\\
&= \Gamma((A^{-1})^*), &(319)
\end{aligned}$$

where (313) and (318) use (312), (314) and (319) follow from (291), (315) and (317) take into account the fact that $U\mathcal{M}^\perp = (U\mathcal{M})^\perp$ for any $\mathcal{M} \subseteq \mathcal{H}$, which is proven in Step 2 of the proof of Theorem 2.2, and (317) follows from the fact that for any $h, g \in \mathcal{H}$:

$$\begin{aligned}
VU(h,g) &= V(g,-h) &(320)\\
&= (-h,g), &(321)
\end{aligned}$$

and

$$\begin{aligned}
UV(h,g) &= U(g,h) &(322)\\
&= (h,-g), &(323)
\end{aligned}$$

so that

$$\begin{aligned} VU\Gamma(A)^\perp &= \{(h,\tilde{h})|\langle(g,\tilde{g})|(-h,\tilde{h})\rangle_{\mathcal{H}\times\mathcal{H}} = 0\ \forall(g,\tilde{g})\in\Gamma(A)\} && (324)\\ &= \{(h,\tilde{h})|\langle g|h\rangle_{\mathcal{H}} = \langle\tilde{g}|\tilde{h}\rangle_{\mathcal{H}}\ \forall(g,\tilde{g})\in\Gamma(A)\} && (325)\\ &= UV\Gamma(A)^\perp. && (326)\end{aligned}$$

Therefore, we conclude that $(A^*)^{-1} = (A^{-1})^*$.

Step 2. If A is closable, and its closure $\overline{A}$ is injective, then

$$\begin{aligned} \Gamma(\overline{A}^{-1}) &= V\Gamma(\overline{A}) && (327)\\ &= \overline{V\Gamma(A)} && (328)\\ &= \Gamma(\overline{A^{-1}}), && (329)\end{aligned}$$

and we conclude that $\overline{A}^{-1} = \overline{A^{-1}}$. □

Lemma 2.7. *Let $A:\mathcal{D}_A\to\mathcal{H}$ be a self-adjoint injective operator. Then A^{-1} is also self-adjoint.*

Proof. Since A is self-adjoint, i.e., $A = A^*$, Lemma 2.1 suggests that $\mathrm{ran}(A)^\perp = \ker(A)$. Since A is also injective, $\ker(A) = \{0\}$, hence, $\mathrm{ran}(A)^\perp = \{0\}$, and $\mathrm{ran}(A)$ is dense in $\mathcal{H}$. Therefore, applying Lemma 2.6, we conclude that $A^{-1} = (A^{-1})^*$, i.e., A^{-1} is self-adjoint. □

Theorem 2.4. *Let $A:\mathcal{D}_A\to\mathcal{H}$ be a symmetric operator. It is essentially self-adjoint if and only if, for some $z\in\mathbb{C}\setminus\mathbb{R}$,*

$$\overline{\mathrm{ran}(A+\mathsf{z})} = \overline{\mathrm{ran}(A+\overline{\mathsf{z}})} = \mathcal{H}, \tag{330}$$

or equivalently,

$$\ker(A^*+\mathsf{z}) = \ker(A^*+\overline{\mathsf{z}}) = \{0\}. \tag{331}$$

where $\mathsf{z} := z\mathrm{id}$ and $\overline{\mathsf{z}} := \overline{z}\mathrm{id}$, with $\mathrm{id}: d\mapsto d$ for any $d\in\mathcal{D}_A$.

Proof. First of all, (330) and (331) are equivalent by virtue of Lemma 2.1, hence, it is enough to prove one of them. In what follows, we proceed in two steps for both directions.

Step 1 (⇐). Since A is symmetric, due to Theorem 2.3, it is also closable, and there exists $\overline{A}$. Therefore, it is necessary to prove that $\overline{A}$ is self-adjoint, hence, without loss of generality, we can assume that A is closed. Let $z = x+iy\in\mathbb{C}\setminus\mathbb{R}$, so that $y\neq 0$. Then, for any $h\in\mathcal{H}$, we calculate

$$\begin{aligned} \|(A+\mathsf{z})h\|^2_{\mathcal{H}} &= \|(A+\mathsf{x})h+iyh\|^2_{\mathcal{H}} && (332)\\ &= \langle(A+\mathsf{x})h+iyh|(A+\mathsf{x})h+iyh\rangle_{\mathcal{H}} && (333)\\ &= \langle(A+\mathsf{x})h|(A+\mathsf{x})h\rangle_{\mathcal{H}} + iy\langle(A+\mathsf{x})h|h\rangle_{\mathcal{H}} - iy\langle h|(A+\mathsf{x})h\rangle_{\mathcal{H}} + y^2\langle h|h\rangle_{\mathcal{H}} && (334)\\ &= \|(A+\mathsf{x})h\|^2_{\mathcal{H}} + y^2\|h\|^2_{\mathcal{H}} && (335)\\ &\geq y^2\|h\|^2_{\mathcal{H}}. && (336)\end{aligned}$$

Since $y\neq 0$, we have that $\ker(A+\mathsf{z})$ is trivial. Therefore, $(A+\mathsf{z})$ is an injective operator, and there exists an inverse operator $(A+\mathsf{z})^{-1}$ defined on $\mathrm{ran}(A+\mathsf{z})$. In turn, let $\tilde{h} = (A+\mathsf{z})h$, so that $(A+\mathsf{z})^{-1}\tilde{h} = h$. Then, rewriting (336), we obtain

$$\|\tilde{h}\|^2_{\mathcal{H}} \geq y^2\|(A+\mathsf{z})^{-1}\tilde{h}\|^2_{\mathcal{H}}, \tag{337}$$

and, in turn, for any $\tilde{h}\in\mathrm{ran}(A+\mathsf{z})$,

$$\|(A+\mathsf{z})^{-1}\tilde{h}\|_{\mathcal{H}} \leq |y|^{-1}\|\tilde{h}\|_{\mathcal{H}}, \tag{338}$$

Therefore, we obtain $\|(A+\mathsf{z})^{-1}\|\leq|y|^{-1}$, so that $(A+\mathsf{z})^{-1}$ is bounded and, due to Lemma 2.6, closed. Hence, its domain $\mathrm{ran}(A+\mathsf{z})$ is a closed subset of $\mathcal{H}$ (*exercise*). This means that $\mathrm{ran}(A+\mathsf{z}) =$

$\overline{\operatorname{ran}(A+\mathsf{z})} = \mathcal{H}$. Replacing z by its complex conjugate $\overline{z}$ we conclude that $\operatorname{ran}(A+\overline{\mathsf{z}}) = \mathcal{H}$ as well. Therefore, applying Theorem 2.1, we conclude that A is self-adjoint.

Step 2 ($\Rightarrow$). Let $A = A^*$ and $z = x + iy \in \mathbb{C}\setminus\mathbb{R}$, so that $y \neq 0$. Then, for any $h \in \mathcal{H}$, following (332)–(336), we obtain

$$\|(A^*+\mathsf{z})h\|_{\mathcal{H}}^2 \geq y^2\|h\|_{\mathcal{H}}^2, \tag{339}$$

$$\|(A^*+\overline{\mathsf{z}})h\|_{\mathcal{H}}^2 \geq y^2\|h\|_{\mathcal{H}}^2. \tag{340}$$

Since $y \neq 0$, we have that $\ker(A^*+\mathsf{z}) = \ker(A^*+\overline{\mathsf{z}}) = \{0\}$. □

Corollary 2.3. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator, and $d_\pm := \dim(K^\pm)$ are its* ***defect indices****, where*

$$K^+ := \operatorname{ran}(A+\mathsf{z})^\perp \tag{341}$$

$$= \ker(A^*+\overline{\mathsf{z}}), \tag{342}$$

$$K^- := \operatorname{ran}(A+\overline{\mathsf{z}})^\perp \tag{343}$$

$$= \ker(A^*+\mathsf{z}), \tag{344}$$

where $\mathsf{z} := z\mathrm{id}$ and $\overline{\mathsf{z}} := \overline{z}\mathrm{id}$, with $\mathrm{id} : d \mapsto d$ for any $d \in \mathcal{D}_A$, for some $z \in \mathbb{C}\setminus\mathbb{R}$, which can be taken as $z = i$ without loss of generality. Then A has one self-adjoint extension, namely $\overline{A}$, if $d_+ = d_- = 0$.

Now, we proceed by proving an important result suggesting that a closed unbounded operator cannot be defined on the entire Hilbert space. We start by recalling the following useful theorem.

Theorem 2.5 (Baire's category theorem)**.** *Let V be a Banach space*[5]*. Then V cannot be a countable union of nowhere dense sets, i.e., sets whose closures have empty interiors.*

Proof. Let $\{V_n\}_{n\in\mathbb{N}}$ a cover of V, i.e., $V = \bigcup_{n\in\mathbb{N}} V_n$, such that each V_n is a closed set and does not contain any open ball $B(v,r) := \{v' \in V | \|v'-v\|_V < r\}$. Let us show that this leads to a contradiction by constructing a Cauchy sequence, which does not belong to any V_n, and is convergent due to completeness of Banach space. By construction, the complements $V\setminus V_n$ are open and non-empty sets. Without loss of generality, let us assume $n = 1$: there exists $v_1 \notin V_1$ such that $\overline{B(v_1,r_1)} \subset V\setminus V_1$ for some r_1. On the other hand, by assumption, V_2 cannot contain $B(v_1,r_1)$. Therefore, there exists $v_2 \in B(v_1,r_1)$ such that $v_2 \notin V_2$. Since $B(v_1,r_1)\cap(V\setminus V_2)$ is an open and non-empty set, there exists $\overline{B(v_2,r_2)} \subset B(v_1,r_1)\cap(V\setminus V_2)$ with $r_2 < r_1$. Therefore, by induction, we can construct a sequence $\{B(v_n,r_n)\}_{n\in\mathbb{N}}$ such that

$$\overline{B(v_{n+1},r_{n+1})} \subset B(v_n,r_n)\cap(V\setminus V_{n+1}). \tag{345}$$

In every step, r_n can be chosen arbitrarily small. Therefore, without loss of generality, we can assume $r_n \to 0$. By construction, for any $N \in \mathbb{N}$ and $n \geq N$, we have $v_n \in \overline{B(v_N,r_N)}$. Therefore, $\{v_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence and, hence, there exists $v \in V$ such that $\lim_{n\to\infty} v_n = v$. In turn, for any $n \in \mathbb{N}$, $v \in \overline{B(v_n,r_n)} \subset V\setminus V_n$. Therefore, for any $n \in \mathbb{N}$, $v \notin V_n$, contradicting the assumption that $\{V_n\}_{n\in\mathbb{N}}$ is a cover of V. □

Theorem 2.6 (Banach, Steinhaus / Uniform boundedness principle)**.** *Let $(V, \|\cdot\|_V)$ be a Banach space, $(W, \|\cdot\|_W)$ be a normed space, and $\{A_\alpha\}_{\alpha\in I}$ be a family of operators such that $A_\alpha \in \mathcal{L}(V,W)$ for any $\alpha \in I$. If, for a given $v \in V$, $\|A_\alpha v\|_W \leq C(v) < \infty$ for any $\alpha \in I$, then $\{A_\alpha\}_{\alpha\in I}$ is uniformly bounded, i.e., $\exists C > 0$ such that $\|A_\alpha\| \leq C < \infty$ for any $\alpha \in I$.*

[5] Although Baire's category theorem is formulated for any complete metric space, for the purpose of course, we focus on Banach spaces as a particular case.

Proof. Let us define a family of sets $\{V_n\}_{n\in\mathbb{N}}$ such that

$$V_n = \bigcap_{\alpha\in I} V_n^{(\alpha)}, \tag{346}$$

$$V_n^{(\alpha)} := \{v \in V | \|A_\alpha v\|_W \leq n\}, \tag{347}$$

so that $\{V_n\}_{n\in\mathbb{N}}$ defines a cover of V by assumption, $V = \bigcup_{n\in\mathbb{N}} V_n$. Since every A_α is bounded,

$$\|A_\alpha v\|_W \leq \|A_\alpha\|\|v\|_V, \tag{348}$$

so that it is Lipschitz continuous and, hence, continuous. Therefore, taking into account continuity of the norm, $V_n^{(\alpha)}$ is closed for any $\alpha \in I$, and, moreover, V_n is closed as an intersection of closed sets. By Theorem 2.5, $\exists n \in \mathbb{N}$ such that $B_\varepsilon(v_0) := \{v \in V | \|v - v_0\|_V < \varepsilon\} \subset V_n$ for some $\varepsilon > 0$ and $v_0 \in V$. In turn, let $y \in V$ such that $\|y\| < \varepsilon$. Then we have:

$$\|A_\alpha y\|_V = \|A_\alpha(y + v_0 - v_0)\|_W \tag{349}$$

$$\leq \|A_\alpha(y + v_0)\|_W + \|A_\alpha v_0\|_W \tag{350}$$

$$\leq n + C(v_0). \tag{351}$$

In turn, assuming $y = \varepsilon\frac{x}{\|x\|_V}$ for any $V \ni x \neq 0$, we obtain:

$$\|A_\alpha x\|_W \leq \frac{n + C(v_0)}{\varepsilon}\|x\|_V. \tag{352}$$

Therefore, we conclude that $\|A_\alpha\| \leq \frac{n+C(v_0)}{\varepsilon}$ for any $\alpha \in I$. □

Theorem 2.7 (Closed graph theorem)**.** *Let $A : \mathcal{H}_1 \to \mathcal{H}_2$ be an operator defined on the entire Hilbert space $\mathcal{H}_1$. Then A is bounded if and only if it is closed.*

Proof. In what follows, we proceed in two steps for both directions.

Step 1 (⇒). Suppose that A is bounded. Then it is closed if and only if its domain is closed. Since A is defined on the entire Hilbert space $\mathcal{H}_1$, which is closed, we conclude that A is closed.

Step 2 (⇐). Let us assume that A is closed, hence, A^* is well-defined[6]. In turn, let $\tilde{h} \in \mathcal{D}_{A^*} \subseteq \mathcal{H}_2$ such that $\|\tilde{h}\|_{\mathcal{H}_1} = 1$ and define $\mathtt{f}_{\tilde{h}} \in \mathcal{H}_1^*$ such that $\mathtt{f}_{\tilde{h}} h = \langle A^*\tilde{h}|h\rangle_{\mathcal{H}_1}$, for any $h \in \mathcal{H}_1$. Then

$$|\mathtt{f}_{\tilde{h}} h| = |\langle A^*\tilde{h}|h\rangle_{\mathcal{H}_1}| \tag{353}$$

$$= |\langle\tilde{h}|Ah\rangle_{\mathcal{H}_2}| \tag{354}$$

$$\leq \|\tilde{h}\|_{\mathcal{H}_2}\|Ah\|_{\mathcal{H}_2} \tag{355}$$

$$= \|Ah\|_{\mathcal{H}_2}. \tag{356}$$

Hence, applying Theorem 2.6, we have that there exists $C > 0$ such that $\|\mathtt{f}_{\tilde{h}}\| < C$. Therefore, $\|A^*\tilde{h}\|_{\mathcal{H}_1} < C$, i.e., A^* is bounded, and, in turn, $A = A^{**}$ is bounded. □

Definition 2.9. *We call* ***Cayley transform*** *the mapping*

$$A \mapsto V_z := (A + \bar{\mathtt{z}})(A + \mathtt{z})^{-1} : \operatorname{ran}(A + \mathtt{z}) \to \operatorname{ran}(A + \bar{\mathtt{z}}), \tag{357}$$

where $\mathtt{z} := z\mathrm{id}$ *and* $\bar{\mathtt{z}} := \bar{z}\mathrm{id}$, *with* $\mathrm{id} : d \mapsto d$ *for any* $d \in \mathcal{D}_A$, *for some* $z \in \mathbb{C} \setminus \mathbb{R}$,.

In what follows, for the sake of simplicity, we focus on the Cayley transform $V_{z=i} := V$.

[6]Definition 2.1 can be straightforwardly generalized to an operator mapping $\mathcal{D}_A \subseteq \mathcal{H}_1$ to $\mathcal{H}_2$ as an operator $A^* : \mathcal{D}_{A^*} \to \mathcal{H}_1$, where $\mathcal{D}_{A^*} = \{h \in \mathcal{H}_2 | \exists\tilde{h} \in \mathcal{H}_1 : \langle h|Ag\rangle_{\mathcal{H}_2} = \langle\tilde{h}|g\rangle_{\mathcal{H}_1} \forall g \in \mathcal{D}_A\}$, so that $A^*h = \tilde{h}$ for any $h \in \mathcal{D}_{A^*}$.

Lemma 2.8. *Cayley transform* (357) *is a bijection between the set of symmetric operators A and the set of operators V that preserve the norm, $\|Vh\|_{\mathcal{H}} = \|h\|_{\mathcal{H}}$ for any $h \in \mathcal{D}_V$, such that* $\operatorname{ran}(\mathrm{id} - V)$ *is dense.*

Proof. Since A is symmetric, for any $h \in \mathcal{D}_A$, we have

$$\begin{aligned}
\|(A + i\ \mathrm{id})h\|^2_{\mathcal{H}} &= \langle (A + i\ \mathrm{id})h | (A + i\ \mathrm{id})h\rangle_{\mathcal{H}} && (358)\\
&= \langle Ah|Ah\rangle_{\mathcal{H}} + i\langle Ah|h\rangle_{\mathcal{H}} - i\langle h|Ah\rangle_{\mathcal{H}} + \langle h|h\rangle_{\mathcal{H}} && (359)\\
&= \langle Ah|Ah\rangle_{\mathcal{H}} + \langle h|h\rangle_{\mathcal{H}} && (360)\\
&= \|Ah\|^2_{\mathcal{H}} + \|h\|^2_{\mathcal{H}}, && (361)
\end{aligned}$$

and

$$\begin{aligned}
\|(A - i\ \mathrm{id})h\|^2_{\mathcal{H}} &= \langle (A - i\ \mathrm{id})h | (A - i\ \mathrm{id})h\rangle_{\mathcal{H}} && (362)\\
&= \langle Ah|Ah\rangle_{\mathcal{H}} - i\langle Ah|h\rangle_{\mathcal{H}} + i\langle h|Ah\rangle_{\mathcal{H}} + \langle h|h\rangle_{\mathcal{H}} && (363)\\
&= \langle Ah|Ah\rangle_{\mathcal{H}} + \langle h|h\rangle_{\mathcal{H}} && (364)\\
&= \|Ah\|^2_{\mathcal{H}} + \|h\|^2_{\mathcal{H}}. && (365)
\end{aligned}$$

Therefore, for any $\tilde{h} \in \mathcal{D}_V = \operatorname{ran}(A + i\ \mathrm{id})$, we obtain

$$\begin{aligned}
\|V\tilde{h}\|_{\mathcal{H}} &= \|(A + i\ \mathrm{id})h\|_{\mathcal{H}} && (366)\\
&= \sqrt{\|Ah\|^2_{\mathcal{H}} + \|h\|^2_{\mathcal{H}}} && (367)\\
&= \|(A - i\ \mathrm{id})h\|_{\mathcal{H}} && (368)\\
&= \|\tilde{h}\|_{\mathcal{H}}, && (369)
\end{aligned}$$

so that V indeed preserves the norm.

$$\begin{aligned}
\mathrm{id} + V &= (A + i\ \mathrm{id})(A + i\ \mathrm{id})^{-1} + (A - i\ \mathrm{id})(A + i\ \mathrm{id})^{-1} && (370)\\
&= 2A(A + i\ \mathrm{id})^{-1}, && (371)
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{id} - V &= (A + i\ \mathrm{id})(A + i\ \mathrm{id})^{-1} - (A - i\ \mathrm{id})(A + i\ \mathrm{id})^{-1} && (372)\\
&= 2i(A + i\ \mathrm{id})^{-1}. && (373)
\end{aligned}$$

Since A is a densely defined operator by Definition 2.3, we conclude that $\operatorname{ran}(\mathrm{id} - V)$ is dense, and A defines V via

$$A = i(\mathrm{id} + V)(\mathrm{id} - V)^{-1}. \tag{374}$$

Step 2. Let A be given by (374), where V is an operator that preserves norm on $\mathcal{D}_V$. Hence, for any $\tilde{h} \in \mathcal{D}_V$,

$$\begin{aligned}
\langle (\mathrm{id} \pm V)\tilde{h} | (\mathrm{id} \mp V)\tilde{h}\rangle_{\mathcal{H}} &= \langle \tilde{h}|\tilde{h}\rangle_{\mathcal{H}} \pm \langle V\tilde{h}|\tilde{h}\rangle_{\mathcal{H}} \mp \langle \tilde{h}|V\tilde{h}\rangle_{\mathcal{H}} - \langle V\tilde{h}|V\tilde{h}\rangle_{\mathcal{H}} && (375)\\
&= \pm\langle V\tilde{h}|\tilde{h}\rangle_{\mathcal{H}} \mp \langle \tilde{h}|V\tilde{h}\rangle_{\mathcal{H}} && (376)\\
&= \pm 2i\operatorname{Im}(\langle V\tilde{h}|\tilde{h}\rangle_{\mathcal{H}}). && (377)
\end{aligned}$$

Now let us assume that $h = (1 - V)\tilde{h} \in \mathcal{D}_A = \text{ran}(1 - V)$. Then we obtain:

$$\begin{aligned}
\langle Ah|h\rangle_{\mathcal{H}} &= \langle i(\text{id} + V)(\text{id} - V)^{-1}h|h\rangle_{\mathcal{H}} &(378)\\
&= \langle i(\text{id} + V)\tilde{h}|(\text{id} - V)\tilde{h}\rangle_{\mathcal{H}} &(379)\\
&= -i\langle(\text{id} + V)\tilde{h}|(\text{id} - V)\tilde{h}\rangle_{\mathcal{H}} &(380)\\
&= 2\text{Im}(\langle V\tilde{h}|\tilde{h}\rangle_{\mathcal{H}}) &(381)\\
&= i\langle(\text{id} - V)\tilde{h}|(\text{id} + V)\tilde{h}\rangle_{\mathcal{H}} &(382)\\
&= \langle(\text{id} - V)\tilde{h}|i(\text{id} + V)\tilde{h}\rangle_{\mathcal{H}} &(383)\\
&= \langle h|i(\text{id} + V)(\text{id} - V)^{-1}h\rangle_{\mathcal{H}} &(384)\\
&= \langle h|Ah\rangle_{\mathcal{H}}, &(385)
\end{aligned}$$

hence, proving that A is symmetric. □

Corollary 2.4. *A symmetric operator $A : \mathcal{D}_A \to \mathcal{H}$ is self-adjoint if and only if the corresponding Cayley transform V is unitary, i.e., norm-preserving and $\mathcal{D}_V = \mathcal{H}$.*

Corollary 2.4 suggests that finding a self-adjoint extension of a symmetric operator A is equivalent to finding a unitary extension of the corresponding Cayley transform V. Due to Theorem 1.6, this means closing it and finding a unitary operator from $\mathcal{D}_V^{\perp}$ to $\text{ran}(V)^{\perp}$. Recalling Corollary 2.3, this is true if and only if $d_+ = d_-$. This leads to the following recipe of construction of a self-adjoint extension.

Corollary 2.5. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a closed symmetric operator with $d_+ = d_-$. Then a self-adjoint extension of A can be constructed as an operator $A' : \mathcal{D}_{A'} \to \mathcal{H}$ defined on*

$$\mathcal{D}_{A'} = \mathcal{D}_A + (\text{id} - V')K_+, \tag{386}$$

where V' is the Cayley transform of A', and K_+ is defined by (341)–(342), and acts on it as

$$A'h' = Ah + ig + iV'g, \tag{387}$$

where $h \in \mathcal{D}_A$ and $g \in \ker(A^* - i)$, with $\tilde{h} = h + g$.

Proof. First, we construct the domain of A':

$$\begin{aligned}
\mathcal{D}_{A'} &= \text{ran}(\text{id} - V') &(388)\\
&= \text{ran}(\text{id} - V) + (\text{id} - V')K_+ &(389)\\
&= \mathcal{D}_A + (\text{id} - V')K_+ &(390)\\
&= \{h' \in \mathcal{H}|h' = h + (\text{id} - V')g,\ h \in \mathcal{D}_A,\ g \in \ker(A^* - i\,\text{id})\}, &(391)
\end{aligned}$$

where (389) uses Theorem 1.6 with respect to linear subspace $\text{ran}(A + i\,\text{id})^{\perp} = \ker(A^* - i\,\text{id})$, which is closed by Lemma 1.3, and its orthogonal complement $\overline{\text{ran}(A + i\,\text{id})}$, and the fact that $V \subseteq V'$ following from $A \subseteq A'$. In turn, for any $h' \in \mathcal{D}_{A'}$, we have

$$\begin{aligned}
A'h' &= A'h + A'(\text{id} - V')g &(392)\\
&= Ah + i(\text{id} + V')(\text{id} - V')^{-1}(\text{id} - V')g &(393)\\
&= Ah + i(\text{id} + V')g &(394)\\
&= Ah + ig + V'g, &(395)
\end{aligned}$$

where $h \in \mathcal{D}_A$ and $g \in \ker(A^* - i\,\text{id})$. □

2.3 Resolvents, spectra, and spectral theorem

We start by setting the playground for spectral theorem and providing necessary basic definitions.

Definition 2.10. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. We call* ***resolvent set*** *of A:*

$$\rho(A) = \{z \in \mathbb{C} | (A - \mathbf{z}) \text{ is bijective, } (A - \mathbf{z})^{-1} \text{ is bounded}\}. \tag{396}$$

Definition 2.11. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. We call* ***spectrum*** *of A the set $\sigma(A) := \mathbb{C} \setminus \rho(A)$.*

Definition 2.12. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. An element $z \in \sigma(A)$ is called* ***eigenvalue*** *of A if $\ker(A - \mathbf{z}) \neq \{0\}$, so that there exists an element $h \in \ker(A - \mathbf{z})$ called* ***eigenvector*** *such that*

$$Ah = zh. \tag{397}$$

Definition 2.13. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a densely defined operator. The map $R_A : \rho(A) \to \mathcal{L}(\mathcal{H})$ is called* ***resolvent*** *of A if*

$$R_A(z) = (A - \mathbf{z})^{-1}. \tag{398}$$

Lemma 2.9 (First resolvent formula)**.** *Let $A : \mathcal{D}_A \to \mathcal{H}$ be an operator. Then, for any $z, z' \in \rho(A)$, its resolvent $R_A(z)$ satisfies:*

$$R_A(z) - R_A(z') = (z - z')R_A(z)R_A(z') = (z - z')R_A(z')R_A(z). \tag{399}$$

Proof. Let us consider:

$$\begin{aligned}
R_A(z) - (z - z')R_A(z)R_A(z') &= (A - z)^{-1} - (z - z')(A - z)^{-1}(A - z')^{-1} && (400)\\
&= (A - z)^{-1}\Big(\mathrm{id} - (z - z')(A - z')^{-1}\Big) && (401)\\
&= (A - z)^{-1}\Big(\mathrm{id} + (A - z)(A - z')^{-1} - (A - z')(A - z')^{-1}\Big) && (402)\\
&= (A - z')^{-1} && (403)\\
&= R_A(z'), && (404)
\end{aligned}$$

so that $R_A(z) - R_A(z') = (z - z')R_A(z)R_A(z')$. The second equality follows by permutation of z and z'. □

Theorem 2.8. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. Then it is self-adjoint if and only if $\sigma(A) \subseteq \mathbb{R}$.*

Proof. We proceed in two steps for each direction.

Step 1. ($\Leftarrow$) Let $\sigma(A) \subseteq \mathbb{R}$. Then $\mathbb{C} \setminus \mathbb{R} \subseteq \rho(A)$. Hence, from Definition 2.10, $\operatorname{ran}(A - z) = \mathcal{H}$ for any $z \in \mathbb{C} \setminus \mathbb{R}$. Therefore, applying Theorem 2.1, we conclude that A is self-adjoint.

Step 2. ($\Rightarrow$) Let A be self-adjoint and $z \in \mathbb{C} \setminus \mathbb{R}$, so that $z = x + iy$ with $y \neq 0$. Following (332)–(336), we have that $\ker(A - \mathbf{z})$ is trivial, so that $(A - \mathbf{z})$ is injective, and there exists $(A - \mathbf{z})^{-1} : \operatorname{ran}(A - z) \to \mathcal{D}_A$. Therefore, due to Definition 2.13, for any $z \in \mathbb{C} \setminus \mathbb{R}$, the resolvent $R_A(z)$ exists, meaning that $\mathbb{C} \setminus \mathbb{R} \subseteq \rho(A)$. Hence, recalling Definition 2.11, we conclude that $\sigma(A) \subseteq \mathbb{R}$. □

Now we proceed with derivation of spectral theorem, which we construct step by step. We start by introducing a new notion of measure that assigns to every element of the σ-algebra a bounded operator on $\mathcal{H}$ as its "volume" instead of an element of $\mathbb{R}$ or $\mathbb{C}$.

Definition 2.14. *Let $\mathcal{H}$ be a Hilbert space, and $\mathfrak{B}$ be a Borel σ-algebra on $\mathbb{R}$. A map $P : \mathfrak{B} \to \mathcal{L}(\mathcal{H})$ is called* ***projection-valued measure (PVM)*** *if is satisfies:*

1. *For any $\Omega \in \mathfrak{B}$, $P(\Omega)^* = P(\Omega)$.*

2. *For any* $\Omega \in \mathfrak{B}$, $P(\Omega) \circ P(\Omega) = P(\Omega)$.

3. $P(\mathbb{R}) = \mathrm{id}$.

4. *If* Ω *is a pairwisely disjoint union, i.e.,* $\Omega = \bigcup_i \Omega_i$ *with* $\Omega_i \cap \Omega_j = \emptyset$ *for any* $i \neq j$, *then*

$$\forall h \in \mathcal{H} : \sum_i P(\Omega_i)h = P(\Omega)h. \tag{405}$$

Corollary 2.6. *Let* $P : \mathfrak{B} \to \mathcal{L}(\mathcal{H})$ *be a PVM with respect to a Borel* σ*-algebra* $\mathfrak{B}$ *on* $\mathbb{R}$ *and a Hilbert space* $\mathcal{H}$. *Then* P *satisfies the following properties:*

1. $P(\emptyset) = 0$.

2. *For any* $\Omega \in \mathfrak{B}$, $P(\mathbb{R} \setminus \Omega) = \mathrm{id} - P(\Omega)$.

3. *For any* $\Omega_1, \Omega_2 \in \mathfrak{B}$, $P(\Omega_1 \cup \Omega_2) = P(\Omega_1) + P(\Omega_2) - P(\Omega_1 \cap \Omega_2)$.

4. *For any* $\Omega_1, \Omega_2 \in \mathfrak{B}$, $P(\Omega_1 \cap \Omega_2) = P(\Omega_1) \circ P(\Omega_2)$.

Proof. We proceed in four steps in order to prove every statement of the Corollary.

Step 1. Let $h \in \mathcal{H}$. Then we have:

$$\begin{aligned} P(\emptyset)h &= P(\emptyset \cup \emptyset)h && (406) \\ &= P(\emptyset)h + P(\emptyset)h, && (407) \end{aligned}$$

where we have used (405) in the Property 4 in Definition 2.14 and the fact that $\emptyset \cap \emptyset = \emptyset$ and $\emptyset \cup \emptyset = \emptyset$. In turn, this means that

$$P(\emptyset)h = 0. \tag{408}$$

Since h is arbitrary, we conclude that $P(\emptyset) = 0$.

Step 2. We notice that, for any $\Omega \in \mathfrak{B}$,

$$\begin{aligned} P(\mathbb{R}) &= P((\mathbb{R} \setminus \Omega) \cup \Omega) && (409) \\ &= P(\mathbb{R} \setminus \Omega) + P(\Omega), && (410) \end{aligned}$$

where we have used (405) in the Property 4 in Definition 2.14. Since $P(\mathbb{R}) = \mathrm{id}$ due to the Property 3 in Definition 2.14, we conclude that

$$P(\mathbb{R} \setminus \Omega) = \mathrm{id} - P(\Omega). \tag{411}$$

Step 3. Let $\Omega_1, \Omega_2 \in \mathfrak{B}$. Then we have:

$$\begin{aligned} P(\Omega_1) &= P((\Omega_1 \cap \Omega_2) \cup (\Omega_1 \setminus \Omega_2)) && (412) \\ &= P(\Omega_1 \cap \Omega_2) + P(\Omega_1 \setminus \Omega_2), && (413) \end{aligned}$$

and

$$\begin{aligned} P(\Omega_2) &= P((\Omega_1 \cap \Omega_2) \cup (\Omega_2 \setminus \Omega_1)) && (414) \\ &= P(\Omega_1 \cap \Omega_2) + P(\Omega_2 \setminus \Omega_1), && (415) \end{aligned}$$

where we have used (405) in the Property 4 in Definition 2.14 and the fact that $(A \cap B) \cap (A \setminus B) = \emptyset$. On the other hand, we notice that:

$$\begin{aligned} P(\Omega_1 \cup \Omega_2) &= P((\Omega_1 \setminus \Omega_2) \cup (\Omega_2 \setminus \Omega_1) \cup (\Omega_1 \cap \Omega_2)) && (416) \\ &= P(\Omega_1 \setminus \Omega_2) + P(\Omega_2 \setminus \Omega_1) + P(\Omega_1 \cap \Omega_2), && (417) \end{aligned}$$

where we have used (405) in the Property 4 in Definition 2.14. Then, taking into account (413) and (415), we conclude that

$$P(\Omega_1 \cup \Omega_2) = P(\Omega_1) + P(\Omega_2) - P(\Omega_1 \cap \Omega_2). \tag{418}$$

Step 4. First, let us consider a pair of disjoint Borel sets $\Omega_1, \Omega_2 \in \mathfrak{B}$, so that $\Omega_1 \cap \Omega_2 = \emptyset$. Then we have:

$$\begin{aligned} P(\Omega_1) + P(\Omega_2) &= P(\Omega_1 \cup \Omega_2) && (419)\\ &= P(\Omega_1 \cup \Omega_2) \circ P(\Omega_1 \cup \Omega_2) && (420)\\ &= \Big(P(\Omega_1) + P(\Omega_2)\Big) \circ \Big(P(\Omega_1) + P(\Omega_2)\Big) && (421)\\ &= P(\Omega_1) \circ P(\Omega_1) + P(\Omega_2) \circ P(\Omega_1) + P(\Omega_1) \circ P(\Omega_2) + P(\Omega_2) \circ P(\Omega_2) && (422)\\ &= P(\Omega_1) + P(\Omega_2) \circ P(\Omega_1) + P(\Omega_1) \circ P(\Omega_2) + P(\Omega_2), && (423) \end{aligned}$$

where (419) and (421) use (405) in the Property 4 in Definition 2.14, and (420) and (423) use the Property 2 in Definition 2.14. Therefore, we find that

$$P(\Omega_2) \circ P(\Omega_1) = -P(\Omega_1) \circ P(\Omega_2). \tag{424}$$

In turn, taking a composition with $P(\Omega_2)$ on both sides, we obtain:

$$P(\Omega_2) \circ P(\Omega_1) \circ P(\Omega_2) = -P(\Omega_1) \circ P(\Omega_2) \circ P(\Omega_2). \tag{425}$$

Taking into account Property 2 in Definition 2.14 and the fact that

$$\begin{aligned} P(\Omega_2) \circ P(\Omega_1) \circ P(\Omega_2) &= -P(\Omega_2) \circ P(\Omega_2) \circ P(\Omega_1) && (426)\\ &= -P(\Omega_2) \circ P(\Omega_1), && (427) \end{aligned}$$

due to (424), we rewrite (425) as

$$P(\Omega_2) \circ P(\Omega_1) = P(\Omega_1) \circ P(\Omega_2). \tag{428}$$

Comparing (424) and (428), we conclude that

$$P(\Omega_1) \circ P(\Omega_2) = \emptyset, \tag{429}$$

for disjoint Ω_1 and Ω_2. Now, let us assume that $\Omega_1 \cap \Omega_2 \neq \emptyset$. Then, applying (413) and (415), we obtain:

$$\begin{aligned} P(\Omega_1) \circ P(\Omega_2) &= \Big(P(\Omega_1 \cap \Omega_2) + P(\Omega_1 \setminus \Omega_2)\Big) \circ \Big(P(\Omega_1 \cap \Omega_2) + P(\Omega_2 \setminus \Omega_1)\Big) && (430)\\ &= P(\Omega_1 \cap \Omega_2) \circ P(\Omega_1 \cap \Omega_2) + P(\Omega_1 \setminus \Omega_2) \circ P(\Omega_1 \cap \Omega_2)\\ &+ P(\Omega_1 \cap \Omega_2) \circ P(\Omega_2 \setminus \Omega_1) + P(\Omega_1 \setminus \Omega_2) \circ P(\Omega_2 \setminus \Omega_1) && (431)\\ &= P(\Omega_1 \cap \Omega_2), && (432) \end{aligned}$$

where we have taken into account that $(\Omega_1 \setminus \Omega_2) \cap (\Omega_2 \setminus \Omega_1) =$, $(\Omega_1 \setminus \Omega_2) \cap (\Omega_1 \cap \Omega_2) = \emptyset$ and $(\Omega_2 \setminus \Omega_1) \cap (\Omega_1 \cap \Omega_2) = \emptyset$, and applied (429). □

Definition 2.15. *Given a Borel σ-algebra $\mathfrak{B}$ on $\mathbb{R}$, a Hilbert space $\mathcal{H}$, and the corresponding PVM $P : \mathfrak{B} \to \mathcal{L}(\mathcal{H})$, for any $h, g \in \mathcal{H}$, we define the associated complex measure $\mu_{h,g} : \mathfrak{B} \to \mathbb{C}$ as follows:*

$$\mu_{h,g}(\Omega) = \langle h | P(\Omega) g \rangle_{\mathcal{H}}, \tag{433}$$

and a real-valued measure $\mu_h := \mu_{h,h}$.

Exercise 2.4. *Prove that $\mu_{h,g}$ fulfills the properties of a complex-valued measure.*

A natural step further is to develop integration over PVMs: following the construction of Lebesgue integral, we start by considering simple functions.

Definition 2.16. *Let $\mathcal{S}$ be a space of simple functions $f:\mathbb{R}\to\mathbb{C}$, i.e., $f\in\mathcal{S}$ if it can be decomposed as*

$$f=\sum_{i=1}^{n} f_i\chi_{\Omega_i} \tag{434}$$

for some $n\in\mathbb{N}$, $\{f_i\}_{i=1}^{n}\subset\mathbb{C}$, and $\{\Omega_i\}_{i=1}^{n}\subset\mathfrak{B}$, where χ_{Ω_i} is the characteristic function of $\Omega_i\in\mathfrak{B}$ and $\mathfrak{B}$ is a Borel σ-algebra on $\mathbb{R}$. Then, given a Hilbert sapce $\mathcal{H}$ we define an integral over PVM $P:\mathfrak{B}\to\mathcal{L}(\mathcal{H})$ as a map $\int dP:\mathcal{S}\to\mathcal{L}(\mathcal{H})$ such that for any $f\in\mathcal{S}$

$$\int f dP := \sum_{i=1}^{n} f_i P(\Omega_i). \tag{435}$$

Theorem 2.9. *$\int dP$ is a bounded operator with a unit norm.*

Proof. Let $f\in\mathcal{S}$ and $h\in\mathcal{H}$. Then we obtain:

$$\begin{aligned}
\left\|\Big(\int fdP\Big)h\right\| &= \sqrt{\left\langle\Big(\int fdP\Big)h\Big|\Big(\int fdP\Big)h\right\rangle_{\mathcal{H}}} && (436)\\
&= \sqrt{\left\langle\sum_{i=1}^{n} f_iP(\Omega_i)h\Big|\sum_{i=1}^{n} f_iP(\Omega_i)h\right\rangle_{\mathcal{H}}} && (437)\\
&= \sqrt{\left\langle h\Big|\sum_{i,j=1}^{n} \overline{f_i}f_jP(\Omega_i)P(\Omega_j)h\right\rangle_{\mathcal{H}}} && (438)\\
&= \sqrt{\left\langle h\Big|\sum_{i=1}^{n} |f_i|^2P(\Omega_i)h\right\rangle_{\mathcal{H}}} && (439)\\
&= \sqrt{\sum_{i=1}^{n} |f_i|^2\left\langle h\Big|P(\Omega_i)h\right\rangle_{\mathcal{H}}} && (440)\\
&\leq \|f\|_\infty\|h\|_{\mathcal{H}}. && (441)
\end{aligned}$$

Therefore, we obtain:

$$\begin{aligned}
\left\|\int dP\right\| &= \sup_{f\in\mathcal{S}}\frac{\left\|\int fdP\right\|}{\|f\|_{\mathcal{S}}} && (442)\\
&= \sup_{f\in\mathcal{S}}\sup_{h\in\mathcal{H}}\frac{\left\|\left(\int fdP\right)h\right\|}{\|f\|_{\mathcal{S}}\|h\|_{\mathcal{H}}} && (443)\\
&= 1. && (444)
\end{aligned}$$

□

Once the integral over PVMs is defined for simple functions, we can immediately define it for any bounded Borel-measurable function $f:\mathbb{R}\to\mathbb{C}$ via the following Corollary.

Corollary 2.7. *Let $\mathfrak{B}$ be a Borel σ-algebra on $\mathbb{R}$, $\mathcal{H}$ be a Hilbert space, and $P:\mathfrak{B}\to\mathcal{L}(\mathcal{H})$ be a PVM. The integral $\int dP$ over it (as given in Definition 2.16) can be uniquely extended to the set $B(\mathbb{R},\mathbb{C})$ of bounded Borel-measurable functions.*

Proof. First, we notice that $\overline{\mathcal{S}} = B(\mathbb{R}, \mathbb{C})$, so that $\mathcal{S}$ is a dense subset of the space of bounded Borel-measurable functions. Due to Theorem 2.9, $\int dP$ is a bounded operator, hence, it can be uniquely extended to $B(\mathbb{R}, \mathbb{C})$ by virtue of the BLT theorem (Theorem 1.2). □

Definition 2.17. *Let $f : \mathbb{R} \to \mathbb{C}$ be a Borel-measurable function. Then we define a linear map $\int f dP : \mathcal{D}_{\int f dP} \to \mathcal{H}$ such that*

$$\mathcal{D}_{\int f dP} = \left\{ h \in \mathcal{H} \middle| \int |f|^2 d\mu_h < \infty \right\}, \tag{445}$$

$$\left(\int f dP \right) h = \lim_{n \to \infty} \left(\int f_n dP \right) h, \tag{446}$$

where $f_n = \chi_{\Omega_n} f$, with $\Omega_n := \{x \in \mathbb{R} | |f(x)| < n\}$, so that $\{f_n\}_{n \in \mathbb{N}}$ and $(\int f_n dP)h$ are Cauchy sequences in $L^2(\mathbb{R}, d\mu_h)$ and $\mathcal{H}$, respectively.

Lemma 2.10. *Let $P : \mathfrak{B} \to \mathcal{L}(\mathcal{H})$ be a PVM with respect to a Borel σ-algebra on $\mathbb{R}$ and Hilbert space $\mathcal{H}$. Then $\int f dP$ satisfies*

$$\left(\int f dP \right)^* = \int \overline{f} dP, \tag{447}$$

and is a normal operator, i.e., for any $h \in \mathcal{D}_{(\int f dP)^*} = \mathcal{D}_{\int f dP}$:

$$\left\| \left(\int f dP \right)^* h \right\|_{\mathcal{H}} = \left\| \left(\int f dP \right) h \right\|_{\mathcal{H}}. \tag{448}$$

Proof. First, for any $h' \in \mathcal{D}_{\int f dP}$, let $\{f_n\}_{n \in \mathbb{N}}$ be the Cauchy sequence in $L^2(\mathbb{R}, d\mu_{h'})$ as given in Definition 2.17, so that $\lim_{n \to \infty} f_n = f$. Then, for every f_n and for any $h \in \mathcal{D}_{\int f_n dP}$ and $g \in \mathcal{D}_{(\int f_n dP)^*}$, we can calculate

$$\begin{aligned}
\left\langle \left(\int f_n dP \right)^* g \middle| h \right\rangle_{\mathcal{H}} &= \left\langle g \middle| \left(\int f_n dP \right) h \right\rangle_{\mathcal{H}} && (449)\\
&= \left\langle g \middle| \lim_{n' \to \infty} \left(\int f_{n,n'} dP \right) h \right\rangle_{\mathcal{H}} && (450)\\
&= \lim_{n' \to \infty} \left\langle g \middle| \left(\int f_{n,n'} dP \right) h \right\rangle_{\mathcal{H}} && (451)\\
&= \lim_{n' \to \infty} \left\langle \left(\int \overline{f_{n,n'}} dP \right) g \middle| h \right\rangle_{\mathcal{H}} && (452)\\
&= \left\langle \lim_{n' \to \infty} \left(\int \overline{f_{n,n'}} dP \right) g \middle| h \right\rangle_{\mathcal{H}} && (453)\\
&= \left\langle \left(\int \overline{f_n} dP \right) g \middle| h \right\rangle_{\mathcal{H}}, && (454)
\end{aligned}$$

where $\{f_{n,n'}\}_{n' \in \mathbb{N}}$ is a Cauchy sequence of simple functions such that $\lim_{n' \to \infty} f_{n,n'} = f_n$, whereas (451) and (453) follow from continuity of inner product, and (453) follows from sesquilinearity of inner product applied to simple functions $f_{n,n'}$ with respect to (435). This proves (447) for bounded Borel-measurable functions and, in turn,

$$\left\langle g \middle| \left(\int f dP \right) h \right\rangle_{\mathcal{H}} = \left\langle \left(\int \overline{f} dP \right) g \middle| h \right\rangle_{\mathcal{H}}, \tag{455}$$

for any $h, g \in \mathcal{D}_{\int f dP} = \mathcal{D}_{\int \overline{f} dP}$ by continuity. On the other hand, in order to show that $\mathcal{D}_{(\int f_n dP)^*} \subseteq (\mathcal{D}_{\int f_n dP}$ let $h \in \mathcal{D}_{(\int f dP)^*}$, so that there exists $\tilde{h} \in \mathcal{H}$ such that

$$\left\langle h \middle| \left(\int f dP \right) g \right\rangle_{\mathcal{H}} = \langle \tilde{h} | g \rangle_{\mathcal{H}}, \tag{456}$$

for any $g \in \mathcal{D}_{\int f dP}$. Therefore, for any $g \in \mathcal{H}$, we can calculate

$$\begin{aligned} \left\langle \left(\int f_n dP\right)^* h \middle| g \right\rangle_{\mathcal{H}} &= \left\langle h \middle| \left(\int f_n dP\right) g \right\rangle_{\mathcal{H}} && (457) \\ &= \left\langle h \middle| \left(\int f dP\right) P(\Omega_n) g \right\rangle_{\mathcal{H}} && (458) \\ &= \langle \tilde{h} | P(\Omega_n) g \rangle_{\mathcal{H}} && (459) \\ &= \langle P(\Omega_n) \tilde{h} | g \rangle_{\mathcal{H}}, && (460) \end{aligned}$$

where (458) follows from $\int f_n dP = \left(\int f dP\right) P(\Omega_n)$ by construction. Since g is arbitrary, we conclude that $\left(\int f_n dP\right)^* h = P(\Omega_n)\tilde{h}$. Let us recall that, for any simple function $f' \in \mathcal{S}$ and $h' \in \mathcal{H}$,

$$\begin{aligned} \left\| \left(\int f' dP\right) h' \right\|^2 &= \left\langle \left(\int f' dP\right) h' \middle| \left(\int f' dP\right) h' \right\rangle_{\mathcal{H}} && (461) \\ &= \left\langle \sum_{i=1}^n f'_i P(\Omega_i) h \middle| \sum_{i=1}^n f'_i P(\Omega_i) h' \right\rangle_{\mathcal{H}} && (462) \\ &= \left\langle h' \middle| \sum_{i,j=1}^n \overline{f'_i} f'_j P(\Omega_i) P(\Omega_j) h' \right\rangle_{\mathcal{H}} && (463) \\ &= \left\langle h' \middle| \sum_{i=1}^n |f'_i|^2 P(\Omega_i) h' \right\rangle_{\mathcal{H}} && (464) \\ &= \sum_{i=1}^n |f'_i|^2 \left\langle h' \middle| P(\Omega_i) h' \right\rangle_{\mathcal{H}} && (465) \\ &= \sum_{i=1}^n |f'_i|^2 \mu_{h'}(\Omega_i) && (466) \\ &= \int |f'|^2 d\mu_{h'}, && (467) \end{aligned}$$

which is straightforwardly extended to bounded Borel-measurable functions via BLT theorem (Theorem 1.2). Therefore, we have

$$\begin{aligned} \lim_{n\to\infty} \int_{\mathbb{R}} |f_n|^2 d\mu_h &= \lim_{n\to\infty} \left\| \left(\int f_n dP\right) h \right\|_{\mathcal{H}}^2 && (468) \\ &= \lim_{n\to\infty} \|P(\Omega_n)\tilde{h}\|_{\mathcal{H}}^2 && (469) \\ &= \|\tilde{h}\|_{\mathcal{H}}^2. && (470) \end{aligned}$$

Hence, by monotone convergence, we have that $f \in L^2(\mathbb{R}, d\mu_h)$, and $h \in \mathcal{D}_{\int f dP}$. Therefore, $\mathcal{D}_{(\int f dP)^*} =$

$\mathcal{D}_{\int f dP}$. Moreover, we have

$$\begin{aligned}
\left\| \left(\int f dP \right) h \right\|_{\mathcal{H}}^2 &= \lim_{n\to\infty} \left\| \left(\int f_n dP \right) h \right\|_{\mathcal{H}}^2 && (471)\\
&= \lim_{n\to\infty} \int_{\mathbb{R}} |f_n|^2 d\mu_h && (472)\\
&= \lim_{n\to\infty} \int_{\mathbb{R}} |\overline{f_n}|^2 d\mu_h && (473)\\
&= \lim_{n\to\infty} \left\| \left(\int \overline{f_n} dP \right) h \right\|_{\mathcal{H}}^2 && (474)\\
&= \left\| \left(\int \overline{f} dP \right) h \right\|_{\mathcal{H}}^2, && (475)
\end{aligned}$$

concluding the proof. □

Now, Lemma 2.10 allows us to prove the inverted version of spectral theorem, which guarantees existence of a self-adjoint operator associated with any PVM.

Theorem 2.10 (Inverse spectral theorem). *Let $P : \mathfrak{B} \to \mathcal{L}(\mathcal{H})$ be a PVM with respect to a Borel σ-algebra on $\mathbb{R}$ and Hilbert space $\mathcal{H}$. Then there exists a self-adjoint operator $A_P : \mathcal{D}_{A_P} \to \mathcal{H}$ such that*

$$A_P = \int \imath_{\mathbb{R}} dP, \tag{476}$$

where $\imath_{\mathbb{R}} : \mathbb{R} \hookrightarrow \mathbb{C}$ is inclusion of $\mathbb{R}$ into $\mathbb{C}$, so that $\imath_{\mathbb{R}}(\lambda) = \lambda$ for any $\lambda \in \mathbb{R}$.

Proof. In order to prove self-adjointness of A_P, we notice that:

$$\begin{aligned}
A_P^* &= \left(\int \imath_{\mathbb{R}} dP \right)^* && (477)\\
&= \int \overline{\imath_{\mathbb{R}}} dP && (478)\\
&= \int \imath_{\mathbb{R}} dP && (479)\\
&= A_P, && (480)
\end{aligned}$$

where (478) follows from Lemma 2.10. Hence, A_P is self-adjoint. □

On the other hand, spectral theorem suggests a recipe to construct a PVM out of a given self-adjoint operator. Before to proceed with it, we provide the following definition.

Definition 2.18. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a self-adjoint operator. It is called **spectrally decomposable** if there exists a PVM $P : \mathfrak{B} \to \mathcal{L}(\mathcal{H})$ with respect to the Borel σ-algebra $\mathfrak{B}$ on $\mathbb{R}$ and Hilbert space $\mathcal{H}$ such that*

$$A = \int \imath_{\mathbb{R}} dP. \tag{481}$$

Given a Borel-measurable function $f : \mathbb{R} \to \mathbb{C}$, we define an operator

$$f(A) := \int (f \circ \imath_{\mathbb{R}}) dP. \tag{482}$$

Exercise 2.5. *Given a spectrally decomposable operator $A : \mathcal{D}_A \to \mathcal{H}$ and a Borel-measurable real-valued function $f : \mathbb{R} \to \mathbb{R}$, show that $f(A)$ is self-adjoint.*

Theorem 2.11 (Spectral theorem)**.** *Any self-adjoint operator $A : \mathcal{D}_A \to \mathcal{H}$ is spectrally decomposable with respect to some corresponding PVM P_A.*

Proof. The proof of spectral theorem has constructive nature. In what follows, we proceed in two major steps:

Step 1. Given a self-adjoint operator $A : \mathcal{D}_A \to \mathcal{H}$, we construct the corresponding complex-valued measure $\mu_{h,g}$ for any $h, g \in \mathcal{H}$.

Step 2. Recalling Definition 2.15, we aim at inverting it and construct the PVM P_A from the complex-valued measure $\mu_{h,g}$. □

In order to proceed with Step 1 of the proof of spectral theorem, we need to recall several useful facts from measure theory and complex analysis.

Definition 2.19. *Let μ be a finite Borel measure on $\mathbb{R}$. We call its* ***Borel transform*** *the map:*

$$z \mapsto F(z) = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda). \tag{483}$$

The following Lemma provide a recipe of reconstruction of a finite Borel measure out of its Borel transform.

Lemma 2.11 (Stieltjes inversion formula)**.** *Let μ be a finite Borel measure on $\mathbb{R}$. Then it can be reconstructed from its Borel transform (483) as:*

$$\mu((-\infty, \lambda']) = \lim_{\delta \to 0^+} \lim_{\varepsilon \to 0^+} \frac{1}{\pi} \int_{-\infty}^{\lambda'+\delta} dt \, \mathrm{Im} F(t + i\varepsilon), \tag{484}$$

where $\lambda' \in \mathbb{R}$.

Proof. Let $F(z)$ be given by (483). First, we notice that its imaginary part can be given in the following way,

$$\begin{aligned}
\mathrm{Im}[F(z)] &= \mathrm{Im}\left[\int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda)\right] && (485)\\
&= \int_{\mathbb{R}} \mathrm{Im}\Big[\frac{1}{\lambda - z}\Big] d\mu(\lambda) && (486)\\
&= \int_{\mathbb{R}} \frac{\mathrm{Im}[z]}{|\lambda - z|^2} d\mu(\lambda). && (487)
\end{aligned}$$

Now, let us assume that $z = t + i\varepsilon$, with $t \in \mathbb{R}$ and $\varepsilon \in \mathbb{R}^+$, and calculate the integral

$$\begin{aligned}
\lim_{\varepsilon \to 0^+} \frac{1}{\pi} \int_{t_1}^{t_2} dt \, \mathrm{Im}\Big[F(t + i\varepsilon)\Big] &= \lim_{\varepsilon \to 0^+} \frac{1}{\pi} \int_{t_1}^{t_2} dt \int_{\mathbb{R}} \frac{\varepsilon}{(\lambda - t)^2 + \varepsilon^2} d\mu(\lambda) && (488)\\
&= \int_{\mathbb{R}} \lim_{\varepsilon \to 0^+} \left(\frac{1}{\pi} \int_{t_1}^{t_2} dt \frac{\varepsilon}{(\lambda - t)^2 + \varepsilon^2}\right) d\mu(\lambda) && (489)\\
&= \int_{\mathbb{R}} \lim_{\varepsilon \to 0^+} \left(\frac{1}{\pi}\left[\arctan\Big(\frac{t_2 - \lambda}{\varepsilon}\Big) - \arctan\Big(\frac{t_1 - \lambda}{\varepsilon}\Big)\right]\right) d\mu(\lambda) && (490)\\
&= \int_{\mathbb{R}} \frac{1}{2}\Big(\chi_{(t_1,t_2)}(\lambda) + \chi_{[t_1,t_2]}(\lambda)\Big) d\mu(\lambda), && (491)
\end{aligned}$$

where (489) uses Fubini theorem, and (491) follows from the fact that the function inside the limit in (490) converges to the function

$$\frac{1}{2}\Big(\chi_{(t_1,t_2)}(\lambda) + \chi_{[t_1,t_2]}(\lambda)\Big) = \begin{cases} 0, & \lambda \in (-\infty, t_1) \cup (t_2, \infty), \\ \frac{1}{2}, & \lambda = t_{1,2}, \\ 1, & \lambda \in (t_1, t_2). \end{cases} \tag{492}$$

Now, taking the limit $t_1 \to -\infty$ and setting $t_2 = \lambda' - \delta$ with $\delta \to 0^+$, in order to guarantee right continuity of μ, we obtain:

$$\lim_{\delta\to 0^+}\lim_{\varepsilon\to 0^+}\frac{1}{\pi}\int_{-\infty}^{\lambda'-\delta} dt\,\mathrm{Im}[F(t+i\varepsilon)] = \lim_{\delta\to 0^+}\int_{\mathbb{R}}\frac{1}{2}\Big(\chi_{(-\infty,\lambda'-\delta)}(\lambda)+\chi_{(-\infty,\lambda'-\delta]}(\lambda)\Big)d\mu(\lambda) \quad (493)$$

$$= \mu((-\infty,\lambda']), \quad (494)$$

where we use the fact that $\lim_{\delta\to 0^+}\chi_{(-\infty,\lambda'-\delta)} = \chi_{(-\infty,\lambda']} = \lim_{\delta\to 0^+}\chi_{(-\infty,\lambda'-\delta]}$. □

Now, let us show that a finite Borel measure can be constructed via the Stieltjes inversion formula in Lemma 2.11 for any complex function once it satisfies certain properties on boundedness and symmetry with respect to the real line.

Lemma 2.12. *Let $F(z)$ be a Herglotz (Nevanlinna) function, i.e., a holomorphic function mapping the upper complex half-plane into itself. If there exists $0 \le M < \infty$ such that for any $z \in \mathbb{C}_+$:*

$$|F(z)| \le \frac{M}{\mathrm{Im}(z)}, \quad (495)$$

then there exists a Borel measure μ such that $\mu(\mathbb{R}) \le M$, and $F(z)$ is its Borel transform.

Proof. First, we take into account that $F(z)$ is a holomorphic function, so that, using Cauchy's integral formula, we can represent it as

$$F(z) = \frac{1}{2\pi i}\int_{\gamma}\frac{F(\zeta)}{\zeta - z}d\zeta, \quad (496)$$

for any contour γ containing z. Assuming $R > 0$ and $\varepsilon > 0$, and decomposing $z = x + iy$ with $x, y \in \mathbb{R}$, we choose the contour

$$\gamma = \{x + i\varepsilon + \lambda | \lambda \in [-R, R]\} \cup \{x + i\varepsilon + Re^{i\varphi} | \varphi \in [0, \pi]\}. \quad (497)$$

Choosing $0 < \varepsilon < y < R$, we have that z lies inside γ, while the point $\overline{z} + 2i\varepsilon$ lies outside it. Therefore, using (496) and Cauchy's integral theorem, we can write

$$F(z) = \frac{1}{2\pi i}\int_{\gamma}\Big(\frac{1}{\zeta - z} - \frac{1}{\zeta - \overline{z} - 2i\varepsilon}\Big)F(\zeta)\, d\zeta. \quad (498)$$

Taking into account (497), we can further represent it as

$$F(z) = \frac{1}{\pi}\int_{-R}^{R}\frac{y-\varepsilon}{\lambda^2 + (y-\varepsilon)^2}F(x + i\varepsilon + \lambda)\, d\lambda + \frac{i}{\pi}\int_{\pi}^{0}\frac{y-\varepsilon}{R^2 e^{2i\varphi} + (y-\varepsilon)^2}F(x + i\varepsilon + Re^{i\varphi})Re^{i\varphi}\, d\varphi. \quad (499)$$

Under the limit $R \to \infty$, the second integral in (499) vanishes, so that

$$F(z) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{y-\varepsilon}{(\lambda - x)^2 + (y-\varepsilon)^2}F(i\varepsilon + \lambda)\, d\lambda, \quad (500)$$

where the change $\lambda \mapsto \lambda + x$ of variable has been performed. Decomposing $F(z)$ into its real and imaginary parts as $F(z) = r(z) + iw(z)$, we focus on the latter and apply the bound (495),

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{y(y-\varepsilon)}{(\lambda - x)^2 + (y-\varepsilon)^2}w(i\varepsilon + \lambda)\, d\lambda \le M. \quad (501)$$

Taking the limit $y \to \infty$, we obtain

$$\frac{1}{\pi}\int_{-\infty}^{\infty} w(i\varepsilon + \lambda)d\lambda \le M. \quad (502)$$

On the other hand, denoting $\frac{y-\varepsilon}{(\lambda-x)^2+(y-\varepsilon)^2} := \phi_\varepsilon(\lambda)$, we have a bound

$$|\phi_\varepsilon(\lambda) - \phi_0(\lambda)| \leq C(x, y, \varepsilon)\varepsilon, \tag{503}$$

where $C(x, y, \varepsilon)$ is a constant. Therefore, taking $\mu_\varepsilon(\lambda) = \frac{1}{\pi}\int_{-\infty}^{\lambda} w(i\varepsilon + \lambda')d\lambda'$, we have

$$w(z) = \lim_{\varepsilon\to 0^+} \int_{-\infty}^{\infty} \phi_0(\lambda)d\mu_\varepsilon(\lambda). \tag{504}$$

In turn, (502) suggests that $\mu_\varepsilon(\mathbb{R}) \leq M$. Since it holds for any suitable ε, there exists a subsequence μ_n that converges vaguely to some measure μ such that $\mu(\mathbb{R}) \leq M$, i.e.,

$$\int_{-\infty}^{\infty} f d\mu_n \to \int_{-\infty}^{\infty} f d\mu, \tag{505}$$

for any continuous f with compact support[7]. Moreover, (505) holds for any continuous f vanishing at infinity, therefore, we can write[8]

$$w(z) = \int_{-\infty}^{\infty} \phi_0(\lambda)d\mu(\lambda). \tag{506}$$

Since $\phi_0(\lambda) = \mathrm{Im}\Big(\frac{1}{\lambda - z}\Big)$, we conclude that

$$\mathrm{Im}(F(z)) = \mathrm{Im}\Big(\int_{-\infty}^{\infty} \phi_0(\lambda)d\mu(\lambda)\Big). \tag{507}$$

Therefore, $F(z)$ and Borel transform of μ differ only by a real constant, which, due to the bound (495), is zero. □

Now, we exploit the fact that the resolvent of a self-adjoint operator defines a Herglotz (Nevanlinna) function that satisfies (495), so that a family of real-valued measurer can be associated with it via Lemma 2.11 and Lemma 2.12.

Theorem 2.12. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a self-adjoint operator, and $h \in \mathcal{D}_A$. If $R_A(z)$ is resolvent of A, there exists a measure μ_h such that*

$$F_h(z) = \langle h|R_A(z)h\rangle_{\mathcal{H}} \tag{508}$$

is its Borel transform.

Proof. Let $F_h(z) = \langle h|R_A(z)h\rangle_{\mathcal{H}}$, which is holomorphic for $z \in \rho(A)$ by definition. First, we notice that

$$\begin{aligned} R_A(z)^* &= ((A - \mathsf{z})^{-1})^* && (509)\\ &= ((A - \mathsf{z})^*)^{-1} && (510)\\ &= (A - \overline{\mathsf{z}})^{-1} && (511)\\ &= R_A(\overline{z}), && (512) \end{aligned}$$

where (510) follows from Lemma 2.6 since $R_A(z)$ is bijective, and its range is dense in $\mathcal{H}$. This translates into the following property $F_h(y)$:

$$\begin{aligned} F_h(\overline{z}) &= \langle h|R_A(\overline{z})h\rangle_{\mathcal{H}} && (513)\\ &= \langle h|R_A(z)^*h\rangle_{\mathcal{H}} && (514)\\ &= \langle R_A(z)h|h\rangle_{\mathcal{H}} && (515)\\ &= \overline{F_h(z)}. && (516) \end{aligned}$$

[7] Proof of the corresponding lemma from measure theory can be found in Lemma A.35 in [1] (Lemma A.26 in the first edition of [1]).

[8] Proof of the corresponding lemma from measure theory can be found in Lemma A.36 in [1] (Lemma A.27 in the first edition of [1]).

In order to check whether $F_h(z)$ is a Herglotz (Nevanlinna) function, we have to investigate behaviour of its imaginary part,

$$\begin{aligned}
\mathrm{Im}[F_h(z)] &= -i(F_h(z) - \overline{F_h(z)}) && (517)\\
&= -i(F_h(z) - F_h(\overline{z})) && (518)\\
&= -i\Big(\langle h|R_A(z)h\rangle_{\mathcal{H}} - \langle h|R_A(\overline{z})h\rangle_{\mathcal{H}}\Big) && (519)\\
&= -i\langle h|(R_A(z) - R_A(\overline{z}))h\rangle_{\mathcal{H}} && (520)\\
&= -i(z-\overline{z})\langle h|R_A(\overline{z})R_A(z)h\rangle_{\mathcal{H}} && (521)\\
&= \mathrm{Im}[z]\langle h|R_A(\overline{z})R_A(z)h\rangle_{\mathcal{H}} && (522)\\
&= \mathrm{Im}[z]\langle R_A(\overline{z})^* h|R_A(z)h\rangle_{\mathcal{H}} && (523)\\
&= \mathrm{Im}[z]\langle R_A(z)h|R_A(z)h\rangle_{\mathcal{H}} && (524)\\
&= \mathrm{Im}[z]\|R_A(z)h\|_{\mathcal{H}}, && (525)
\end{aligned}$$

where (521) follows from the first resolvent formula (Lemma 2.9). Since norm is a non-negative function by definition, $F_h(z)$ maps the upper complex half-plane into itself and is indeed a Herglotz (Nevanlinna) function. Moreover, we find that

$$\begin{aligned}
|F_h(z)| &\leq \|h\|_{\mathcal{H}}\|R_A(z)h\|_{\mathcal{H}} && (526)\\
&\leq \|h\|^2_{\mathcal{H}}\|R_A(z)\| && (527)\\
&\leq \frac{\|h\|^2_{\mathcal{H}}}{|\mathrm{Im}(z)|}, && (528)
\end{aligned}$$

where (526) follows from Cauchy-Schwarz inequality in Lemma 1.1, (527) follows from the definition of operator norm, and (528) follows from (338) in the proof of Theorem 2.4, so that $\|(A-\mathrm{z})^{-1}\| \leq |\mathrm{Im}[z]|^{-1}$. Therefore, by virtue of Lemma 2.12, there exists a measure μ_h such that $\langle h|R_A(z)h\rangle_{\mathcal{H}}$ is its Borel transform, so that μ_h can be constructed from $R_A(z)$ connected via Stieltjes inversion formula (Lemma 2.11). □

Once the real-valued measure μ_h is constructed out of $R_A(z)$, it can be immediately extended to the complex-valued measure $\mu_{h,g}$.

Corollary 2.8. *For any $h, g \in \mathcal{H}$, there exists a complex measure $\mu_{h,g}$ such that*

$$\langle h|R_A(z)g\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_{h,g}(\lambda). \tag{529}$$

Proof. First, we notice that $s_A(h,g) := \langle h|R_A(z)g\rangle_{\mathcal{H}}$ is a sesquilinear form that has an associated quadratic form $q_A(h) := \langle h|R_A(z)h\rangle_{\mathcal{H}}$. Therefore, it can be decomposed into a sum of quadratic forms via generalization of the polarization identity (113) to arbitrary sesquilinear forms (*exercise*):

$$s_A(h,g) = \frac{1}{4}\Big(q_A(h+g) - q_A(h-g) + iq_A(h-ig) - iq_A(h+ig)\Big). \tag{530}$$

This allows us to translate polarization identity to the measure by defining

$$\mu_{h,g}(\Omega) := \frac{1}{4}\Big(\mu_{h+g}(\Omega) - \mu_{h-g}(\Omega) + i\mu_{h-ig}(\Omega) - i\mu_{h+ig}(\Omega)\Big), \tag{531}$$

recovering (530) and, in turn, (529). □

This concludes Step 1 of the proof of spectral theorem, and we proceed with Step 2 by associating a PVM with the constructed complex-valued measure. First, we prove that it can be associated with some family of self-adjoint operators.

Lemma 2.13. *For the complex-valued measure $\mu_{h,g}$, there exists a family of self-adjoint operators $P_A(\Omega)$ such that*

$$0 \leq \langle h|P_A(\Omega)h\rangle_{\mathcal{H}} \leq \|h\|^2_{\mathcal{H}}, \tag{532}$$

and

$$\langle h|P_A(\Omega)g\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{h,g}(\lambda). \tag{533}$$

Proof. Let us define a sesquilinear form s_Ω such that for any $h, g \in \mathcal{H}$,

$$s_\Omega(h,g) = \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{h,g}(\lambda), \tag{534}$$

and the associated quadratic form

$$\begin{aligned} q_\Omega(h) &= s_\Omega(h,h) && (535) \\ &= \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_h(\lambda). && (536) \end{aligned}$$

Since $q_\Omega(h) = \mu_h(\Omega) \geq 0$, we can use the generalization of Cauchy-Schwarz inequality to sesquilinear forms:

$$\begin{aligned} |s_\Omega(h,g)| &\leq \sqrt{q_\Omega(h)}\sqrt{q_\Omega(g)} && (537) \\ &= \sqrt{\mu_h(\Omega)}\sqrt{\mu_g(\Omega)} && (538) \\ &\leq \sqrt{\mu_h(\mathbb{R})}\sqrt{\mu_g(\mathbb{R})} && (539) \\ &\leq \|h\|_{\mathcal{H}}\|g\|_{\mathcal{H}}. && (540) \end{aligned}$$

Therefore, s_Ω is bounded. By fixing one of its arguments, for example, as $s_\Omega(\cdot, g)$ for some $g \in \mathcal{H}$, it can be seen as bounded linear functional on $\mathcal{H}$. Therefore, by Riesz representation theorem (Theorem 1.7), there exists a vector g' such that

$$s_\Omega(h,g) = \langle h|g'\rangle_{\mathcal{H}}, \tag{541}$$

and, in turn, there exists a bounded operator $P_A(\Omega)$ with $\|P_A(\Omega)\| = C$ such that $h' = P_A(\Omega)h$, where

$$|s_\Omega(h,g)| \leq C\|h\|_{\mathcal{H}}\|g\|_{\mathcal{H}}, \tag{542}$$

so that $C = 1$ due to (540). Therefore, we have that $0 \leq \langle h|P_A(\Omega)h\rangle_{\mathcal{H}} \leq \|h\|^2_{\mathcal{H}}$ and

$$s_\Omega(h,g) = \langle h|P_A(\Omega)g\rangle. \tag{543}$$

Moreover, since $\mu_{h,g} = \overline{\mu_{g,h}}$, the sesquilinear form $s_\Omega(h,g)$ is symmetric, i.e., $s_\Omega(h,g) = \overline{s_\Omega(g,h)}$, so that $P_A(\Omega)$ are self-adjoint. □

Theorem 2.13. *The family of operators $P_A(\Omega)$ forms a PVM.*

Proof. In order to prove that $P_A(\Omega)$ indeed form a PVM, we proceed in four steps corresponding to each property of PVM due to Definition 2.14.

Step 1. Self-adjointness of $P_A(\Omega)$ follows immediately from Lemma 2.13.

Step 2. In order to show that $P_A(\Omega) \circ P_A(\Omega) = P_A(\Omega)$, we assume that $z, z' \in \rho(A)$ and $h, g \in \mathcal{H}$ and calculate the following integral:

$$\begin{aligned} \int_{\mathbb{R}} \frac{1}{\lambda - z'} d\mu_{R_A(\overline{z})h,g}(\lambda) &= \langle R_A(\overline{z})h|R_A(z')g\rangle_{\mathcal{H}} && (544) \\ &= \langle h|R_A(z)R_A(z')g\rangle_{\mathcal{H}} && (545) \\ &= \frac{1}{z - z'}\Big(\langle h|R_A(z)g\rangle_{\mathcal{H}} - \langle h|R_A(z')g\rangle_{\mathcal{H}}\Big) && (546) \\ &= \frac{1}{z - z'}\int_{\mathbb{R}}\Big(\frac{1}{\lambda - z} - \frac{1}{\lambda - z'}\Big) d\mu_{h,g}(\lambda) && (547) \\ &= \int_{\mathbb{R}} \frac{d\mu_{h,g}(\lambda)}{(\lambda - z)(\lambda - z')}, && (548) \end{aligned}$$

where (546) follows from the first resolvent formula (Lemma 2.9). Hence, we conclude that $d\mu_{R_A(\overline{z})h,g}(\lambda) = (\lambda - z)^{-1} d\mu_{h,g}(\lambda)$. On the other hand, we have

$$\int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_{h,P_A(\Omega)g}(\lambda) = \langle h|R_A(z)P_A(\Omega)g\rangle_{\mathcal{H}} \tag{549}$$

$$= \langle R_A(\overline{z})h|P_A(\Omega)g\rangle_{\mathcal{H}} \tag{550}$$

$$= \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{R_A(\overline{z})h,g}(\lambda) \tag{551}$$

$$= \int_{\mathbb{R}} \frac{\chi_\Omega(\lambda)}{\lambda - z} d\mu_{h,g}(\lambda), \tag{552}$$

where (550) follows from (512). Therefore, we have that $d\mu_{h,P_A(\Omega)g}(\lambda) = \chi_\Omega(\lambda) d\mu_{h,g}(\lambda)$. This allows us to calculate the following inner product,

$$\langle h|P_A(\Omega_1)P_A(\Omega_2)g\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \chi_{\Omega_2}(\lambda) d\mu_{h,P_A(\Omega_1)g}(\lambda) \tag{553}$$

$$= \int_{\mathbb{R}} \chi_{\Omega_2}(\lambda)\chi_{\Omega_1}(\lambda) d\mu_{h,g}(\lambda) \tag{554}$$

$$= \int_{\mathbb{R}} \chi_{\Omega_1 \cap \Omega_2}(\lambda) d\mu_{h,g}(\lambda) \tag{555}$$

$$= \langle h|P_A(\Omega_1 \cap \Omega_2)g\rangle_{\mathcal{H}}, \tag{556}$$

where (555) uses the fact that $\chi_{\Omega_1}(\lambda)\chi_{\Omega_2}(\lambda) = \chi_{\Omega_1 \cap \Omega_2}(\lambda)$. Therefore, we conclude that $P_A(\Omega_1) \circ P_A(\Omega_2) = P_A(\Omega_1 \cap \Omega_2)$. In particular, for $\Omega_1 = \Omega_2 := \Omega$, we have $P_A(\Omega) \circ P_A(\Omega) = P_A(\Omega)$.

Step 3. Let $h \in \ker(P_A(\mathbb{R}))$, so that

$$\mu_h(\mathbb{R}) = \langle h|P_A(\mathbb{R})h\rangle_{\mathcal{H}} \tag{557}$$

$$= 0. \tag{558}$$

Therefore, due to Lemma 2.12, we have that $\langle h|R_A(z)h\rangle_{\mathcal{H}} = 0$. In turn, using (525) we find that $\|R_A(z)h\|_{\mathcal{H}} = 0$ and, in turn, $R_A(z)h = 0$ due to the definition of norm. In turn, this implies $h = 0$, meaning that the kernel of $P_A(\mathbb{R})$ is trivial, and $P_A(\mathbb{R}) = \mathrm{id}$.

Step 4. Let $\Omega = \cup_{i \in \mathbb{N}} \Omega_i$ with $\Omega_i \cap \Omega_j = \emptyset$ for $i \neq j$. First, let us consider a finite sum of $P_A(\Omega_i)$ and calculate the following inner product:

$$\left\langle h \middle| \Big(\sum_{i=1}^n P_A(\Omega_i)\Big) h \right\rangle_{\mathcal{H}} = \sum_{i=1}^n \langle h|P_A(\Omega_i)h\rangle_{\mathcal{H}} \tag{559}$$

$$= \sum_{i=1}^n \mu_h(\Omega_i). \tag{560}$$

Due to σ-additivity of the measure μ_h, we can consider the limit $n \to \infty$, so that

$$\lim_{n \to \infty} \sum_{i=1}^n \mu_h(\Omega_i) = \mu_h(\Omega), \tag{561}$$

and, in turn,

$$\lim_{n \to \infty} \sum_{i=1}^n \langle h|P_A(\Omega_i)h\rangle_{\mathcal{H}} = \mu_h(\Omega). \tag{562}$$

On the other hand, by definition, $\mu_h(\Omega) = \langle h|P_A(\Omega)h\rangle_{\mathcal{H}}$. Therefore, we conclude that

$$\lim_{n \to \infty} \sum_{i=1}^n \langle h|P_A(\Omega_i)h\rangle_{\mathcal{H}} = \langle h|P_A(\Omega)h\rangle_{\mathcal{H}}, \tag{563}$$

and the family of operators $P_A(\Omega)$ is weakly σ-additive, i.e., with respect to weak convergence in the sense of Definition 1.9. In order to prove strong σ-additivity required by Definition 2.14, we notice that

$$\begin{aligned}
\lim_{n\to\infty}\Big\|\sum_{i=1}^{n} P(\Omega_i)h\Big\|^2 &= \lim_{n\to\infty}\Big\langle\Big(\sum_{i=1}^{n} P_A(\Omega_i)\Big)h\Big|\Big(\sum_{j=1}^{n} P_A(\Omega_j)\Big)h\Big\rangle_{\mathcal{H}} && (564)\\
&= \lim_{n\to\infty}\Big\langle h\Big|\Big(\sum_{i=1}^{n}\sum_{j=1}^{n} P_A(\Omega_i)P_A(\Omega_j)\Big)h\Big\rangle_{\mathcal{H}} && (565)\\
&= \lim_{n\to\infty}\Big\langle h\Big|\Big(\sum_{i=1}^{n} P_A(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}} && (566)\\
&= \lim_{n\to\infty}\sum_{i=1}^{n}\langle h|P_A(\Omega_i)h\rangle_{\mathcal{H}} && (567)\\
&= \langle h|P_A(\Omega)h\rangle_{\mathcal{H}} && (568)\\
&= \langle h|P_A(\Omega)P_A(\Omega)h\rangle_{\mathcal{H}} && (569)\\
&= \langle P_A(\Omega)h|P_A(\Omega)h\rangle_{\mathcal{H}} && (570)\\
&= \|P(\Omega)h\|^2. && (571)
\end{aligned}$$

This allows us to calculate the norm

$$\begin{aligned}
\lim_{n\to\infty}\Big\|P(\Omega)h-\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\|^2_{\mathcal{H}} &= \lim_{n\to\infty}\Big\langle P(\Omega)h-\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big|P(\Omega)h-\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}} && (572)\\
&= \lim_{n\to\infty}\Bigg(\|P(\Omega)h\|^2_{\mathcal{H}} - 2\mathrm{Re}\Big(\Big\langle P(\Omega)h\Big|\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}}\Big)\\
&+ \Big\|\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\|^2_{\mathcal{H}}\Bigg) && (573)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\lim_{n\to\infty}\mathrm{Re}\Big(\Big\langle P(\Omega)h\Big|\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}}\Big) && (574)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\lim_{n\to\infty}\mathrm{Re}\Big(\Big\langle h\Big|P(\Omega)\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}}\Big) && (575)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\lim_{n\to\infty}\mathrm{Re}\Big(\Big\langle h\Big|\Big(\sum_{i=1}^{n} P(\Omega)P(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}}\Big) && (576)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\lim_{n\to\infty}\mathrm{Re}\Big(\Big\langle h\Big|\Big(\sum_{i=1}^{n} P(\Omega_i)\Big)h\Big\rangle_{\mathcal{H}}\Big) && (577)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\mathrm{Re}\Big(\langle h|P(\Omega)h\rangle_{\mathcal{H}}\Big) && (578)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\mathrm{Re}\Big(\langle h|P(\Omega)P(\Omega)h\rangle_{\mathcal{H}}\Big) && (579)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\mathrm{Re}\Big(\langle P(\Omega)h|P(\Omega)h\rangle_{\mathcal{H}}\Big) && (580)\\
&= 2\|P(\Omega)h\|^2_{\mathcal{H}} - 2\mathrm{Re}\Big(\|P(\Omega)h\|^2_{\mathcal{H}}\Big) && (581)\\
&= 0, && (582)
\end{aligned}$$

where (577) follows from the fact that $\Omega\cap\Omega_i=\Omega_i$, hence, proving strong σ-additivity of $P_A(\Omega)$ and, in turn, concluding that $P_A(\Omega)$ indeed form a PVM. □

3 Schrödinger operators

3.1 Axiomatic construction of quantum mechanics

In this chapter, we focus on applications of the theory we have developed so far. Our aim is to address **non-relativistic quantum mechanics** — a physical theory that seeks to explain phenomena at a microscopic scale under velocities much smaller compared with the speed of light. In particular, microscopic scale usually implies the scale up to atomic one, opposed to motion of objects that we observe at the everyday life scale (e.g., a thrown ball), which is described by **classical mechanics**.

The ultimate goal of any physical theory is to describe the behaviour of the corresponding physical system, including description of its state. This requires setting the playground — a certain configuration space, so that the possible states of the system can be associated to elements thereof. For a given physical system with N degrees of freedom, classical mechanics in its Lagrangian formulation associates its states to elements of a N-dimensional smooth manifold Q. Locally they can be described by N quantities $\{q_i\}_{i=1}^N$ providing information on its spatial configuration, i.e., **position**. In simple cases, the configuration space can be safely reduced to $\mathbb{R}^N$, for example, $\mathbb{R}^3$ for a single free particle. Hamiltonian formulation of classical mechanics operates instead with the symplectic cotangent bundle T^*Q (known as phase space), thus, requiring locally additional N quantities $\{p_i\}_{i=1}^N$ in order to describe the **momentum** of the particle, which replaces velocity in Lagrangian mechanics. Similarly to Lagrangian formulation, in simple cases, the phase space can be reduced to $\mathbb{R}^{2N}$, for example, $\mathbb{R}^6$ for a single free particle. In quantum mechanics, a complex separable Hilbert space is used to describe the states of a physical system. This is stipulated by the first Axiom[9].

Axiom 1

The configuration space of a physical system is a complex separable Hilbert space $\mathcal{H} = L^2(\mathbb{R}^N, d\mu)$, with physical state being represented by normalized elements $f \in \mathcal{H}$, i.e., $\|f\|_{\mathcal{H}} = 1$.

Apart from determining the state of the system, a physical theory has to provide information on its **observables** — physical properties or quantities of the system that can be measured in an experiment. In classical mechanics, any observable a is described by a real-valued function on the corresponding configuration space. In quantum mechanics, these are substituted by self-adjoint operators, as Axiom 2 suggests.

Axiom 2

An observable a corresponds to a self-adjoint operator $A : \mathcal{D}_A \to \mathcal{H}$.

In classical mechanics, any property of the physical system exists independently on our actions as observers and can be revealed by measuring the corresponding observable. For example, the position of a thrown ball or the colour of the Prof. Bertlmann's sock[10] can be determined with an arbitrary precision which is limited only by sensitivity of our eyes. Imprecision of the measurement and the corresponding lack of knowledge on the observable of interest requires framework of probability theory. However, in classical mechanics, nothing prevents one to reduce it by improving the experimental technique and, in turn, perfectly learn the corresponding physical property. Quantum mechanics instead is incompatible with local pre-defined physical properties of a system and has an intrinsic

[9] Strictly speaking, a physical state in quantum mechanics is associated to a **ray** in Hilbert space, i.e., an equivalence class under the equivalence relation $h \sim h'$ if $h' = \lambda h$ for some $\lambda \in \mathbb{C}$, with $h, h' \in \mathcal{H}$. This definition reflects $U(1)$-invariance of probabilistic predictions of quantum mechanics (physicists mention it as independence on overall phase of the quantum state). Nevertheless, for the sake of simplicity, we stick to the formulation of Axiom 1 in terms of normalized elements of $\mathcal{H}$.

[10] This is a reference to Bertlmann's socks, a famous example named after Prof. Reinhold Bertlmann of the University of Vienna and provided by John Bell in his 1980 paper "Bertlmann's socks and the nature of reality" in order to illustrate the difference between classical and quantum mechanics.

probabilistic nature which cannot be avoided in a measurement[11]. It is reflected by Axiom 3 which constraints information on a physical system that can be obtained in a measurement.

Axiom 3

If the physical system is in the state $f \in \mathcal{D}_A$, the expectation value for a measurement of a is given by

$$\mathbb{E}_f(A) = \langle f|Af\rangle. \tag{583}$$

The obtained axiomatic construction deals so far with the properties of a physical system which are independent of time. However, one of ultimate goals of a physical theory is ability of prediction of dynamical behaviour of the physical system, i.e., its evolution in time. For example, knowing where and when a ball has been thrown, we can predict its trajectory using classical mechanics. Quantum mechanics, for this purpose, introduces a family of unitary operators sharing certain properties stipulated by Axiom 4. Moreover, it provides a fundamental connection between the energy of the system and its time evolution.

Axiom 4

The time evolution of the physical system is given by strongly continuous one-parameter unitary group $U(t)$ with $t \in \mathbb{R}$, i.e., a group of unitary operators such that

$$U(0) = \mathrm{id}, \tag{584}$$
$$U(t+s) = U(t)U(s), \tag{585}$$
$$\lim_{t\to t_0} U(t)f = U(t_0)f,\ \forall f \in \mathcal{H}. \tag{586}$$

The energy of the system corresponds to the generator of $U(t)$.

The generator H of $U(t)$ mentioned in Axiom 4 is called **Hamiltonian** and can be defined by

$$Hf = \lim_{t\to 0} \frac{i}{t}\Big(U(t)f - f\Big), \tag{587}$$
$$\mathcal{D}_H = \Big\{f \in \mathcal{H}\Big|\exists \lim_{t\to 0}\frac{i}{t}\Big(U(t)f - f\Big)\Big\}. \tag{588}$$

In turn, the dynamics of the state of a physical system is governed by a parameterized family of elements $\{f(t)\}_{t\in\mathbb{R}}$ of the Hilbert space $\mathcal{H}$: under assumption $f(0) \in \mathcal{D}_H$, it is provided via differential equation known as **Schrödinger equation**:

$$i\hbar\frac{d}{dt}f(t) = Hf(t), \tag{589}$$

where $\hbar$ is the Planck constant. One of the central problems in quantum mechanics is to predict time evolution of the state of a given system by solving Schrödinger equation, which requires characterization of H.

Focusing on a single particle as a physical system of interest, its canonical observables, i.e., its position and momentum, correspond[12] to multiplication (position) vector-valued operator $\vec{\mathfrak{x}}$ such that

$$\mathfrak{x}_i : \mathcal{D}_{\mathfrak{x}_i} \to L^2(\mathbb{R}^N, d\mu), \tag{590}$$
$$(\mathfrak{x}_i f)(x) = x_i f(x), \tag{591}$$

[11]Explanation of the probabilistic nature of quantum mechanics constitutes one of the main subjects of quantum foundations — a subfield of quantum theory in the intersection of physics and philosophy. In particular, there exist interpretations of quantum mechanics aiming at introduction of determinism, for example, Bohmian mechanics, which allows for pre-defined physical properties by abandoning the principle of locality, i.e., allowing for instantaneous action at a distance.

[12]This correspondence is guaranteed by Stone-von Neumann theorem, a treatment whereof, however, goes beyond scope of this course.

and differential (momentum) vector-valued operator $\vec{\mathfrak{p}}$ such that

$$\begin{aligned} \mathfrak{p}_i : \mathcal{D}_{\mathfrak{p}_i} &\rightarrow L^2(\mathbb{R}^N, d\mu), && (592)\\ (\mathfrak{p}_i f)(x) &= -i\hbar \frac{\partial}{\partial x_i} f(x), && (593) \end{aligned}$$

where $i \in \{1, \dots, N\}$ corresponds to the i-th component of the corresponding vector in certain orthonormal basis on $\mathbb{R}^N$. In terms of these operators, the Hamiltonian operator can be represented in the following form,

$$H = \frac{1}{2m}\vec{\mathfrak{p}}^2 + V(\vec{\mathfrak{r}}). \quad (594)$$

where the first term represents kinetic energy of the particle, with m being its mass, and the second terms corresponds to its potential energy (the "functions" of operators $\vec{\mathfrak{p}}$ and $\vec{\mathfrak{r}}$ have to be treated with respect to Definition 2.18 as soon as they are proven to be self-adjoint). Therefore, analysis of dynamics of a quantum particle requires analysis of self-adjointness and spectrum of the differential operator which we define in what follows.

Definition 3.1. *We call* ***Schrödinger operator*** *an operator*

$$H = -\frac{\hbar^2}{2m}\Delta + \mathcal{V}, \quad (595)$$

where $\Delta : \mathcal{D}_\Delta \rightarrow L^2(\mathbb{R}^N, d\mu)$ *is a differential operator defined as*

$$(\Delta f)(x) = \sum_{i=1}^{n} \frac{\partial^2}{\partial x^2} f(x), \quad (596)$$

and $\mathcal{V} : \mathcal{D}_\mathcal{V} \rightarrow L^2(\mathbb{R}^N, d\mu)$ *is a multiplication operator defined as*

$$(\mathcal{V} f)(x) = V(x) f(x), \quad (597)$$

where $V : \mathbb{R}^N \rightarrow \mathbb{R}$ *is a measurable function.*

The rest of the course we dedicate to examination of Schrödinger operators using the theory developed in Sections 1 and 2.

3.2 Momentum operator

Before to proceed with Schrödinger operators, we consider first the momentum operator $\vec{\mathfrak{p}}$ in order to get insights into properties of a differential operator. For the sake of simplicity, we fix $N = 1$ and focus on a compact interval $I \subseteq \mathbb{R}$ as a toy model of physical space — this is the case, e.g., for a quantum particle moving along the bottom of a well. Without loss of generality, we assume $I = [0, 2\pi]$ and fix the corresponding Hilbert space as $\mathcal{H} = L^2(0, 2\pi)$. Therefore, we consider the momentum operator $\mathfrak{p}$ defined as

$$\begin{aligned} \mathfrak{p} : \mathcal{D}_{\mathfrak{p}} &\rightarrow L^2(0, 2\pi), && (598)\\ (\mathfrak{p} f)(x) &= -i\hbar \frac{d}{dx} f(x). && (599) \end{aligned}$$

First, it is necessary to define the domain of $\mathfrak{p}$. Since the function has to be differentiable, and we would expect it to vanish on boundaries, we define an operator $\mathfrak{p}_0 : \mathcal{D}_{\mathfrak{p}_0} \rightarrow L^2(0, 2\pi)$ as a candidate such that

$$\begin{aligned} (\mathfrak{p}_0 f)(x) &= -i\hbar \frac{d}{dx} f(x), && (600)\\ \mathcal{D}_{\mathfrak{p}_0} &= \{f \in C^1[0, 2\pi] | f(0) = f(2\pi) = 0\}. && (601) \end{aligned}$$

We have immediately the following fact.

Lemma 3.1. *The operator $\mathfrak{p}_0$ is symmetric.*

Proof. Let $f, g \in \mathcal{D}_{\mathfrak{p}_0}$. Then a straightforward calculation shows:

$$\begin{aligned} \langle g|\mathfrak{p}_0 f\rangle_{L^2(0,2\pi)} &= \int_0^{2\pi} dx\; \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) && (602)\\ &= -\int_0^{2\pi} dx\; f(x)\Big(-i\hbar\frac{d}{dx}\Big)\overline{g(x)} + (-i\hbar)\overline{g(x)}f(x)\Big|_0^{2\pi} && (603)\\ &= \int_0^{2\pi} dx\; f(x)\overline{\Big(-i\hbar\frac{d}{dx}\Big)g(x)} && (604)\\ &= \langle \mathfrak{p}_0 g|f\rangle_{L^2(0,2\pi)}. && (605)\end{aligned}$$

□

Since $\mathfrak{p}_0$ is symmetric, Lemma 2.3 suggests that $\mathfrak{p}_0 \subseteq \mathfrak{p}_0^*$. Therefore, in order to check whether $\mathfrak{p}_0$ is self-adjoint, we have to determine $\mathcal{D}_{\mathfrak{p}_0^*}$ and analyse the behaviour of $\mathfrak{p}_0^*$ outside $\mathcal{D}_{\mathfrak{p}_0}$. First, let us define $\mathfrak{p}_0^*$ more precisely,

$$\begin{aligned} \mathfrak{p}_0^* : \mathcal{D}_{\mathfrak{p}_0^*} &\to L^2(0,2\pi) && (606)\\ (\mathfrak{p}_0^* f)(x) &= -i\hbar\frac{d}{dx}f(x). && (607)\end{aligned}$$

By Definition 2.1, for any $g \in \mathcal{D}_{\mathfrak{p}_0^*}$, there exists $\tilde{g} \in L^2(0,2\pi)$ such that $\langle g|\mathfrak{p}_0 f\rangle_{L^2(0,2\pi)} = \langle \tilde{g}|f\rangle_{L^2(0,2\pi)}$, i.e.,

$$\int_0^{2\pi} dx\; \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) = \int_0^{2\pi} dx\; \overline{\tilde{g}(x)}f(x). \quad (608)$$

Using integration by parts, we find

$$\int_0^{2\pi} dx\; \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) = -\int_0^{2\pi} dx \int_0^x dt\; \overline{\tilde{g}(t)}\frac{d}{dx}f(x) + \int_0^x dt\; \overline{\tilde{g}(t)}f(x)\Big|_0^{2\pi}, \quad (609)$$

or, equivalently,

$$\int_0^{2\pi} dx\; \overline{\Big(g(x) - \frac{i}{\hbar}\int_0^x dt\; \tilde{g}(t)\Big)}\frac{d}{dx}f(x) = 0. \quad (610)$$

This means that

$$\Big\langle g(x) - i\int_0^x dt\; \tilde{g}(t)\Big| f'\Big\rangle_{\mathcal{H}} = 0, \quad (611)$$

so that $g(x) - \frac{i}{\hbar}\int_0^x dt\; \tilde{g}(t) \in \{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}^\perp$, where f' indicates derivative of f. In order to characterize this set, we need several new tools.

Definition 3.2. *Let $I \subset \mathbb{R}$. A function $g : I \to \mathbb{C}$ is called **absolutely continuous** if there exists an integrable function $\tilde{g} : I \to \mathbb{C}$ such that*

$$g(x) = g(a) + \int_a^x dt\; \tilde{g}(t), \quad (612)$$

for any local compact subset $[a, x] \subseteq I$. The set of all absolutely continuous functions on I is denoted by $AC(I) \subset L^2(I)$.

Definition 3.3. *Let $I \subset \mathbb{R}$ be open. A measurable function $g : I \to \mathbb{C}$ is called p-**locally integrable** for $1 \le p \le \infty$ if*

$$\int_\Omega |g(x)|^p dx < \infty, \quad (613)$$

for any local compact subset $\Omega \subset I$. The set of all p-locally integrable functions on I is denoted by $L^p_{\text{loc}}(I)$.

Definition 3.4. *Let $I \subset \mathbb{R}$ be open, and $g \in L^1_{\text{loc}}(I)$. It is called **weakly differentiable** if there exists $\tilde{g} \in L^1_{\text{loc}}(I)$ called **weak derivative** of g such that*

$$\int_I dx\, g(x) f'(x) dx = - \int_I dx\, \tilde{g}(x) f(x), \tag{614}$$

for any $f \in C^\infty(I)$ such that f vanishes on limits of integration. The set of all weakly differentiable functions on I is denoted by $W^1(I) \subset L^1_{\text{loc}}(I)$. By induction, $W^k(I) \subset L^1_{\text{loc}}(I)$ is the set of all locally integrable functions f such that weak derivatives of f of order α for any $\alpha \leq k$ exist, i.e., functions $\tilde{g} \in L^1_{\text{loc}}(I)$ such that

$$\int_I dx\, g(x) f^{(\alpha)}(x) dx = (-1)^\alpha \int_I dx\, \tilde{g}(x) f(x), \tag{615}$$

where $f^{(\alpha)}$ denotes derivative of f of order α.

We are interested in integrable functions which admit integrable weak derivatives. This motivates introduction of a new subspace of L^p in the following Definition.

Definition 3.5. *Let $I \subset \mathbb{R}$ be open, $k \in \mathbb{N}$, and $1 \leq p \leq \infty$. We call the $(k,p)-$**Sobolev space** the space of functions*

$$W^{k,p}(I) = \{f \in L^p(I) \cap W^k(I) | f^{(\alpha)} \in L^p(I),\ \forall \alpha \leq k\}. \tag{616}$$

For $p = 2$, the Sobolev spaces are denoted $H^k(I) := W^{k,2}(I)$.

Exercise 3.1. *Prove that $H^k(I)$ is a Hilbert space.*

Exercise 3.2. *Prove that $\{f \in AC(I) | f' \in L^2(I)\} \subseteq H^1(I)$.*

Now we are ready to characterize the set $\{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}^\perp$ defining the domain of $\mathfrak{p}_0^*$. First, let us provide several useful results.

Lemma 3.2. *Let $\{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}$ be the set of derivatives of functions from the domain of $\mathfrak{p}_0$. Then*

$$\{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\} = \left\{ h \in C[0, 2\pi] \middle| \int_0^{2\pi} dt\, h(t) = 0 \right\}. \tag{617}$$

Proof. Let $f' \in \{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}$. Then, by (601),

$$\int_0^{2\pi} dx\, f'(x) = f(x)\big|_0^{2\pi} \tag{618}$$

$$= 0, \tag{619}$$

so that $f' \in \{h \in C[0, 2\pi] | \int_0^{2\pi} dt\, h(t) = 0\}$. On the other hand, let $h \in \{h \in C[0, 2\pi] | \int_0^{2\pi} dt\, h(t) = 0\}$. Since $h \in C[0, 2\pi]$, we have:

$$\tilde{h}(x) := \int_0^x dt\, h(t) \in C^1[0, 2\pi]. \tag{620}$$

Moreover, $\tilde{h}(0) = \tilde{h}(2\pi) = 0$, so that $\tilde{h}(x) \in \mathcal{D}_{\mathfrak{p}_0}$ and, in turn, $h \in \{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}$. This proves the statement of the Lemma. □

Lemma 3.3. *Let $\{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}$ be the set of derivatives of functions from the domain of $\mathfrak{p}_0$. Then*

$$\overline{\{f' | f \in \mathcal{D}_{\mathfrak{p}_0}\}} = \{\mathbb{1}\}^\perp, \tag{621}$$

where $\mathbb{1} \in L^2(0, 2\pi)$ is a constant function such that $\mathbb{1}(x) = 1$ for any $x \in [0, 2\pi]$.

Proof. From Lemma 3.2 we have:

$$\{f'|f \in \mathcal{D}_{\mathfrak{p}_0}\} = \{h \in C[0,2\pi] | \langle \mathbb{1}|h\rangle_{L^2(0,2\pi)} = 0\}. \tag{622}$$

Taking the closure, we obtain:

$$\begin{aligned}
\overline{\{f'|f \in \mathcal{D}_{\mathfrak{p}_0}\}} &= \overline{\{h \in C[0,2\pi] | \langle \mathbb{1}|h\rangle_{L^2(0,2\pi)} = 0\}} && (623)\\
&= \{h \in \overline{C[0,2\pi]} | \langle \mathbb{1}|h\rangle_{L^2(0,2\pi)} = 0\} && (624)\\
&= \{h \in L^2(0,2\pi) | \langle \mathbb{1}|h\rangle_{L^2(0,2\pi)} = 0\} && (625)\\
&= \{\mathbb{1}\}^{\perp}. && (626)
\end{aligned}$$

□

Theorem 3.1. $\mathfrak{p}_0^*$ *is defined on (1,2)-Sobolev space, so that* $\mathcal{D}_{\mathfrak{p}_0^*} = H^1(0,2\pi) \neq \mathcal{D}_{\mathfrak{p}_0}$*, and* $\mathfrak{p}_0$ *is not self-adjoint.*

Proof. First, let us show that any function from $\mathcal{D}_{\mathfrak{p}_0^*}$ is absolutely continuous.

$$\begin{aligned}
g(x) - \frac{i}{\hbar}\int_0^x dt\ \tilde{g}(t) &\in \{f'|f \in \mathcal{D}_{\mathfrak{p}_0}\}^{\perp} && (627)\\
&= \overline{\{f'|f \in \mathcal{D}_{\mathfrak{p}_0}\}^{\perp}} && (628)\\
&= \{f'|f \in \mathcal{D}_{\mathfrak{p}_0}\}^{\perp\perp\perp} && (629)\\
&= \overline{\{f'|f \in \mathcal{D}_{\mathfrak{p}_0}\}}^{\perp} && (630)\\
&= \{\mathbb{1}\}^{\perp\perp} && (631)\\
&= \overline{\{\mathbb{1}\}} && (632)\\
&= \mathrm{span}(\mathbb{1}). && (633)
\end{aligned}$$

Therefore, any $g(x) - \frac{i}{\hbar}\int_0^x dt\ \tilde{g}(t)$ is a constant function $x \mapsto g(0) \in \mathbb{C}$. Hence, we conclude that $g(x) = g(0) + \frac{i}{\hbar}\int_0^x dt\ \tilde{g}(t)$, so that, recalling Definition 3.2, $g \in AC[0,2\pi]$, and, in turn, $\mathcal{D}_{\mathfrak{p}_0^*} \subseteq AC[0,2\pi]$. Moreover, recalling that $\mathfrak{p}_0^*$ maps its domain to $L^2(0,2\pi)$, we conclude that $\mathcal{D}_{\mathfrak{p}_0^*} \subseteq H^1(0,2\pi)$ using Exercise 3.2. On the other hand, we take into account that all integrations by parts in Lemma 3.1 are of the form

$$\int_I dx\ g(x) f'(x) dx = -\int_I dx\ g'(x) f(x), \tag{634}$$

for arbitrary $f \in C^1(0,2\pi)$ vanishing on limits of integration. Since $C^\infty(0,2\pi) \subset C^1(0,2\pi)$, it is also valid for arbitrary $f \in C^\infty(0,2\pi)$ vanishing on limits of integration. Recalling Definition 3.4, this is the condition of weak derivative. Hence, due to Definition 3.5, we conclude that $\mathcal{D}_{\mathfrak{p}_0^*} = H^1(0,2\pi)$, so that $\mathcal{D}_{\mathfrak{p}_0} \neq \mathcal{D}_{\mathfrak{p}_0^*}$, and $\mathfrak{p}_0$ is not self-adjoint. □

Since $\mathfrak{p}_0$ is symmetric yet not a self-adjoint operator, we can question its self-adjoint extensions. First, we check whether it is essentially self-adjoint that would guarantee a unique self-adjoint extension due to Corollary 2.2.

Theorem 3.2. $\mathfrak{p}_0$ *is not essentially self-adjoint.*

Proof. Due to Definition 2.8, we have to check whether $\overline{\mathfrak{p}_0}$ is a self-adjoint operator. First, due to Theorem 2.2, we have $\overline{\mathfrak{p}_0} = \mathfrak{p}_0^{**}$. Recalling Definition 2.1, $\mathfrak{p}_0^{**}$ is defined in such a way that any $g \in \mathcal{D}_{\mathfrak{p}_0^{**}}$ satisfies

$$\langle g|\mathfrak{p}_0^* f\rangle_{L^2(0,2\pi)} = \langle \mathfrak{p}_0^{**} g|f\rangle_{L^2(0,2\pi)}. \tag{635}$$

for any $f \in \mathcal{D}_{\mathfrak{p}_0^*} = H^1(0,2\pi)$. On the other hand, since $\mathfrak{p}_0$ is symmetric due to Lemma 3.1, Lemma 2.5 suggests that $\mathfrak{p}_0 \subseteq \mathfrak{p}_0^{**} \subseteq \mathfrak{p}_0^*$, so that, for any $g \in \mathcal{D}_{\mathfrak{p}_0^{**}}$,

$$\langle \mathfrak{p}_0^{**} g | f \rangle_{L^2(0,2\pi)} = \langle \mathfrak{p}_0^* g | f \rangle_{L^2(0,2\pi)}, \tag{636}$$

by Definition 1.10. Therefore, we obtain:

$$\langle g | \mathfrak{p}_0^* f \rangle_{L^2(0,2\pi)} = \langle \mathfrak{p}_0^* g | f \rangle_{L^2(0,2\pi)}, \tag{637}$$

for any $g \in \mathcal{D}_{\mathfrak{p}_0^{**}}$ and $f \in \mathcal{D}_{\mathfrak{p}_0^*}$. Calculation of the inner products on $L^2(0,2\pi)$ results in:

$$\int_0^{2\pi} dx\ \overline{g(x)} \Big(-i\hbar \frac{d}{dx}\Big) f(x) = \int_0^{2\pi} dx\ f(x) \overline{\Big(-i\hbar \frac{d}{dx}\Big) g(x)}, \tag{638}$$

and, performing integration by parts, we obtain:

$$\overline{g}(2\pi) f(2\pi) - \overline{g}(0) f(0) = 0. \tag{639}$$

Since there are no constraints on values of $f \in \mathcal{D}_{\mathfrak{p}_0^*} = H^1(0,2\pi)$ on boundaries, we conclude that $\overline{g}(0) = g(0) = \overline{g}(2\pi) = g(2\pi) = 0$, so that

$$\begin{aligned} \mathcal{D}_{\mathfrak{p}_0^{**}} &= \{ f \in H^1(0,2\pi) | f(0) = f(2\pi) = 0 \} && (640) \\ &\neq \mathcal{D}_{\mathfrak{p}_0^*}. && (641) \end{aligned}$$

Therefore, we have $\overline{\mathfrak{p}_0} \neq \mathfrak{p}_0^*$. On the other hand, we notice that $\overline{\mathfrak{p}_0}^* = \mathfrak{p}_0^{***} = \overline{\mathfrak{p}_0^*}$. Moreover, due to Theorem 2.2, we have $\overline{\mathfrak{p}_0^*} = \mathfrak{p}_0^*$. Therefore, we conclude that $\overline{\mathfrak{p}_0} \subseteq \overline{\mathfrak{p}_0}^*$, and $\mathfrak{p}_0$ is not essentially self-adjoint. □

This means that the choice (601) of the domain of $\mathfrak{p}_0$ is not optimal to define the momentum operator. In order to overcome this problem, we can slightly weaken the boundary conditions by defining $\tilde{\mathfrak{p}}_0 : \mathcal{D}_{\tilde{\mathfrak{p}}_0} \to L^2(0,2\pi)$ as a candidate for momentum operator such that

$$\begin{aligned} (\tilde{\mathfrak{p}}_0 f)(x) &= -i\hbar \frac{d}{dx} f(x), && (642) \\ \mathcal{D}_{\tilde{\mathfrak{p}}_0} &= \{ f \in C^1[0,2\pi] | f(0) = f(2\pi) \}, && (643) \end{aligned}$$

i.e., treating $I = [0,2\pi]$ as a circle and, hence, extending previous candidate operator, $\mathfrak{p}_0 \subset \tilde{\mathfrak{p}}_0$. First, we notice that Lemma 3.1 remains valid for $\tilde{\mathfrak{p}}_0$ as well.

Lemma 3.4. *The operator* $\tilde{\mathfrak{p}}_0$ *is symmetric.*

Proof. Let $f, g \in \mathcal{D}_{\tilde{\mathfrak{p}}_0}$. Then a straightforward calculation shows:

$$\begin{aligned} \langle g | \tilde{\mathfrak{p}}_0 f \rangle_{L^2(0,2\pi)} &= \int_0^{2\pi} dx\ \overline{g(x)} \Big(-i\hbar \frac{d}{dx}\Big) f(x) && (644) \\ &= -\int_0^{2\pi} dx\ f(x) \Big(-i\hbar \frac{d}{dx}\Big) \overline{g(x)} + (-i\hbar) \overline{g(x)} f(x) \Big|_0^{2\pi} && (645) \\ &= -\int_0^{2\pi} dx\ f(x) \Big(-i\hbar \frac{d}{dx}\Big) \overline{g(x)} + (-i\hbar) \overline{g(2\pi)} f(2\pi) - (-i\hbar) \overline{g(0)} f(0) && (646) \\ &= -\int_0^{2\pi} dx\ f(x) \Big(-i\hbar \frac{d}{dx}\Big) \overline{g(x)} + (-i\hbar) \overline{g(0)} f(0) - (-i\hbar) \overline{g(0)} f(0) && (647) \\ &= \int_0^{2\pi} dx\ f(x) \overline{\Big(-i\hbar \frac{d}{dx}\Big) g(x)} && (648) \\ &= \langle \tilde{\mathfrak{p}}_0 g | f \rangle_{L^2(0,2\pi)}. && (649) \end{aligned}$$

□

In order to check whether $\tilde{\mathfrak{p}}_0$ is self-adjoint, we recall Definition 2.1 suggesting that any $g \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^*}$ and $f \in \mathcal{D}_{\tilde{\mathfrak{p}}_0}$ satisfy $\langle g|\tilde{\mathfrak{p}}_0 f\rangle_{L^2(0,2\pi)} = \langle \tilde{\mathfrak{p}}_0^* g|f\rangle_{L^2(0,2\pi)}$. On the other hand, we notice that $\tilde{\mathfrak{p}}_0^* \subset \mathfrak{p}_0^*$ due to Lemma 2.2. Therefore, for any $g \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^*}$ and $f \in \mathcal{D}_{\tilde{\mathfrak{p}}_0}$, we have:

$$\langle g|\tilde{\mathfrak{p}}_0 f\rangle_{L^2(0,2\pi)} = \langle \mathfrak{p}_0^* g|f\rangle_{L^2(0,2\pi)}. \tag{650}$$

Calculation of the inner products on $L^2(0,2\pi)$ results in:

$$\int_0^{2\pi} dx\, \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) \;=\; \int_0^{2\pi} dx\, f(x)\overline{\Big(-i\hbar\frac{d}{dx}\Big)g(x)}, \tag{651}$$

and, performing integration by parts, we find:

$$\int_0^{2\pi} dx\, \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) \;=\; \int_0^{2\pi} dx\, \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) + i\hbar\overline{g(x)}f(x)\Big|_0^{2\pi}, \tag{652}$$

which straightforwardly is equivalent to:

$$\overline{g(2\pi)}f(2\pi) = \overline{g(0)}f(0). \tag{653}$$

Since $f \in \mathcal{D}_{\tilde{\mathfrak{p}}_0}$, we take into account that $f(0) = f(2\pi)$, meaning that $g(0) = g(2\pi)$. On the other hand, Theorem 3.1 suggests that $\mathcal{D}_{\mathfrak{p}_0^*} = H^1(0,2\pi)$, thus, we already know that $\mathcal{D}_{\tilde{\mathfrak{p}}_0^*} \subset H^1(0,2\pi)$. Therefore, we conclude that

$$\mathcal{D}_{\tilde{\mathfrak{p}}_0^*} = \{f \in H^1(0,2\pi) | f(0) = f(2\pi)\}, \tag{654}$$

obviously suggesting that $\mathcal{D}_{\tilde{\mathfrak{p}}_0^*} \neq \mathcal{D}_{\tilde{\mathfrak{p}}_0}$ and $\tilde{\mathfrak{p}}_0$ is not self-adjoint. However, we have the following result.

Theorem 3.3. $\tilde{\mathfrak{p}}_0$ *is an essentially self-adjoint operator.*

Proof. Due to Definition 2.8, we have to check whether $\overline{\tilde{\mathfrak{p}}_0}$ is a self-adjoint operator. First, due to Theorem 2.2, we have $\overline{\tilde{\mathfrak{p}}_0} = \tilde{\mathfrak{p}}_0^{**}$. Recalling Definition 2.1, $\tilde{\mathfrak{p}}_0^{**}$ is defined in such a way that any $g \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^{**}}$ satisfies

$$\langle g|\tilde{\mathfrak{p}}_0^* f\rangle_{L^2(0,2\pi)} = \langle \tilde{\mathfrak{p}}_0^{**} g|f\rangle_{L^2(0,2\pi)}. \tag{655}$$

for any $f \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^*} = H^1(0,2\pi)$. On the other hand, since $\tilde{\mathfrak{p}}_0$ is symmetric due to Lemma 3.4, Lemma 2.5 suggests that $\tilde{\mathfrak{p}}_0 \subseteq \tilde{\mathfrak{p}}_0^{**} \subseteq \tilde{\mathfrak{p}}_0^*$, so that, for any $g \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^{**}}$,

$$\langle \tilde{\mathfrak{p}}_0^{**} g|f\rangle_{L^2(0,2\pi)} = \langle \tilde{\mathfrak{p}}_0^* g|f\rangle_{L^2(0,2\pi)}, \tag{656}$$

by Definition 1.10. Therefore, we obtain:

$$\langle g|\tilde{\mathfrak{p}}_0^* f\rangle_{L^2(0,2\pi)} = \langle \tilde{\mathfrak{p}}_0^* g|f\rangle_{L^2(0,2\pi)}, \tag{657}$$

for any $g \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^{**}}$ and $f \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^*}$. Calculation of the inner products on $L^2(0,2\pi)$ results in:

$$\int_0^{2\pi} dx\, \overline{g(x)}\Big(-i\hbar\frac{d}{dx}\Big)f(x) = \int_0^{2\pi} dx\, f(x)\overline{\Big(-i\hbar\frac{d}{dx}\Big)g(x)}, \tag{658}$$

and, performing integration by parts, we obtain:

$$\overline{g}(2\pi)f(2\pi) - \overline{g}(0)f(0) = 0. \tag{659}$$

Since $f \in \mathcal{D}_{\tilde{\mathfrak{p}}_0^*}$, we have $f(0) = f(2\pi)$, so that we obtain a condition on g:

$$g(2\pi) = g(0). \tag{660}$$

Therefore, we conclude that

$$\mathcal{D}_{\tilde{\mathfrak{p}}_0^{**}} = \{f \in H^1(0,2\pi) | f(0) = f(2\pi)\} \tag{661}$$

$$= \mathcal{D}_{\tilde{\mathfrak{p}}_0^*}. \tag{662}$$

and $\overline{\tilde{\mathfrak{p}}_0} = \tilde{\mathfrak{p}}_0^*$. This means that $\overline{\tilde{\mathfrak{p}}_0} \subseteq \tilde{\mathfrak{p}}_0^*$ and $\tilde{\mathfrak{p}}_0^* \subseteq \overline{\tilde{\mathfrak{p}}_0}$. Hence, applying Lemma 2.2 and taking into account again that $\tilde{\mathfrak{p}}_0^{**} = \overline{\tilde{\mathfrak{p}}_0}$, we find that $\overline{\tilde{\mathfrak{p}}_0} \subseteq \overline{\tilde{\mathfrak{p}}_0}^*$ and $\overline{\tilde{\mathfrak{p}}_0}^* \subseteq \overline{\tilde{\mathfrak{p}}_0}$. Therefore, we have that $\overline{\tilde{\mathfrak{p}}_0}^* = \overline{\tilde{\mathfrak{p}}_0}$, and $\tilde{\mathfrak{p}}_0$ is essentially self-adjoint. ∎

Therefore, we conclude that $\tilde{\mathfrak{p}}_0^*$ can be considered as the momentum operator $\mathfrak{p}$ on $L^2(0, 2\pi)$, which we define as:

$$\mathfrak{p}: \; H_c^1(0, 2\pi) \;\to\; L^2(0, 2\pi), \tag{663}$$

$$(\mathfrak{p}f)(x) \;=\; -i\hbar \frac{d}{dx} f(x), \tag{664}$$

where $H_c^1(0, 2\pi) := \{f \in H^1(0, 2\pi) | f(0) = f(2\pi)\}$.

Exercise 3.3. *Solving the equation $\mathfrak{p}u = zu$, show that the eigenvalues of $\mathfrak{p}$ are given by $n \in \mathbb{Z}$ with the corresponding eigenvectors $u_n(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}nx}$ forming an orthonormal basis on $L^2(0, 2\pi)$.*

Before to conclude the discussion of momentum operator, we notice that the momentum operator $\mathfrak{p}$ can be constructed for $L^2(I)$ on any closed interval I in the way guaranteed by Theorem 3.3, and the eigenvalue problem in Exercise 3.3 can be in principle solved. From the physical point of view, this allows one to model dynamics of a particle moving along the bottom of a well of arbitrary length. However, a naive transition to the case of a free particle by considering a "well with infinitely separated walls", i.e., $L^2(\mathbb{R})$ leads to a problem with the eigenvalue equation for the momentum operator which has no solution in $L^2(\mathbb{R})$. An additional structure known as rigged Hilbert space (or Gelfand triple) is introduced in order to overcome this problem by extending the standard Hilbert space L^2 of quantum mechanics. Before to define it for $\mathbb{R}^N$, we introduce the following notation:

$$\partial_\alpha f \;:=\; \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}}, \tag{665}$$

$$x^\alpha \;:=\; x_1^{\alpha_1} \dots x_n^{\alpha_n}, \tag{666}$$

$$|\alpha| \;:=\; \alpha_1 + \dots + \alpha_n, \tag{667}$$

where $\alpha \in \mathbb{N}_0^N$, with $\mathbb{N}_0^N := \times^N \mathbb{N}_0 := \times^N(\mathbb{N} \cup \{0\})$. First, we define a new space $\mathcal{S}(\mathbb{R}^N) \subset C^\infty(\mathbb{R}^N)$ of smooth functions, which (including their derivatives) decay rapidly.

Definition 3.6. *We call the **Schwartz space** the space of functions*

$$\mathcal{S}(\mathbb{R}^N) = \{f \in C^\infty(\mathbb{R}^N) | \sup_x |x^\alpha (\partial_\beta f)(x)| < \infty, \; \forall \alpha, \beta \in \mathbb{N}_0^N\}. \tag{668}$$

Exercise 3.4. *Prove that $\mathcal{S}(\mathbb{R}^N)$ is a dense subset of $L^p(\mathbb{R}^N)$ for $1 \leq p < \infty$.*

Definition 3.7. *The triple of spaces*

$$\mathcal{S}(\mathbb{R}^N) \subset L^2(\mathbb{R}^N) \subset \mathcal{S}^*(\mathbb{R}^N) \tag{669}$$

*is called **rigged Hilbert space** or **Gelfand triple**.*

In particular, it allows one to associate continuous spectrum with elements of $\mathcal{S}^*(\mathbb{R}^N)$ — Schwartz distributions, which are treated as so-called generalized eigenvectors. Treatment of eigenvectors as Schwartz distributions allows one to solve rigorously the eigenvalue problem for position and momentum operators for a free particle. However, the famous Schwartz impossibility result suggests that Schwartz distributions do not form an algebra, so that no multiplication operation can be defined on $\mathcal{S}^*(\mathbb{R}^N)$. We return to this problem in Section 4.

3.3 Free Schrödinger operator

The free Schrödinger operator is a particular case of Schrödinger operator provided in Definition 3.1 with $\mathcal{V} = 0$,

$$H_0 = -\frac{\hbar^2}{2m} \Delta. \tag{670}$$

From the physical point of view, this operator defines the energy of a free particle, which does not experience action of any external potential. In order to study its properties, we introduce an important tool which will simplify the analysis.

Definition 3.8. *We call the* ***Fourier operator*** *an operator* $\mathcal{F}:\mathcal{S}(\mathbb{R}^N)\to\mathcal{S}(\mathbb{R}^N)$ *which acts on* $f\in\mathcal{S}(\mathbb{R}^N)$ *in the following way:*

$$(\mathcal{F}f)(p)=\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,e^{-ipx}f(x). \tag{671}$$

First, we recall several useful properties of Fourier operator that we will need in calculations.

Lemma 3.5. *Let* $f\in\mathcal{S}(\mathbb{R}^N)$ *and* $\alpha\in\mathbb{N}_0^N$. *Then:*

$$(\mathcal{F}(\partial_\alpha f))(p) = (ip)^\alpha(\mathcal{F}f)(p), \tag{672}$$

$$(\mathcal{F}(x^\alpha f(x)))(p) = i^{|\alpha|}\partial_\alpha(\mathcal{F}f)(p). \tag{673}$$

Proof. Let $|\alpha|=1$, so that $\partial_\alpha=\frac{\partial}{\partial x_j}$ for arbitrary j. Then we calculate:

$$\begin{aligned}\Big(\mathcal{F}\Big(\frac{\partial}{\partial x_j}f(x)\Big)\Big)(p) &= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,e^{-ipx}\frac{\partial}{\partial x_j}f(x) &(674)\\ &= -\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,\Big(\frac{\partial}{\partial x_j}e^{-ipx}\Big)f(x) &(675)\\ &= ip_j\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,e^{-ipx}f(x) &(676)\\ &= ip_j(\mathcal{F}f)(p), &(677)\end{aligned}$$

where (676) follows from integration by parts. In turn, the generalization to arbitrary α follows by induction. On the other hand, for $|\alpha|=1$, we calculate:

$$\begin{aligned}\Big(\mathcal{F}\Big(x_jf(x)\Big)\Big)(p) &= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,e^{-ipx}x_jf(x) &(678)\\ &= i\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,\Big(\frac{\partial}{\partial p_j}e^{-ipx}\Big)f(x) &(679)\\ &= i\frac{\partial}{\partial p_j}\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,e^{-ipx}f(x) &(680)\\ &= i\frac{\partial}{\partial p_j}(\mathcal{F}f)(p), &(681)\end{aligned}$$

where (680) follows from the fact that $\left|\frac{\partial}{\partial p_j}e^{-ipx}f(x)\right|\le x_jf(x):=g(x)$, and $g(x)$ is integrable since $f(x)\in\mathcal{S}(\mathbb{R}^N)$. In turn, the generalization to arbitrary α follows by induction. ☐

Lemma 3.6. *Let* $f\in\mathcal{S}(\mathbb{R}^N)$, $a\in\mathbb{R}^n$, *and* $\lambda>0$. *Then:*

$$(\mathcal{F}f(x+a))(p) = e^{iap}(\mathcal{F}f(x))(p), \tag{682}$$

$$(\mathcal{F}f(\lambda x))(p) = \frac{1}{\lambda^N}(\mathcal{F}f(x))\Big(\frac{p}{\lambda}\Big). \tag{683}$$

Proof. First, we calculate:

$$\begin{aligned}(\mathcal{F}f(x+a))(p) &= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Nx\,e^{-ipx}f(x+a) &(684)\\ &= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Ny\,e^{-ip(y-a)}f(y) &(685)\\ &= e^{iap}\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N}d^Ny\,e^{-ipy}f(y) &(686)\\ &= e^{iap}(\mathcal{F}f(x))(p), &(687)\end{aligned}$$

where (685) uses change of variable $y := x - a$. On the other hand, we calculate:

$$(\mathcal{F}f(\lambda x))(p) = \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} d^N x \, e^{-ipx} f(\lambda x) \tag{688}$$

$$= \frac{1}{(2\pi\lambda^2)^{N/2}} \int_{\mathbb{R}^N} d^N y \, e^{-\frac{ipy}{\lambda}} f(y) \tag{689}$$

$$= \frac{1}{\lambda^N} (\mathcal{F}f(x))\Big(\frac{p}{\lambda}\Big), \tag{690}$$

where (685) uses change of variable $y := \lambda x$. □

Lemma 3.7. *Let $z \in \mathbb{C}$ such that* $\mathrm{Re}[z] > 0$. *Then:*

$$(\mathcal{F}e^{-zx^2/2})(p) = \frac{1}{z^{N/2}} e^{-zp^2/2}. \tag{691}$$

Proof. First, we notice that $e^{-zx^2/2} = \prod_{j=1}^N e^{-zx_j^2/2}$. Therefore, without loss of generality, it is enough to provide the proof for a single coordinate $x_j := x$. Let $\phi_z(x) = e^{-zx^2/2}$. Then a straightforward calculation reveals:

$$\phi_z'(x) + zx\phi_z(x) = 0. \tag{692}$$

In turn, applying Fourier operator and taking into account Lemma 3.5, we obtain an ordinary differential equation:

$$i(p(\mathcal{F}\phi_z)(p) + z(\mathcal{F}\phi_z')(p)) = 0. \tag{693}$$

Solving it, we find:

$$(\mathcal{F}\phi_z)(p) = (\mathcal{F}\phi_z)(0)\phi_{1/z}(p), \tag{694}$$

where

$$(\mathcal{F}\phi_z)(0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx \, e^{-zx^2/2} \tag{695}$$

$$= \frac{1}{\sqrt{z}} \tag{696}$$

for $z > 0$. However, since ϕ_z is holomorphic with respect to z and measurable with respect to y, and $|\phi_z(x)| \le e^{-\mathrm{Re}[z]x^2/2} \le e^{-x^2/2} := g(x)$, with $g(x)$ being integrable for any compact subset $V \subset U$, where $U := \{z \in \mathbb{C} | \mathrm{Re}[z] > 0\}$, we conclude that the integral in (695) is holomorphic for $\mathrm{Re}[z] > 0$. Therefore, (696) holds for any $z \in U$ as soon as the branch cut of the root $\sqrt{z}$ is chosen along the negative real axis. □

Theorem 3.4. *Let $\mathcal{F} : \mathcal{S}(\mathbb{R}^N) \to \mathcal{S}(\mathbb{R}^N)$ be the Fourier operator. It is a bijection, and there exists the inverse $\mathcal{F}^{-1} : \mathcal{S}(\mathbb{R}^N) \to \mathcal{S}(\mathbb{R}^N)$ defined as:*

$$(\mathcal{F}^{-1}g)(x) = \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} d^N p \, e^{ipx} f(p). \tag{697}$$

Proof. Let $\phi_\varepsilon(p) = e^{-\varepsilon p^2/2}$, so that $\lim_{\varepsilon\to 0}\phi_\varepsilon(p) = 1$. We calculate:

$$\begin{aligned}
(\mathcal{F}^{-1}(\mathcal{F}f))(x) &= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N p\, e^{ipx}(\mathcal{F}f)(p) && (698)\\
&= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N p\, \lim_{\varepsilon\to 0}\phi_\varepsilon(x)e^{ipx}(\mathcal{F}f)(p) && (699)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N p\, \phi_\varepsilon(p)e^{ipx}(\mathcal{F}f)(p) && (700)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{N}}\int_{\mathbb{R}^N} d^N p\, \phi_\varepsilon(p)e^{ipx}\int_{\mathbb{R}^N} d^N y\, e^{-ipy}f(y) && (701)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{N}}\int_{\mathbb{R}^N} d^N y\, f(y)\int_{\mathbb{R}^N} d^N p\, e^{-ip(y-x)}\phi_\varepsilon(p) && (702)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{N}}\int_{\mathbb{R}^N} d^N z\, f(z+x)\int_{\mathbb{R}^N} d^N p\, e^{-ipz}\phi_\varepsilon(p) && (703)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N z\, f(z+x)(\mathcal{F}(\phi_\varepsilon(p))(z) && (704)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi\varepsilon)^{N/2}}\int_{\mathbb{R}^N} d^N z\, f(z+x)\phi_{1/\varepsilon}(z) && (705)\\
&= \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N \tilde{z}\, f(\sqrt{\varepsilon}\tilde{z}+x)\phi_1(\tilde{z}) && (706)\\
&= \frac{f(x)}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N \tilde{z}\, \phi_1(\tilde{z}) && (707)\\
&= f(x), && (708)
\end{aligned}$$

where (700) and (707) follow from dominated convergence theorem, (702) uses Fubini theorem, (703) applies the change of variable $z := y - x$, (705) and (708) use Lemma 3.7, and (706) applies the change of variable $\tilde{z} := z/\sqrt{\varepsilon}$. □

Now, we prove that Fourier operator $\mathcal{F}$ can be defined on the entire Hilbert space $L^2(\mathbb{R}^N)$. For this purpose, we derive the following useful identity.

Lemma 3.8 (Plancherel's identity)**.** *Let $f \in \mathcal{S}(\mathbb{R}^N)$. Then:*

$$\int_{\mathbb{R}^N} d^N p\, |(\mathcal{F}f)(p)|^2 = \int_{\mathbb{R}^N} d^N x\, |f(x)|^2. \tag{709}$$

Proof. We calculate:

$$\begin{aligned}
\int_{\mathbb{R}^N} d^N p\, |(\mathcal{F}f)(p)|^2 &= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N p\int_{\mathbb{R}^N} d^N x\, e^{ipx}\overline{f(x)}(\mathcal{F}f)(p) && (710)\\
&= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} d^N x\, \overline{f(x)}\int_{\mathbb{R}^N} d^N p\, e^{ipx}(\mathcal{F}f)(p) && (711)\\
&= \int_{\mathbb{R}^N} d^N p\int_{\mathbb{R}^N} d^N x\, |f(x)|^2, && (712)
\end{aligned}$$

where (711) follows from Fubini's theorem. and (712) uses Theorem 3.4. □

Theorem 3.5. *Fourier operator $\mathcal{F} : \mathcal{S}(\mathbb{R}^N) \to \mathcal{S}(\mathbb{R}^N)$ is bounded with $\|\mathcal{F}\| = 1$.*

Proof. We calculate the norm of Fourier operator:

$$\|\mathcal{F}\| = \sup_{f\in\mathcal{S}(\mathbb{R}^N)} \sqrt{\frac{\|\mathcal{F}f\|^2_{\mathcal{S}(\mathbb{R}^N)}}{\|f\|^2_{\mathcal{S}(\mathbb{R}^N)}}} \tag{713}$$

$$= \sup_{f\in\mathcal{S}(\mathbb{R}^N)} \sqrt{\frac{\int_{\mathbb{R}^N} d^N p\, |(\mathcal{F}f)(p)|^2}{\int_{\mathbb{R}^N} d^N x\, |f(x)|^2}} \tag{714}$$

$$= 1, \tag{715}$$

where (714) follows from Lemma 3.8. □

We conclude that Fourier operator is densely defined (see Exercise 3.4) on $L^2(\mathbb{R}^N)$ and bounded. Therefore, we can uniquely extend it to the operator $\mathcal{F} : L^2(\mathbb{R}^N) \to L^2(\mathbb{R}^N)$ defined on the entire Hilbert space by virtue of Theorem 1.2 (BLT theorem). Moreover, since $\mathcal{F}^{-1}$ extends uniquely as well, and Lemma 3.8 remains valid due to continuity of norm, we conclude that $\mathcal{F}$ defined on the entire Hilbert space $L^2(\mathbb{R}^N)$ is a unitary operator.

Now, we proceed with analysis of the free Schrödinger operator (670). In order to find a suitable domain, recalling Definition 3.5, we notice that Lemma 3.5 can be connected to the notion of (inhomohogenous) Sobolev space, which we can represent as

$$H^k(\mathbb{R}^N) = \{f \in L^2(\mathbb{R}^N) | |p|^k(\mathcal{F}f)(p) \in L^2(\mathbb{R}^N)\}. \tag{716}$$

In turn, for any $f \in H^k(\mathbb{R}^N)$ and $\alpha \in \mathbb{N}_0^n$ such that $|\alpha| \le k$, we can use Fourier operator in order to define

$$\partial_\alpha f := \mathcal{F}^{-1}\Big((ip)^\alpha(\mathcal{F}f)(p)\Big). \tag{717}$$

Therefore, for any $f \in H^2(\mathbb{R}^N)$, we can represent the action of free Schrödinger operator (670) in the following form, exploiting unitarity of Fourier operator $\mathcal{F}$,

$$H_0 f = \frac{\hbar^2}{2m}\mathcal{F}^{-1}(p^2(\mathcal{F}f)(p))(x). \tag{718}$$

In other words, assuming its domain $\mathcal{D}_{H_0} = H^2(\mathbb{R}^N)$, free Schrödinger operator is unitarily equivalent to the maximally defined multiplication operator:

$$(\mathcal{F}^{-1} \circ H_0 \circ \mathcal{F})\tilde{f}(p) = \frac{\hbar^2}{2m}p^2\tilde{f}(p), \tag{719}$$

for any $\tilde{f} \in \mathcal{D}_{p^2}$, with $\mathcal{D}_{p^2} = \{\tilde{f} \in L^2(\mathbb{R}^N) | p^2\tilde{f} \in L^2(\mathbb{R}^N)\}$. On the other hand, we can state the following result for multiplication operators.

Theorem 3.6. *Let $A(x) : \mathbb{R}^N \to \mathbb{R}$ be a real measurable function, and $A : \mathcal{D}_A \to L^2(\mathbb{R}^N)$ be a real multiplication operator such that*

$$\mathcal{D}_A = \{f \in L^2(\mathbb{R}^N) | Af \in L^2(\mathbb{R}^N)\}, \tag{720}$$

$$(Af)(x) = A(x)f(x), \tag{721}$$

for any $f \in \mathcal{D}_A$. Then A is self-adjoint.

Proof. First, we notice that $\mathcal{D}_A$ is dense since any $f \in L^2(\mathbb{R}^N)$ can be constructed as a limit of a sequence $\{f_n = \chi_{\Omega_n} f \in \mathcal{D}_A\}_{n\in\mathbb{N}}$, where $\Omega_n = \{x \in \mathbb{R}^N | |A(x)| \le n\}$. Therefore, we can check whether A is a symmetric operator. Indeed, for any $h, g \in \mathcal{D}_A$, we have:

$$\langle h|Ag\rangle_{L^2(\mathbb{R}^N)} = \int_{\mathbb{R}^N} d^N x\, \overline{h(x)}A(x)g(x) \tag{722}$$

$$= \int_{\mathbb{R}^N} d^N x\, \overline{A(x)h(x)}g(x) \tag{723}$$

$$= \langle Ah|g\rangle_{L^2(\mathbb{R}^N)}. \tag{724}$$

On the other hand, if $h \in \mathcal{D}_{A^*}$, then there exists $\tilde{h} \in L^2(\mathbb{R}^N)$ such that

$$\langle h|Ag\rangle_{L^2(\mathbb{R}^N)} = \langle \tilde{h}|g\rangle_{L^2(\mathbb{R}^N)}, \tag{725}$$

for any $h \in \mathcal{D}_A$. Calculating the inner product in $L^2(\mathbb{R}^N)$, we obtain

$$\int d^N x\ \overline{(A(x)h(x) - \tilde{h}(x))} g(x) = 0. \tag{726}$$

Using $\Omega_n \nearrow \mathbb{R}^N$, we can write

$$\int d^N x\ \chi_{\Omega_n}(x)\overline{(A(x)h(x) - \tilde{h}(x))} g(x) = 0, \tag{727}$$

for any $g \in L^2(\mathbb{R}^N)$, so that $\chi_{\Omega_n}\overline{(A(x)h(x) - \tilde{h}(x))} \in L^2(\mathbb{R}^N)$ vanishes. Moreover, since n is arbitrary, we conclude that $A(x)h(x) = \tilde{h}(x) \in L^2(\mathbb{R}^N)$, so that $A^* = A$. □

Theorem 3.6 guarantees self-adjointness of the operator (719), which is unitarily equivalent to the free Schrödinger operator. Therefore, we conclude that the energy of a free particle can be associated to the operator

$$H_0:\ H^2(\mathbb{R}^N) \ \to \ L^2(\mathbb{R}^N), \tag{728}$$

$$(H_0 f)(x) \ = \ -\frac{\hbar^2}{2m}\Delta f(x). \tag{729}$$

In turn, possible values of the energy of a free particle are defined by the spectrum of H_0, which is characterized by the following Theorem.

Theorem 3.7. *The spectrum of H_0 is characterized by $\sigma(H_0) = [0, \infty)$.*

Proof. First, we notice that, since H_0 is self-adjoint, due to Theorem 2.11 (spectral theorem) there exists a PVM P_{H_0} such that

$$H_0 = \int \lambda\ dP_{H_0}(\lambda), \tag{730}$$

which, in turn, defines a real measure $\mu_h = \langle h|P_{H_0}h\rangle_{L^2(\mathbb{R}^N)}$ for any $h \in L^2(\mathbb{R}^N)$. Moreover, Theorem 2.12 suggests that μ_h can be connected to the resolvent $R_{H_0}(z)$ of H_0 via Borel transform,

$$\langle h|R_{H_0}(z)h\rangle_{L^2(\mathbb{R}^N)} = \int_{\mathbb{R}} \frac{d\mu_h(\lambda)}{\lambda - z}. \tag{731}$$

On the other hand, the inner product $\langle h|R_{H_0}(z)h\rangle_{L^2(\mathbb{R}^N)}$ can be calculated directly using the properties of H_0:

$$\langle h|R_{H_0}(z)h\rangle_{L^2(\mathbb{R}^N)} \ = \ \langle \mathcal{F}h|R_{p^2}(z)\mathcal{F}h\rangle_{L^2(\mathbb{R}^N)} \tag{732}$$

$$= \ \int_{\mathbb{R}^N} d^N p\ \frac{|(\mathcal{F}h)(p)|^2}{p^2 - z} \tag{733}$$

$$= \ \int_0^\infty dr\ \frac{r^{N-1}}{r^2 - z} \int_{S^{n-1}} d^{N-1}\omega\ |(\mathcal{F}h)(r\omega)|^2 \tag{734}$$

$$= \ \int_{\mathbb{R}} \frac{\chi_{[0,\infty)} r^{N-1}}{r^2 - z} \int_{S^{n-1}} d^{N-1}\omega\ |(\mathcal{F}h)(r\omega)|^2, \tag{735}$$

where (732) follows from Lemma 3.8, and (733) uses Definition 2.18 providing the spectral decomposition of the multiplication operator p^2 and Definition 2.13. Finally, performing change of variable $\lambda := \sqrt{p}$, we obtain:

$$\langle h|R_{H_0}(z)h\rangle_{L^2(\mathbb{R}^N)} = \frac{1}{2}\int_{\mathbb{R}} d\lambda\ \frac{\chi_{[0,\infty)} \lambda^{N/2-1}}{\lambda - z} \int_{S^{n-1}} d^{N-1}\omega\ |(\mathcal{F}h)(\sqrt{\lambda}\omega)|^2, \tag{736}$$

concluding that

$$d\mu_h = \frac{d\lambda}{2} \frac{\chi_{[0,\infty)}\lambda^{N/2-1}}{\lambda - z} \int_{S^{n-1}} d^{N-1}\omega \; |(\mathcal{F}h)(\sqrt{\lambda}\omega)|^2, \tag{737}$$

which is absolutely continuous with respect to Lebesgue measure and supported on $[0, \infty)$, which corresponds to the spectrum of H_0. □

Theorem 3.7 suggests that H_0 has a continuous spectrum, which covers the entire real half-line. This means that a free quantum particle can take any positive value of energy.

3.4 Schrödinger operators with a potential

Being at the basis of quantum mechanics, free Schrödinger operator (670) represents a highly important example of Schrödinger operators introduced in Definition 3.1. Nevertheless, in most practical applications, the physical system is subject to a certain potential, which is modelled by a non-trivial multiplication operator $\mathcal{V}$. However, analysis of the corresponding Schrödinger operator

$$H = H_0 + \mathcal{V}, \tag{738}$$

is, generally speaking, a complicated problem. In quantum mechanics, apart from several particular models, e.g., harmonic oscillator (described by $V(x) = kx^2/2$, where k is the force constant) and hydrogen atom (described by $V(r) = -e/r$ in $\mathbb{R}^3$, where e is the charge of electron in Gaussian units, and spherical coordinates are used), (738) is analyzed using approximation methods (e.g., asymptotic series) by treating $\mathcal{V}$ as a so-called perturbation of the free Schrödinger operator. This implies that the former is "smaller" in a certain sense than H_0. In order to formalize this, we provide first a new definition that extends the notion of boundedness proposed in Definition 1.7 and introduces the notion of relative boundedness.

Definition 3.9. *Let $A : \mathcal{D}_A \to \mathcal{H}$ and $B : \mathcal{D}_B \to \mathcal{H}$ be operators. B is called A-**bounded** if $\mathcal{D}_A \subseteq \mathcal{D}_B$ and there exist $a, b \geq 0$ such that for any $h \in \mathcal{D}_A$*

$$\|Bh\|_{\mathcal{H}} \leq a\|Ah\|_{\mathcal{H}} + b\|h\|_{\mathcal{H}}, \tag{739}$$

and the value

$$\mathbf{B}_A = \inf_{\substack{\exists b \geq 0:\, \forall h \in \mathcal{H} \\ \|Bh\|_{\mathcal{H}} \leq a\|Ah\|_{\mathcal{H}} + b\|h\|_{\mathcal{H}}}} (a) \tag{740}$$

*is called A-**bound** of B.*

Lemma 3.9. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a closed operator with $\rho(A) \neq \emptyset$, and $B : \mathcal{D}_B \to \mathcal{H}$ be closable. Then B is A-bounded if and only if $BR_A(z)$ is a bounded operator for some $z \in \rho(A)$. The A-bound of B is given by:*

$$\mathbf{B}_A \leq \inf_{z \in \rho(A)} \|BR_A(z)\|. \tag{741}$$

Proof. In what follows, we proceed in two steps for both directions.

Step 1 ($\Rightarrow$). Let B be a closable A-bounded operator. Then, by Definition 3.9, $\mathcal{D}_A \subseteq \mathcal{D}_B$. On the other hand, let A be a closed operator, and $z \in \rho(A)$. Then $BR_A(z)$ is a closed operator *(exercise!)* defined on entire Hilbert space $\mathcal{H}$. Recalling Theorem 2.7, we conclude that $BR_A(z)$ is bounded.

Step 2 ($\Leftarrow$). Let $h \in \mathcal{D}_A$ and $z \in \rho(A)$, for which $BR_A(z)$ is bounded. Then

$$\begin{aligned} \|Bh\|_{\mathcal{H}} &= \|BR_A(z)(A - z)h\|_{\mathcal{H}} && (742) \\ &\leq \|BR_A(z)\|\|(A - z)h\|_{\mathcal{H}} && (743) \\ &:= a\|(A - z)h\|_{\mathcal{H}} && (744) \\ &\leq a\|Ah\|_{\mathcal{H}} + a|z|\|h\|_{\mathcal{H}}. && (745) \end{aligned}$$

By Definition 3.9, the A-bound of B is given by the lower bound on a such that (745) is satisfied. On the other hand, Lemma 2.9 suggests that, if $BR_A(z)$ is bounded for some $z \in \rho(A)$, it is bounded for any $z \in \rho(A)$. Therefore,

$$\mathbf{B}_A \leq \inf_{z\in\rho(A)} a \tag{746}$$

$$= \inf_{z\in\rho(A)} \|BR_A(z)\|. \tag{747}$$

□

Definition 3.10. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a symmetric operator. It is called* ***bounded from below*** *if the exists $\gamma \in \mathbb{R}$ such that*

$$\langle h|Ah\rangle_{\mathcal{H}} \geq \gamma\|h\|^2_{\mathcal{H}} \tag{748}$$

for any $h \in \mathcal{D}_A$.

Lemma 3.10. *Let $A : \mathcal{D}_A \to \mathcal{H}$ be a self-adjoint operator, and $B : \mathcal{D}_B \to \mathcal{H}$ be A-bounded. Then the A-bound of B is given by*

$$\mathbf{B}_A = \lim_{\lambda\to\infty} \|BR_A(\pm i\lambda)\|, \tag{749}$$

or, if A is bounded from below, equivalently,

$$\mathbf{B}_A = \lim_{\lambda\to\infty} \|BR_A(-\lambda)\|. \tag{750}$$

Proof. We proceed in two steps.

Step 1. First, we notice that A is a self-adjoint operator, so that $\mathbb{C} \setminus \mathbb{R} \subseteq \rho(A)$ due to Theorem 2.8, and the resolvent $R_A(\pm i\lambda)$ is well-defined for any $\lambda > 0$. Let $h \in \mathcal{H}$ and $g = BR_A(\pm i\lambda)h$ for some $\lambda > 0$. Since B is A-bounded, by Definition 3.9, there exist $a, b \geq 0$ such that:

$$\|BR_A(\pm i\lambda)h\|_{\mathcal{H}} \leq a\|AR_A(\pm i\lambda)h\|_{\mathcal{H}} + b\|R_A(\pm i\lambda)h\|_{\mathcal{H}} \tag{751}$$

$$= a\Big\|\Big(\int \frac{\lambda'}{\pm i\lambda + \lambda'} dP(\lambda')\Big)h\Big\|_{\mathcal{H}} + b\Big\|\Big(\int \frac{1}{\pm i\lambda + \lambda'} dP(\lambda')\Big)h\|_{\mathcal{H}} \tag{752}$$

$$\leq \Big(a \sup_{\lambda'\in\sigma(A)}\Big|\frac{\lambda'}{\pm i\lambda + \lambda'}\Big| + b \sup_{\lambda'\in\sigma(A)}\Big|\frac{1}{\pm i\lambda + \lambda'}\Big|\Big)\|h\|_{\mathcal{H}} \tag{753}$$

$$\leq \Big(a + \frac{b}{\lambda}\Big)\|h\|_{\mathcal{H}}, \tag{754}$$

where (752) uses Definition 2.18 and Theorem 2.11 (spectral theorem) and (753) follows from (441). Therefore, taking into account the expression (739) for the relative bound, we conclude that

$$\limsup_\lambda \|BR_A(\pm i\lambda)\| \leq \mathbf{B}_A. \tag{755}$$

On the other hand, Lemma 3.9 suggests that $\mathbf{B}_A \leq \inf_\lambda \|BR_A(\pm i\lambda)\|$. Therefore, we conclude that (749) is true.

Step 2. If A is bounded from below by γ, Theorem 2.11 (spectral theorem) suggests that for any $\lambda > 0$, $-\lambda \in \rho(A)$ if $-\lambda < \gamma$, and the resolvent $R_A(-\lambda)$ is well-defined for the corresponding values of λ. Let $h \in \mathcal{H}$ and $g = BR_A(-\lambda)h$ for some $-\lambda < \gamma$. Since B is A-bounded, by Definition 3.9, there exist $a, b \geq 0$ such that:

$$\|BR_A(-\lambda)h\|_{\mathcal{H}} \leq a\|AR_A(-\lambda)h\|_{\mathcal{H}} + b\|R_A(-\lambda)h\|_{\mathcal{H}} \tag{756}$$

$$= a\Big\|\Big(\int \frac{\lambda'}{\lambda + \lambda'} dP(\lambda')\Big)h\Big\|_{\mathcal{H}} + b\Big\|\Big(\int \frac{1}{\lambda + \lambda'} dP(\lambda')\Big)h\|_{\mathcal{H}} \tag{757}$$

$$\leq \Big(a \sup_{\lambda'\in\sigma(A)}\Big|\frac{\lambda'}{\lambda + \lambda'}\Big| + b \sup_{\lambda'\in\sigma(A)}\Big|\frac{1}{\lambda + \lambda'}\Big|\Big)\|h\|_{\mathcal{H}} \tag{758}$$

$$\leq \Big(a \max\Big(1, \frac{|\gamma|}{\lambda + \gamma}\Big) + \frac{b}{\lambda + \gamma}\Big)\|h\|_{\mathcal{H}}, \tag{759}$$

where (757) uses Definition 2.18 and Theorem 2.11 (spectral theorem), (758) follows from (441), and (759) takes into account that the lower bound of the spectrum of A is given by γ due to Definition 3.10. Therefore, we conclude that (750) is true. □

Definition 3.9 allows us to formalize "smallness" of the operator $\mathcal{V}$ in (738) with respect to free Schrödinger operator H_0 as smallness of its H_0-bound $\mathbf{V}_{H_0}$. Self-adjointness of the Schrödinger operator (738) in this case is guaranteed by the following important result based on Lemma 3.10.

Theorem 3.8 (Kato-Rellich theorem). *Let $A : \mathcal{D}_A \to \mathcal{H}$ be (essentially) self-adjoint operator, and $B : \mathcal{D}_B \to \mathcal{H}$ be a symmetric A-bounded operator with $\mathbf{B}_A < 1$. Then $A + B$ with $\mathcal{D}_{A+B} = \mathcal{D}_A$ is (essentially) self-adjoint. If A is bounded from below by γ, then $A + B$ is bounded from below by*

$$\gamma - \max\Big(a|\gamma| + b, \frac{b}{1-a}\Big). \tag{760}$$

Proof. We proceed in two steps.

Step 1. We start by noticing that if B is A-bounded due to Definition 3.9, then the graph norm of A (as introduced in Definition 2.5) dominates the one of B as well as $A + B$. Therefore, $\mathcal{D}_{\overline{A}} \subseteq \mathcal{D}_{\overline{B}}$ and $\mathcal{D}_{\overline{A}} \subseteq \mathcal{D}_{\overline{A+B}}$. Therefore, without loss of generality, we can assume that the (essentially self-adjoint by assumption of the Theorem) operator A is closed and, thus, self-adjoint. On the other hand, since $\mathbf{B}_A < 1$, Lemma 3.10 suggests that there exists $\lambda > 0$ such that $\|BR_A(\mp i\lambda)\| < 1$. Since $BR_A(\mp i\lambda)$ is bounded, there exists a Neumann series which converges to $R_{BR_A(\mp i\lambda)}(z')$ for any $z' \in \mathbb{C}$ such that $|z'| > \|BR_A(\mp i\lambda)\|$, so that $z' \in \rho(BR_A(\mp i\lambda))$[13]. Therefore, we conclude that $-1 \in \rho(BR_A(\mp i\lambda))$. Hence, by Definition 2.10, the operator $BR_A(\mp i\lambda) + \mathrm{id}$ is bijective, so that

$$\mathrm{ran}(BR_A(\mp i\lambda) + \mathrm{id}) = \mathcal{H}, \tag{761}$$

since $R_A(\mp i\lambda)$ is defined on entire $\mathcal{H}$. On the other hand, we have

$$A + B \pm i\lambda\,\mathrm{id} = (BR_A(\mp i\lambda) + \mathrm{id})(A \pm i\lambda\,\mathrm{id}). \tag{762}$$

Therefore, we conclude that

$$\mathrm{ran}(A + B \pm i\lambda\,\mathrm{id}) = \mathcal{H}. \tag{763}$$

Recalling the sufficient criterion of self-adjointness provided by Theorem 2.1, we find that the operator $A + B$ is self-adjoint.

Step 2. Let us assume that A is bounded from below by γ. Then Theorem 2.11 (spectral theorem) suggests that for any $\lambda > 0$, $-\lambda \in \rho(A)$ if $-\lambda < \gamma$, and the resolvent $R_A(-\lambda)$ is well-defined for the corresponding values of λ. On the other hand, since $\mathbf{B}_A < 1$, Lemma 3.10 suggests that there exists $\lambda > 0$ such that $\|BR_A(-\lambda)\| < 1$. Taking into account the estimation given by (759), we choose such λ that

$$a\max\Big(1, \frac{|\gamma|}{\lambda+\gamma}\Big) + \frac{b}{\lambda+\gamma} < 1. \tag{764}$$

Solving (764) with respect to λ, we obtain

$$-\lambda < \gamma - \max\Big(a|\gamma| + b, \frac{b}{1-a}\Big). \tag{765}$$

Therefore, $-\lambda \in \rho(A + B)$ if it satisfies (765), hence, proving the estimate (760). □

As an example of application of Theorem 3.8 to Schrödinger operators (738), we consider a compact interval $I = [0, 2\pi]$ as a toy model of physical space, which has been already used to analyze the momentum operator (598)–(599). Recalling its physical interpretation (a quantum particle moving

[13] See Theorem 2.16 in [1] (Theorem 2.15 in the first edition of [1]).

along the bottom of a well), let us consider a self-adjoint free Schrödinger operator $H_0 : \mathcal{D}_{H_0} \to L^2(0, 2\pi)$ with

$$\mathcal{D}_{H_0} = \{f \in H^2[0, 2\pi] | f(0) = f(2\pi) = 0\}, \tag{766}$$

and the multiplication operator $\mathcal{V} : \mathcal{D}_\mathcal{V} \to L^2(0, 2\pi)$ with respect to some real-valued measurable function $V(x)$. Since any $f \in \mathcal{D}_{H_0}$ is continuous and bounded, we conclude that $\mathcal{D}_{H_0} \subset \mathcal{D}_\mathcal{V}$ if $V(x) \in L^2(0, 2\pi)$, and $\mathcal{V}$ is H_0-bounded.

Exercise 3.5. *Show that any $f \in \mathcal{D}_{H_0}$ satisfies*

$$\|f\|_\infty^2 \leq \frac{\varepsilon}{2}\|f''\|^2_{L^2(0,2\pi)} + \frac{1}{2\varepsilon}\|f\|^2_{L^2(0,2\pi)} \tag{767}$$

for any $\varepsilon > 0$.

Since (767) is satisfied for any $\varepsilon > 0$, recalling Definition 3.9, we find that any $\mathcal{V}$ with respect to $V(x) \in L^2(0, 2\pi)$ is H_0-bounded, and, moreover, $\mathbf{V}_{H_0} = 0$. This allows us to treat $\mathcal{V}$ as a perturbation of H_0, and Theorem 3.8 suggests that the corresponding Schrödinger operator (738) is self-adjoint, hence, representing a physical observable.

4 Applications of nonstandard analysis to operator theory

Nonstandard analysis (NSA) was invented by the logician Abraham Robinson in 1960s. In a nutshell, NSA seeks to provide a rigorous treatment of calculus and classical analysis and use infinitesimal and infinite quantities as numbers, hence, avoiding the $\varepsilon - \delta$ language and referring to the original views of Newton and Leibniz. Interestingly, the NSA-like view on infinitesimals can be found in a plenty of beginner texts on physics (e.g., classical mechanics and electrodynamics) that use differentials interpreting them as "very small" quantities. While NSA is not the only approach to non-Archimedean mathematics (among alternative approaches one can name, e.g., Colombeau's algebras and p-adic number system), it has been extensively studied after its introduction and found a plethora of applications in mathematics (e.g., in stochastics and combinatorics) as well as physics. In what follows, we briefly focus on applications of NSA in operator theory and Schrödinger operators.

4.1 Non-Archimedean fields and construction of hyperreals

We start the discussion on applications of NSA to operator theory by introduction of its fundamental objects, the fields of hyperreal numbers which include infinitely small (infinitesimal) and large (infinite) elements. Obviously, they do not carry the Archimedean property satisfied by the field $\mathbb{R}$ of real numbers, which can be stated in the following way: for any $x, y \in \mathbb{R}$, there exists a positive integer number n such that $nx > y$. Therefore, in order to describe the properties of hyperreals, we have to formalize first the notion of non-Archimedean fields, which is provided by the following Definitions.

Definition 4.1. *Let $(\mathbb{K}, +, \cdot)$ be a field. It is called **ordered** if there exists a set $\mathbb{K}^+ \subset \mathbb{K}$ such that it is closed under the binary operations of $\mathbb{K}$,*

$$\forall x, y \in \mathbb{K}^+ : \; x + y \in \mathbb{K}^+, \; x \cdot y \in \mathbb{K}^+, \tag{768}$$

and $\mathbb{K} = \mathbb{K}^+ \sqcup \{0\} \sqcup \mathbb{K}^-$, where $\mathbb{K}^- = \{x \in \mathbb{K} | -x \in \mathbb{K}^+\}$ and $\sqcup$ denotes disjoint union. The corresponding order relation is defined as:

$$\forall x, y \in \mathbb{K} : \; x < y \Leftrightarrow y - x \in \mathbb{K}^+. \tag{769}$$

Definition 4.2. *Let $\mathbb{K}$ be an ordered field. An element $\xi \in \mathbb{K}$ is called:*

- ***infinitesimal*** *if $|\xi| < \frac{1}{n}$ for any $n \in \mathbb{N}$,*

- ***finite*** *if there exists* $n \in \mathbb{N}$ *such that* $|\xi| < n$*,*
- ***infinite*** *if* $|\xi| > n$ *for any* $n \in \mathbb{N}$*.*

Definition 4.3. *Let* $\mathbb{K}$ *be an ordered field. It is called* ***non-Archimedean*** *if there exists an infinite* $\xi \in \mathbb{K}$*.*

In any non-Archimedean field, it is possible to introduce an equivalence relation with respect to its elements separated by an infinitesimal.

Definition 4.4. *Let* $\mathbb{K}$ *be a non-Archimedean field. Elements* $\xi, \zeta \in \mathbb{K}$ *are called* ***infinitely close*** *if* $\xi - \zeta$ *is infinitesimal, denoted* $\xi \sim \zeta$*.*

Exercise 4.1. *Prove that* $\sim$ *is an equivalence relation.*

Definition 4.5. *Let* $\mathbb{K}$ *be a non-Archimedean field, and* $\xi \in \mathbb{K}$*. The* ***monad*** *of* ξ *is the set of all elements of* $\mathbb{K}$ *infinitely close to it,*

$$\mathfrak{mon}(\xi) = \{\zeta \in \mathbb{K} | \zeta \sim \xi\}, \tag{770}$$

and the ***galaxy*** *of* ξ *is the set*

$$\mathfrak{gal}(\xi) = \{\zeta \in \mathbb{K} | \zeta - \xi \text{ is finite}\}. \tag{771}$$

Theorem 4.1. *Let* $\mathbb{K} \supseteq \mathbb{R}$ *be an ordered field, and* $\xi \in \mathbb{K}$ *is finite. Then there exists a unique* $r \in \mathbb{R}$ *such that* $\xi \sim r$*. It defines the function* $\mathrm{st} : \mathfrak{gal}(0) \to \mathbb{R}$ *called* ***standard part*** *such that* $\mathrm{st}(\xi) = r$*.*

Proof. Let $\xi \in \mathbb{K}$ be finite, and

$$A \quad = \quad \{a \in \mathbb{R} | a < \xi\}. \tag{772}$$

Since ξ is finite, there exist $s, s' \in \mathbb{R}$ such that $s < \xi < s'$. Therefore, $A \neq \emptyset$ and is bounded by s' from above. Taking into account completeness of $\mathbb{R}$, we conclude that there exists a least upper bound $r \in \mathbb{R}$ of A. Now, let $\delta \in \mathbb{R}^+$. Since r is an upper bound of A, we have $r + \delta \notin A$, and $\xi \leq r + \delta$. On the other hand, if $\xi \leq r - \delta$, then $r - \delta$ is an upper bound of A contradicting the fact that r is a least upper bound of A. Hence, we conclude that $r - \delta < \xi \leq r + \delta$ and, in turn, $|\xi - r| \leq \delta$ for any $\delta \in \mathbb{R}^+$. Hence, $\xi - r$ is infinitesimal, so that $\xi \sim r$ by Definition 4.4. Uniqueness of r follows from transitivity of $\sim$ as equivalence relation (Exercise 4.1): let $r' \in \mathbb{R}$ such that $\xi \sim r'$. Therefore, $r \sim r'$, so that $r = r'$ since both are elements of $\mathbb{R}$. □

Corollary 4.1. *Let* $\mathbb{K} \supset \mathbb{R}$ *be an ordered field. Then it is non-Archimedean.*

Proof. Let $\xi \in \mathbb{K} \setminus \mathbb{R}$. If ξ is infinite, then $\mathbb{K}$ is non-Archimedean by Definition 4.3. Otherwise, if ξ is finite, we define an element $\zeta \in \mathbb{K}$ such that

$$\zeta = (\xi - \mathrm{st}(\xi))^{-1}, \tag{773}$$

which is infinite. Therefore, $\mathbb{K}$ is non-Archimedean by Definition 4.3. □

Now we proceed with explicit construction of a hyperreal field out of $\mathbb{R}$. The usual way to construct a hyperreal field in NSA is the **ultrapower construction** which starts with a ring $(\mathbb{R}^\mathbb{N}, +, \cdot)$ of sequences on $\mathbb{R}$. In turn, one defines equivalence classes on $\mathbb{R}^\mathbb{N}$ such that each class consists of sequences that are equal "almost everywhere". In order to formalize this "almost everywhere"-agreement of sequences, one needs to define what are "large" subsets of $\mathbb{N}$, so that agreement of sequences on these subsets can be interpreted as an "almost everywhere"-agreement. Intuitively, any set that contains a large set should be large itself, an intersection of two large sets should be large as well, and a complement of a large set should be "small". These conditions are fulfilled by involving the notion of ultrafilter, the definition whereof requires to provide first the definition of filter.

Definition 4.6. *Let X be a non-empty set. A non-empty set $\mathcal{F} \subseteq 2^X$ is called* ***filter*** *if it satisfies the following conditions.*

1. *Let $A \in \mathcal{F}$ and $B \in \mathcal{F}$. Then $A \cap B \in \mathcal{F}$.*

2. *Let $A \in \mathcal{F}$ and $A \subseteq B$. Then $B \in \mathcal{F}$.*

3. *$\emptyset \notin \mathcal{F}$.*

If $\mathcal{F} \neq 2^X$, it is called ***proper filter****.*

Definition 4.7. *Let $\mathcal{U} \subset 2^S$ be a proper filter on a set S. It is called* ***ultrafilter*** *if, for any $A \in 2^S$, either $A \in \mathcal{U}$ or $A^c \in \mathcal{U}$.*

Lemma 4.1. *Let $\mathcal{U} \subset 2^S$ be a proper filter on a set S. It is an ultrafilter if and only if it cannot be extended to a larger proper filter on S.*

Proof. We proceed with proof of the theorem in both directions.

Step 1 ($\Rightarrow$). Let $\mathcal{U} \subset 2^S$ be an ultrafilter on S, which can be extended to a collection $\mathcal{U}_A \subset 2^S$ such that it includes some $A \subseteq S$ which does not belong to $\mathcal{U}$. By Definition 4.7, $A^c \in \mathcal{U}$, hence, both $A, A^c \in \mathcal{U}_A$. However, $A \cap A^c = \emptyset$, violating property 3 of Definition 4.6. Therefore, $\mathcal{U}_A$ is not a filter, and, since A is arbitrary, $\mathcal{U}$ cannot be extended to a larger proper filter on S.

Step 2. ($\Leftarrow$). Let $\mathcal{F} \subset 2^S$ be a filter on S, which is not an ultrafilter. Therefore, recalling Definition 4.7, $\exists A \subseteq S$ such that $A \notin \mathcal{F}$ and $A^c \notin \mathcal{F}$. Now, let $B, \tilde{B} \in \mathcal{F}$ be elements of the filter such that $B \cap A = \emptyset$ and $\tilde{B} \cap A^c = \emptyset$. Therefore, $B \subseteq A^c$ and $\tilde{B} \subseteq A$. By property 2 of Definition 4.6 this means that $A \in \mathcal{F}$ as well as $A^c \in \mathcal{F}$. This contradicts the fact that A does not belong to the filter, and we conclude that, for any $B \in \mathcal{F}$, $A \cap B \neq \emptyset$ or $A^c \cap B \neq \emptyset$. This means that $A \cup \mathcal{F}$ or $A^c \cup \mathcal{F}$ fulfill *finite intersection property*: for any finite nonempty collection $\{F_i\}_{i=1}^n$, $n \in \mathbb{N}$ of subsets $F_i \in A \cup \mathcal{F}$ or subsets $F_i \in A^c \cup \mathcal{F}$, the condition

$$\bigcap_{i=1}^{n} F_i \neq \emptyset \tag{774}$$

is satisfied. Then, denoting $\mathcal{C} = A \cup \mathcal{F}$ or $\mathcal{C} = A^c \cup \mathcal{F}$, respectively, we build a collection of sets

$$\mathcal{F}^{\mathcal{C}} = \{F \subseteq S | F \supseteq F_1 \cap \cdots \cap F_n \text{ for some } n \in \mathbb{N} \text{ and some } C_i \in \mathcal{C}, i = \ \dots, n\}. \tag{775}$$

First, it is obvious that $\mathcal{C} \in \mathcal{F}^{\mathcal{C}}$. On the other hand, (774) suggests that $\emptyset \notin \mathcal{F}^{\mathcal{C}}$. Now, let $A, A' \in \mathcal{F}^{\mathcal{C}}$, so that, for some $n, n' \in \mathbb{N}$ there exist collections $\{C_i\}_{i=1}^n$ and $\{C'_i\}_{i=1}^{n'}$ of sets in $\mathcal{C}$ such that $A \supseteq C_1 \cap \ldots \cap C_n$ and $A' \supseteq C'_1 \cap \ldots \cap C'_{n'}$. Therefore, $A \cap A' \supseteq C_1 \cap \ldots \cap C_n \cap C'_1 \cap \ldots \cap C'_{n'}$ and, in turn, $A \cap A' \in \mathcal{F}^{\mathcal{C}}$. Finally, let $A \subseteq B$ for some $B \subseteq S$. This means that $B \supset C_1 \cap \ldots \cap C_n$ and, hence, $B \in \mathcal{F}^{\mathcal{C}}$. Therefore, recalling Definition 4.6, we conclude that $\mathcal{F}^{\mathcal{C}}$ is a filter, which properly includes $A \cup \mathcal{F}$ or $A^c \cup \mathcal{F}$, so that $\mathcal{F}$ cannot be maximal. □

Exercise 4.2. *Let S be an infinite set. Show that the Fréchet filter*

$$\mathcal{F}_{\text{co}} = \{A \subseteq S | A^c \textit{ is finite}\} \tag{776}$$

formed by cofinite subsets of S is a proper filter but not an ultrafilter.

Definition 4.8. *Let $\mathcal{U} \subset 2^S$ be an ultrafilter on a set S. It is called* ***non-principal ultrafilter*** *if there exists no $a \in S$ such that $\mathcal{U} = \mathcal{U}^a$, where*

$$\mathcal{U}^a = \{A \subseteq S | a \in A\}. \tag{777}$$

$\mathcal{U}^a$ is called ***principal filter*** *generated by $a \in S$.*

Theorem 4.2. *Let S be an infinite set. Then there exists a non-principal ultrafilter $\mathcal{U} \subset 2^S$.*

Proof. Since S is an infinite set, the Frechét filter (776) can be constructed on it. In turn, the Frechét filter $\mathcal{F}_{\text{co}}$ carries the finite intersection property, i.e., for any finite nonempty collection $\{F_i\}_{i=1}^n$, $n \in \mathbb{N}$ of subsets $F_i \in \mathcal{F}_{\text{co}}$, the condition

$$\bigcap_{i=1}^{n} F_i \neq \emptyset \tag{778}$$

is satisfied. Let us define a collection of filters

$$\mathcal{C} = \{\mathcal{F} \subset 2^S | \mathcal{F}_{\text{co}} \subseteq \mathcal{F},\ \mathcal{F} \text{ is a filter}\}, \tag{779}$$

which is partially ordered by inclusion, and let $\mathcal{C}_t \subseteq \mathcal{C}$ be a totally ordered subcollection. This means that, for any $\mathcal{F}_1, \mathcal{F}_2 \in \mathcal{C}_t$, we have $A_1, A_2 \in \mathcal{F}_1$ or $A_1, A_2 \in \mathcal{F}_2$ for any $A_1 \in \mathcal{F}_1$ and $A_2 \in \mathcal{F}_2$. Therefore, $A_1 \cap A_2 \in \mathcal{F}_1 \cup \mathcal{F}_2$ by property 1 of Definition 4.6. In turn, $A_1 \cap A_2 \in \bigcup_{\mathcal{F} \in \mathcal{C}_t} \mathcal{F} \subseteq \bigcup_{\mathcal{F} \in \mathcal{C}} \mathcal{F}$. Moreover, any $A \in \bigcup_{\mathcal{F} \in \mathcal{C}} \mathcal{F}$ belongs to some filter $\mathcal{F}' \in \mathcal{C}_t$, so that any $B \supseteq A$ fulfills $B \in \mathcal{F}'$ due to property 2 of Definition 4.6 and, in turn, $B \in \bigcup_{\mathcal{F} \in \mathcal{C}} \mathcal{F}$. Finally, since $\emptyset \notin \mathcal{F}$ for any $\mathcal{F} \in \mathcal{C}_t$, we have that $\emptyset \notin \bigcup_{\mathcal{F} \in \mathcal{C}} \mathcal{F}$ and conclude that, for any totally ordered subcollection $\mathcal{C}_t \subseteq \mathcal{C}$, $\bigcup_{\mathcal{F} \in \mathcal{C}} \mathcal{F}$ is a filter by Definition 4.6 and an element of $\mathcal{C}$. Therefore, any $\mathcal{C}_t$ has an upper bound in $\mathcal{C}$, so that $\mathcal{C}$ has a maximal element $\mathcal{U} \in \mathcal{C}$ by Zorn's lemma[14]. Now, let $A \subset S$ such that $A \notin \mathcal{U}$, and suppose that $\mathcal{U}$ can be extended to a filter $\mathcal{F}^A$, so that $\mathcal{A} \in \mathcal{F}^A$. Therefore, $\mathcal{F}_{\text{co}} \subseteq \mathcal{U} \subset \mathcal{F}^A$, and $\mathcal{F}^A \in \mathcal{C}$, contradicting the fact that $\mathcal{U}$ is a maximal element of $\mathcal{C}$. Hence, $\mathcal{U}$ is a maximal filter and, by Lemma 4.1, an ultrafilter on S, and the Frechét filter $\mathcal{F}_{\text{co}}$ is included in it. On the other hand, for any $a \in S$, $S \setminus \{a\} \in \mathcal{F}_{\text{co}}$ and, thus, $S \setminus \{a\} \in \mathcal{U}$. Therefore, for any $a \in S$, $\mathcal{U}$ includes subsets of S which do not contain a, so that, recalling Definition 4.8, $\mathcal{U}$ is a non-principal ultrafilter. □

Theorem 4.2 is an important tool which guarantees that there exists a non-principal ultrafilter $\mathcal{U}$ on $\mathbb{N}$, which can be used to construct hyperreals as a quotient set of $\mathbb{R}^{\mathbb{N}}$ by introducing the following relation.

Definition 4.9. *Let $\mathcal{U} \subset 2^{\mathbb{N}}$ be a non-principal ultrafilter on $\mathbb{N}$, and $\{r_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$ and $\{r'_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$ be sequences on $\mathbb{R}$. They* ***agree almost everywhere modulo $\mathcal{U}$*** *or* ***agree $\mathcal{U}$-eventually*** *if*

$$\{n \in \mathbb{N} | r_n = r'_n\} \in \mathcal{U}, \tag{780}$$

denoted $\{r_n\} \equiv \{r'_n\}$.

Exercise 4.3. *Prove that $\equiv$ is an equivalence relation and congruence on $(\mathbb{R}^{\mathbb{N}}, +, \cdot)$.*

Definition 4.10. *A* ***hyperreal field*** *${}^*\mathbb{R}$ is a quotient set $\mathbb{R}^{\mathbb{N}}/\equiv$.*

Therefore, a hyperreal field ${}^*\mathbb{R}$ constructed in this manner consists of equivalence classes $[a_n] = \{\{b_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}} : \{b_n\} \equiv \{a_n\}\}$. It is naturally equipped with well-defined binary operations

$$+ : \quad [a_n], [b_n] \mapsto [a_n] + [b_n] = [a_n + b_n], \tag{781}$$

$$\cdot : \quad [a_n], [b_n] \mapsto [a_n] \cdot [b_n] = [a_n \cdot b_n]. \tag{782}$$

Indeed, let us take sequences $\{r_n\}_{n\in\mathbb{N}}, \{r'_n\}_{n\in\mathbb{N}}, \{s_n\}_{n\in\mathbb{N}}, \{s'_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$ such that $\{r_n\} \equiv \{r'_n\}$ and $\{s_n\} \equiv \{s'_n\}$. Then, considering $\{r_n + s_n\}_{n\in\mathbb{N}}$ and $\{r'_n + s'_n\}_{n\in\mathbb{N}}$, we find that $\{n \in \mathbb{N} | r_n + s_n = r'_n + s'_n\} \subseteq \{n \in \mathbb{N} | r_n = r'_n\} \cap \{n \in \mathbb{N} | s_n = s'_n\} \in \mathcal{U}$ due to property 1 of Definition 4.6. Similarly, for $\{r_n \cdot s_n\}_{n\in\mathbb{N}}$ and $\{r'_n \cdot s'_n\}_{n\in\mathbb{N}}$, we have $\{n \in \mathbb{N} | r_n \cdot s_n = r'_n \cdot s'_n\} \subseteq \{n \in \mathbb{N} | r_n = r'_n\} \cap \{n \in \mathbb{N} | s_n = s'_n\} \in \mathcal{U}$. Similarly, it is possible to equip ${}^*\mathbb{R}$ with a partial order relation

$$[a_n] < [b_n] \Leftrightarrow \{n \in \mathbb{N} | a_n < b_n\} \in \mathcal{U}. \tag{783}$$

[14] Recall that Zorn's lemma is equivalent to the axiom of choice and states the following: any partially ordered set $\mathcal{C}$ such that any its totally ordered subset $\mathcal{C}_t \subseteq \mathcal{C}$ has an upper bound in $\mathcal{C}$, necessarily contains at least one maximal element.

Indeed, considering again the sequences $\{r_n\}_{n\in\mathbb{N}}, \{r'_n\}_{n\in\mathbb{N}}, \{s_n\}_{n\in\mathbb{N}}, \{s'_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$, we find $\{n \in \mathbb{N}|r_n < s_n\} \supseteq \{n \in \mathbb{N}|r_n = r'_n\} \cap \{n \in \mathbb{N}|s_n = s'_n\} \cap \{n \in \mathbb{N}|r'_n = s'_n\}$ and $\{n \in \mathbb{N}|r'_n < s'_n\} \supseteq \{n \in \mathbb{N}|r_n = r'_n\} \cap \{n \in \mathbb{N}|s_n = s'_n\} \cap \{n \in \mathbb{N}|r_n = s_n\}$. Therefore, $\{n \in \mathbb{N}|r_n < s_n\} \in \mathcal{U}$ if and only if $\{n \in \mathbb{N}|r'_n < s'_n\} \in \mathcal{U}$.

The field $\mathbb{R}$ of real numbers is naturally embedded to $^*\mathbb{R}$ by the mapping $* : \mathbb{R} \hookrightarrow {}^*\mathbb{R}$ that acts as

$$^* :\ r \mapsto {}^*r = [\{r_n|\forall n \in \mathbb{N} :\ r_n = r\}_{n\in\mathbb{N}}] := [r]. \tag{784}$$

In order to provide examples of nonstandard numbers, i.e. elements of $^*\mathbb{R}\backslash\mathbb{R}$, we consider two sequences

$$\{\varepsilon_n\}_{n\in\mathbb{N}} = \left\{\frac{1}{n}\right\}_{n\in\mathbb{N}}, \tag{785}$$

$$\{\omega_n\}_{n\in\mathbb{N}} = \{n\}_{n\in\mathbb{N}}. \tag{786}$$

First, we notice that $\left\{n \in \mathbb{N}\middle|0 < \frac{1}{n}\right\} = \mathbb{N} \in \mathcal{U}$ and $\left\{n \in \mathbb{N}\middle|\frac{1}{n} < r\right\} \in \mathcal{U}$ for any $r \in \mathbb{R}$ since it is a cofinite set, hence, an element of the Frechét filter $\mathcal{F}_{\text{co}}$ which, in turn, is contained in $\mathcal{U}$ (see the proof of Theorem 4.2). Hence, we conclude that $^*0 < [\varepsilon_n] < {}^*r$ for any $r \in \mathcal{R}$, so that, recalling Definition 4.2, $[\varepsilon_n] \in {}^*\mathbb{R}$ is a positive infinitesimal number. In the same manner, $\{n \in \mathbb{N}|r < n\Big\} \in \mathcal{U}$ for any $r \in \mathbb{R}$ as a cofinite set, so that $^*r < [\omega_n]$ for any $r \in \mathcal{R}$ and, hence, $[\omega_n] \in {}^*\mathbb{R}$ is a positive infinite number. Moreover, it is straightforward to demonstrate that $[\omega_n] = [\varepsilon_n]^{-1}$.

Finally, we prove that the constructed hyperreal field in indeed an ordered field.

Theorem 4.3. *$({}^*\mathbb{R}, +, \cdot, <)$ is an ordered field with zero ^{*0} and unity ^{*1}.*

Proof. From the above construction, it is obvious that $^*\mathbb{R}$ is a commutative ring with with zero $^*0 = [0]$, unity $^*1 = [1]$, and inverse such that, for any $[r_n] \in {}^*\mathbb{R}$ with respect to the corresponding $\{r_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$, $-[r_n] = [-r_n]$ with respect to $\{-r_n\}_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$. Therefore, it is necessary to prove that any $[r_n] \neq {}^*0$ has a multiplicative, and $<$ is a total ordering on $^*\mathbb{R}$. For the former, we notice that $[r_n] \neq {}^*0$ means that $\{n \in \mathbb{N}|r_n = 0\} \notin \mathcal{U}$ and $N := \{n \in \mathbb{N}|r_n \neq 0\} \in \mathcal{U}$. Defining a new sequence $\{s_n\}_{n\in\mathbb{N}}$ such that

$$s_n = \begin{cases} \frac{1}{r_n}, & \text{if } n \in N, \\ 0, & \text{if } n \notin N, \end{cases} \tag{787}$$

we have that $\{n \in \mathbb{N}|r_n \cdot s_n = 1\} = N \in \mathcal{U}$, so that $[r_n \cdot s_n] = {}^*1$. Recalling (782), we conclude that

$$[r_n] \cdot [s_n] = {}^*1, \tag{788}$$

so that we can define the multiplicative inverse $[s_n] = [r_n]^{-1}$, and $^*\mathbb{R}$ is a field. For $<$ being total ordering on $^*\mathbb{R}$, we notice that, for any $[r_n], [s_n] \in {}^*\mathbb{R}$,

$$\mathbb{N} = \{n \in \mathbb{N}|r_n < s_n\} \sqcup \{n \in \mathbb{N}|r_n = s_n\} \sqcup \{n \in \mathbb{N}|r_n > s_n\} \tag{789}$$

$$:= \mathbb{N}^<_{r_n,s_n} \sqcup \mathbb{N}^=_{r_n,s_n} \sqcup \mathbb{N}^>_{r_n,s_n}. \tag{790}$$

Combining properties 1 and 3 of Definition 4.6 and Definition 4.7, we have that exactly one of the sets $\mathbb{N}^<_{r_n,s_n}$, $\mathbb{N}^=_{r_n,s_n}$, and $\mathbb{N}^>_{r_n,s_n}$ belongs to the ultrafilter $\mathcal{U}$. In turn, this means that for any $[r_n], [s_n] \in {}^*\mathbb{R}$, exactly one of the relations $[r_n] < [s_n]$, $[r_n] = [s_n]$, and $[r_n] > [s_n]$ is true. Therefore, recalling Definition 4.1, we define $^*\mathbb{R}^+ := \{[r_n] \in {}^*\mathbb{R}|[r_n] < 0\}$, so that $^*\mathbb{R} = {}^*\mathbb{R}^+ \sqcup \{{}^*0\} \sqcup {}^*\mathbb{R}^-\}$ with $^*\mathbb{R}^- = \{[r_n] \in {}^*\mathbb{R}| - [r_n] \in {}^*\mathbb{R}^+\}$. In turn, let $[r_n], [s_n] \in {}^*\mathbb{R}^+$. We have that

$$\{n \in \mathbb{N}|r_n > 0\} \cap \{n \in \mathbb{N}|s_n > 0\} \subseteq \{n \in \mathbb{N}|r_n + s_n > 0\}, \tag{791}$$

$$\{n \in \mathbb{N}|r_n > 0\} \cap \{n \in \mathbb{N}|s_n > 0\} \subseteq \{n \in \mathbb{N}|r_n \cdot s_n > 0\}, \tag{792}$$

so that $[r_n] + [s_n] \in {}^*\mathbb{R}^+$ and $[r_n] \cdot [s_n] \in {}^*\mathbb{R}^+$. Hence, due to Definition 4.1, $^*\mathbb{R}$ is an ordered field. □

It is possible to show that the set of non-principal ultrafilters on $\mathbb{N}$ is as big as the power set $2^{2^{\mathbb{N}}}$ of power set of $\mathbb{N}$. Therefore, a natural question arises: how the choice of the underlying ultrafilter $\mathcal{U}$ affects the properties of hyperreal fields introduced via the ultrapower construction, first of all, whether $^*\mathbb{R}$ is unique? Generally speaking, it is neither provable nor disprovable within the ZFC set theory. However, if the continuum hypothesis is accepted, one can prove that the hyperreal fields constructed under different ultrafilters $\mathcal{U}$ are isomorphic, so that the choice of $\mathcal{U}$ is irrelevant in this case.

The $*$-map can be further generalized to a map associating to standard mathematical objects (such as subsets of $\mathbb{R}^N$ and functions $f:\mathbb{R}^N \to \mathbb{R}$ for some $N \in \mathbb{N}$) their nonstandard extensions on $^*\mathbb{R}$. For example, for a given subset $A \subseteq \mathbb{R}$, we can define its nonstandard extension as $^*A = \{[a_n] \in {^*\mathbb{R}} | \{n \in \mathbb{N} | a_n \in A\} \in \mathcal{U}\}$. However, in order to guarantee that such extended nonstandard objects do not lose the properties carried by the original standard objects, it is necessary to involve the machinery of mathematical logic, first of all, model theory that provides the **transfer principle** for such generalized $*$-map. The former can be informally stated as the following: given standard mathematical objects $A_1, \ldots, A_n$, their elementary property $P(A_1, \ldots, A_n)$ is true if and only if $P(^*A_1, \ldots, {^*A_n})$ is true. In order to simplify introduction of nonstandard objects, the usual ultrapower construction in NSA can be translated into a more intuitive approach called Λ-limit, which parallels construction of the field of real numbers $\mathbb{R}$ via Cauchy limits on the field $\mathbb{Q}$ of rational numbers.

Definition 4.11. *We call **index set** an infinite set $\Lambda \supset \mathbb{R}$ such that*

$$\Lambda = \bigcup_{n \in \mathbb{N}_0} \Lambda_n(\mathbb{R}) \tag{793}$$

such that $\Lambda_0(\mathbb{R}) = \mathbb{R}$ and $\Lambda_{n+1}(\mathbb{R}) = \Lambda_n(\mathbb{R}) \cup 2^{\Lambda_n(\mathbb{R})}$.

We can single out finite sets from the index set Λ generating a family $\mathfrak{L} = \mathcal{P}_{\text{fin}}(\Lambda) \subset 2^\Lambda$. It is naturally equipped with a partial order relation $\subset$ making $\mathfrak{L}$ a directed set. In turn, we can introduce a set $\mathfrak{F}(\mathfrak{L}, \mathbb{R})$ of functions (nets) $\varphi : \mathfrak{L} \to \mathbb{R}$ equipped with natural pointwise binary operations $+$ and $\cdot$ and partial order relation. For the nets, we can introduce the standard Cauchy limit extending Definition 3, so that, for any $\varphi \in \mathfrak{F}(\mathfrak{L}, \mathbb{R})$,

$$L = \lim_{\lambda \to \Lambda} \varphi(\lambda) \tag{794}$$

if and only if for any $\varepsilon > 0$ there exists $\lambda_0 \in \mathfrak{L}$ such that for any $\lambda \supset \lambda_0$

$$|\varphi(\lambda) - L| < \varepsilon. \tag{795}$$

Therefore, the index set Λ can be seen as a "point at infinity" with respect to $\mathfrak{L}$. This suggests a construction of a hyperreal field considering limits of nets on $\mathfrak{L}$. However, the Cauchy limit does not necessarily exist for arbitrary net $\varphi \in \mathfrak{F}(\mathfrak{L}, \mathbb{R})$, and we need some additional structure provided iby the following Exercise.

Exercise 4.4. *Let $\mathcal{U}$ be a non-principal ultrafilter on $\mathfrak{L}$. Then*[15]

$$I_{\mathcal{U}} = \left\{ \varphi \in \mathfrak{F}(\mathfrak{L}, \mathbb{R}) \middle| \exists U \in \mathcal{U} : \ \varphi(\lambda) = 0 \ \forall \lambda \in U \right\} \tag{796}$$

is a maximal ideal on the ring $\mathfrak{F}(\mathfrak{L}, \mathbb{R})$, so that the quotient set $\mathfrak{F}(\mathfrak{L}, \mathbb{R})/I_{\mathcal{U}}$ is a field.

The quotient set $\mathfrak{F}(\mathfrak{L}, \mathbb{R})/I_{\mathcal{U}}$ with elements $[\varphi]_{\mathcal{U}} \in \mathfrak{F}(\mathfrak{L}, \mathbb{R})/I_{\mathcal{U}}$, which are equivalence classes with respect to the corresponding net $\varphi \in \mathfrak{F}(\mathfrak{L}, \mathbb{R})$, can be associated to a hyperreal field, whose elements are called Euclidean numbers[16] in order to highlight the used approach to their construction.

[15] Generalizing Definition 4.9 to nets, the condition (796) can be seen as requirement for φ to agree with a zero net $\mathcal{U}$-eventually.

[16] The name "Euclidean numbers" reflects their origin as an extension of ordinal numbers which satisfies the five common notions of Euclid's Elements (in particular, the principle "The whole is greater than the part" which is incompatible with Cantor's theory of cardinality). For more details, the reader can refer to arXiv:1702.04163.

Definition 4.12. *A field* $\mathbb{E} \supset \mathbb{R}$ *is called* ***field of Euclidean numbers*** *if there exists an isomorphism*

$$J: \mathfrak{F}(\mathfrak{L}, \mathbb{R})/I_{\mathcal{U}} \to \mathbb{E} \tag{797}$$

such that for any $r \in \mathbb{R}$ *and the corresponding constant net* $\varphi_r(\lambda) = r$ *it fulfills* $J([\varphi_r]_{\mathcal{U}}) = r$.

The isomorphism J allows us to define a new notion of limit of nets on $\mathfrak{L}$, which we denote by vertical arrow in order to distinguish it from the usual Cauchy limit.

Definition 4.13. *Let* $\varphi \in \mathfrak{F}(\mathfrak{L}, \mathbb{R})$ *be a net. Then its* Λ***-limit*** *is*

$$\lim_{\lambda \uparrow \Lambda} \varphi(\lambda) = J([\varphi]_{\mathcal{U}}). \tag{798}$$

Importantly, Λ-limit and the standard Cauchy limit can be connected, as suggested by the following Exercise.

Exercise 4.5. *Let* $\varphi \in \mathfrak{F}(\mathfrak{L}, \mathbb{R})$ *be a net such that it admits the Cauchy limit. Then*

$$\lim_{\lambda \to \Lambda} \varphi(\lambda) = \mathrm{st}\Big(\lim_{\lambda \uparrow \Lambda} \varphi(\lambda)\Big). \tag{799}$$

Having a proper definition of the hyperreal field $\mathbb{E}$ and Λ-limit of nets on $\mathbb{R}$, we can use the former to construct extensions of standard mathematical objects, starting with extensions of subsets of $\mathbb{R}^N$ for some $N \in \mathbb{N}$.

Definition 4.14. *Let* $N \in \mathbb{N}$, *and* $A \subseteq \mathbb{R}^N$ *be a subset of* $\mathbb{R}^N$. *Then an* ***extension*** ${}^*A \subseteq \mathbb{E}^N$ *of* A *is the set*

$${}^*A = \Big\{\lim_{\lambda \uparrow \Lambda} x_\lambda \Big| x_\lambda \in A,\ \forall \lambda \in \mathfrak{L}\Big\}. \tag{800}$$

In a similar manner, if there is a net of sets $A_\lambda \subseteq \mathbb{R}^N$, we can consider nets $\{x_\lambda\}_{\lambda \in \Lambda}$ of their elements such that each x_λ belongs to the corresponding A_λ and use the corresponding Λ-limits in order to associate to it a set

$$\langle A_\lambda \rangle_{\lambda \in \Lambda} = \Big\{\lim_{\lambda \uparrow \Lambda} x_\lambda \Big| x_\lambda \in A_\lambda,\ \forall \lambda \in \mathfrak{L}\Big\}. \tag{801}$$

This allows us to provide several important definitions via the Λ-limit. First, we define a nonstandard extension of a function.

Definition 4.15. *Let* $f: \mathbb{R}^N \to \mathbb{R}$. *Then its* ***extension*** *is a function* ${}^*f: \mathbb{E}^N \to \mathbb{E}$ *such that*

$${}^*f(x) = \lim_{\lambda \uparrow \Lambda} f(x_\lambda), \tag{802}$$

for any $x = \lim_{\lambda \uparrow \Lambda} x_\lambda$.

Next, we consider the sets which are nonstandard counterparts of finite sets and, therefore, share many useful properties with them.

Definition 4.16. *Let* $N \in \mathbb{N}$. *A set* $F \subset \mathbb{E}^N$ *is called* ***hyperfinite*** *if there exists a net* $\{F_\lambda\}_{\lambda \in \mathfrak{L}}$ *of finite sets such that*

$$F = \Big\{\lim_{\lambda \uparrow \Lambda} x_\lambda \Big| x_\lambda \in F_\lambda\Big\}. \tag{803}$$

One of the crucial properties that, exploiting their nature as nonstandard counterpart of finite sets, the elements of a hyperfinite set can be "summed" by defining a Λ-limit of sums over corresponding finite sets.

Definition 4.17. *Let $N \in \mathbb{N}$, and $F \subset \mathbb{E}^N$ be a hyperfinite set. Then the* ***hyperfinite sum*** *of its elements is*

$$\sum_{x\in F} x = \lim_{\lambda\uparrow\Lambda} \sum_{x\in F_\lambda} x. \tag{804}$$

We can use the notion of hyperfinite set in order to define the following hyperfinite space, which can be intuitively interpreted as a grid of infinitesimally separated elements, and construct functions on it.

Definition 4.18. *Let $N \in \mathbb{N}$. A hyperfinite set Γ such that $\mathbb{R}^N \subset \Gamma \subset \mathbb{E}^N$ is called* ***hyperfinite grid****. Furthermore, for any $\Omega \subset \mathbb{R}^N$, we define*

$$\Omega^\circ := {}^*\Omega \cap \Gamma. \tag{805}$$

Definition 4.19. *Let Γ be a hyperfinite grid with the corresponding net $\{\Gamma_\lambda\}_{\lambda\in\mathfrak{L}}$ of finite subsets of $\mathbb{R}^N$ for some $n \in \mathbb{N}$. The space $\mathfrak{F}(\Gamma,\mathbb{E})$ is called* ***space of grid functions*** *if, for any $u \in \mathfrak{F}(\Gamma,\mathbb{E})$,*

$$u(x) = \lim_{\lambda\uparrow\Lambda} u(x_\lambda), \tag{806}$$

for any net $\{x_\lambda\}_{\lambda\in\mathfrak{L}}$ with $x_\lambda \in \Gamma_\lambda$ such that $x = \lim_{\lambda\uparrow\Lambda} x_\lambda \in \Gamma$.

It is known that, given a function $f : F \to \mathbb{R}$ on a finite set $F \subseteq \mathbb{R}^N$ for some $n \in \mathbb{N}$, can be written in terms of characteristic functions χ_a of each element $a \in F$ as a sum

$$f(x) = \sum_{a\in F} f(a)\chi_a(x). \tag{807}$$

This property can be straightforwardly translate to grid functions as suggested by the following Exercise.

Exercise 4.6. *Prove that any grid function $u : \Gamma \to \mathbb{E}$ can be represented as a hyperfinite sum*

$$u(x) = \sum_{a\in\Gamma} u(a)\chi_a(x), \tag{808}$$

where $\chi_a(x)$ is a characteristic function of $\{a\}$.

This allows us to straightforwardly restrict extensions of standard functions to the given hyperfinite grid. In particular, for a given function $f : \mathcal{D}_f \to \mathbb{R}$, where $\mathcal{D}_f \subseteq \mathbb{R}^N$ we can define the corresponding grid function $f^\circ : \mathcal{D}_f^\circ \to \mathbb{E}$ by restricting ${}^*f$ to Γ as

$$f^\circ(x) = \sum_{a\in{}^*\mathcal{D}_f\cap\Gamma} f(a)\chi_a(x), \tag{809}$$

i.e., setting f° to zero in the points of Γ which do not belong to the extension of $\mathcal{D}_f$.

4.2 Space of ultrafunctions

We have concluded previous section with important definitions of hyperfinite grid Γ and the corresponding abstract functional space $\mathfrak{F}(\Gamma,\mathbb{E})$. Now, our aim is to construct a space of grid functions suitable for the purposes of operator theory, thus, substituting the standard Hilbert space. In particular, for its applications to non-relativistic quantum mechanics, we need a space which contains L^2-functions as well as Schwartz distributions. For the sake of simplicity, we consider the real line $\mathbb{R}$ and build the new space out of two components:

1) a suitable hyperfinite grid Γ constructed, due to Definition 4.16, via a net of finite subsets $\{\Gamma_\lambda\}_{\lambda\in\mathfrak{L}}$ of $\mathbb{R}$ in such a way that $\max(\Gamma) = -\min(\Gamma) = \omega$, where $\omega = \lim_{\lambda\uparrow\Lambda}\omega_\lambda$ with $\omega_\lambda = \max(\Gamma_\lambda)$,

2) a suitable standard functional space $V(\mathbb{R}) \supset \mathcal{C}^0(\mathbb{R})$.

We construct a family $\{V_\lambda(\mathbb{R})\}_{\lambda\in\mathfrak{L}}$ of finite-dimensional subspaces of $V(\mathbb{R})$ such that, for any finite-dimensional subspace $F \subset V(\mathbb{R})$, there exists λ such that $F \subset V_\lambda(\mathbb{R})$, so that

$$V(\mathbb{R}) = \bigcup_{\lambda\in\mathfrak{L}} V_\lambda(\mathbb{R}). \tag{810}$$

The corresponding space $V^\circ(\Gamma)$ of grid functions, which we call **ultrafunctions**, is equipped with several ad hoc properties provided by the following axiomatic definition.

Definition 4.20. *A **space of ultrafunctions** $V^\circ(\Gamma)$ generated by a functional space $V(\mathbb{R})$ and modeled on the family of its finite subspaces $\{V_\lambda(\mathbb{R})\}_{\lambda\in\mathfrak{L}}$ is a space of grid functions $u : \Gamma \to \mathbb{R}$ that satisfy the axioms given below*[17].

We seek to equip the space of ultrafunctions with a structure of algebra. First, it is necessary to ensure that algebra of ultrafunctions extends the algebra of real functions, with identity $\mathbb{1}^\circ$, where $\mathbb{1} \in V(\mathbb{R})$ is a constant function such that $\mathbb{1}(x) = 1$ for any $x \in \mathbb{R}$.

Axiom 1: Extension axiom

For every function $f : \mathbb{R} \to \mathbb{R}$, there exists a unique ultrafunction $f^\circ \in V^\circ(\Gamma)$ such that for any $x \in \mathbb{R}$:

$$f^\circ(x) = f(x). \tag{811}$$

On the other hand, we aim at a space $V^\circ(\Gamma)$ which does not simply consists of extensions of real functions to the hyperfinite grid but contains new objects as well. An example is given by a characteristic function χ_a for any $a \in \Gamma \setminus \mathbb{R}$. Therefore, we require the following Axiom, which also implies that any ultrafunction $u \in V^\circ(\Gamma)$ can be represented as the hyperfinite sum (808).

Axiom 2: χ_a-axiom

For any element $a \in \Gamma$, the corresponding characteristic function $\chi_a \in V^\circ(\Gamma)$.

Finally, we formalize the construction of $V^\circ(\Gamma)$ via the family of finite-dimensional subspaces $\{V_\lambda(\mathbb{R})\}_{\lambda\in\mathfrak{L}}$ of the original functional space $V(\mathbb{R})$.

Axiom 3: Approximation axiom

A function $u : \Gamma \to \mathbb{E}$ is an ultrafunction, so that $u \in V^\circ(\Gamma)$, if and only if there is a net of functions $u_\lambda \in V_\lambda(\mathbb{R})$ such that

$$u(x) = \lim_{\lambda\uparrow\Lambda} u_\lambda(x_\lambda), \tag{812}$$

for every $x = \lim_{\lambda\uparrow\Lambda} x_\lambda \in \Gamma$, where $x_\lambda \in \Gamma_\lambda$.

Next, we equip the space of ultrafunctions with suitable definitions of integral and derivative. First, in order to provide a definition of integral on $V^\circ(\Gamma)$, we require the functional space $V(\mathbb{R})$ to fulfill $V_c(\mathbb{R}) \subset L^1(\mathbb{R}) \subset \overline{V_c(\mathbb{R})}$, where $V_c(\mathbb{R}) \subset V(\mathbb{R})$ is the subspace of functions with a compact support, and the closure is taken in L^1-topology.

Definition 4.21. *Let $u \in V^\circ(\Gamma)$. The **pointwise integral** $\oint : V^\circ(\Gamma) \to \mathbb{E}$ is defined as follows:*

$$\oint u(x)dx = \lim_{\lambda\uparrow\Lambda} \int_{-\omega_\lambda}^{\omega_\lambda} u_\lambda(x)dx. \tag{813}$$

[17] This definition can be straightforwardly generalized to $\mathbb{R}^N$ for arbitrary $N \in \mathbb{N}$ by considering a hyperfinite grid $\mathbb{R}^N \subset \Gamma \subset \mathbb{E}^N$ and a space $\otimes_{i=1}^N V(\mathbb{R}) \subset V(\mathbb{R}^N)$ with a family $\{\otimes_{i=1}^N V_\lambda(\mathbb{R})\}_{\lambda\in\mathfrak{L}}$ of its finite-dimensional subspaces.

The following result demonstrates the origin of the name "pointwise" for the integral since it can be associated to a hyperfinite sum with respect to the values of the ultrafunction in each point of the hyperfinite grid.

Lemma 4.2. *Let* $u \in V^\circ(\Gamma)$. *Then*

$$\oint u(x)dx = \sum_{a\in\Gamma} u(a)d(a), \tag{814}$$

where $d(a) = \oint \chi_a(x)dx$.

Proof. Let $a = \lim_{\lambda\uparrow\Lambda} a_\lambda \in \Gamma$, where $a_\lambda \in \Gamma_\lambda$. We consider a net $\{\sigma_{a_\lambda}\}_{\lambda\in\mathfrak{L}}$ with $\sigma_{a_\lambda} \in V_\lambda(\mathbb{R})$ such that

$$\lim_{\lambda\uparrow\Lambda} \sigma_{a_\lambda}(x_\lambda) = \chi_a(x), \tag{815}$$

for any $x = \lim_{\lambda\uparrow\Lambda} x_\lambda$. Therefore, for any $u \in V^\circ(\Gamma)$, which is generated by a net of functions $\{u_\lambda\}_{\lambda\in\mathfrak{L}}$ due to Axiom 3,

$$u_\lambda(x) = \sum_{a_\lambda\in\Gamma_\lambda} u_\lambda(a_\lambda)\sigma_{a_\lambda}(x). \tag{816}$$

Defining a function $d(a_\lambda) := \int_{-\omega_\lambda}^{\omega_\lambda} \sigma_{a_\lambda}(x)dx$, we have:

$$\begin{aligned}\int_{-\omega_\lambda}^{\omega_\lambda} u_\lambda(x)dx &= \int_{-\omega_\lambda}^{\omega_\lambda}\Big(\sum_{a_\lambda\in\Gamma_\lambda} u_\lambda(a_\lambda)\sigma_{a_\lambda}(x)\Big)dx && (817)\\ &= \sum_{a_\lambda\in\Gamma_\lambda} u_\lambda(a_\lambda)\int_{-\omega_\lambda}^{\omega_\lambda}\sigma_{a_\lambda}(x)dx && (818)\\ &= \sum_{a_\lambda\in\Gamma_\lambda} u_\lambda(a_\lambda)d(a_\lambda). && (819)\end{aligned}$$

Therefore, we conclude that

$$\begin{aligned}\oint u(x)dx &= \lim_{\lambda\uparrow\Lambda}\int_{-\omega_\lambda}^{\omega_\lambda} u_\lambda(x)dx && (820)\\ &= \lim_{\lambda\uparrow\Lambda}\sum_{a_\lambda\in\Gamma_\lambda} u_\lambda(a_\lambda)d(a_\lambda) && (821)\\ &= \sum_{a\in\Gamma} u(a)d(a). && (822)\end{aligned}$$

□

The function $d(a)$ can, hence, be seen as a "measure" of a point $a \in \Gamma$ of the hyperfinite grid. This contrasts with the Lebesgue integral, which, for any $a \in \mathbb{R}$, provides $\int \chi_a(x)dx = 0$. In general, we have the following result connecting pointwise and Lebesgue integrals.

Lemma 4.3. *Let* $f \in L^1(\mathbb{R})$. *Then*

$$\oint f^\circ(x)dx \sim \int f(x)dx. \tag{823}$$

Proof. First, we notice that $V_c(\mathbb{R})$ is dense in $L^1(\mathbb{R})$. Therefore, there exists a net $\{f_\lambda\}_{\lambda\in\mathfrak{L}}$ of functions $f_\lambda \in V_\lambda(\mathbb{R})$ such that

$$\lim_{\lambda\to\Lambda}\int_{-\omega_\lambda}^{\omega_\lambda} |f_\lambda - f| = 0. \tag{824}$$

In turn, we have:

$$\left|\oint f^\circ(x)dx - \int f(x)dx\right| = \left|\lim_{\lambda\uparrow\Lambda}\int_{-\omega_\lambda}^{\omega_\lambda} f_\lambda(x)dx - \lim_{\lambda\to\Lambda}\int_{-\omega_\lambda}^{\omega_\lambda} f_\lambda(x)\right| \quad (825)$$

$$= \left|\lim_{\lambda\to\Lambda}\int_{-\omega_\lambda}^{\omega_\lambda} f_\lambda(x)dx - \lim_{\lambda\to\Lambda}\int_{-\omega_\lambda}^{\omega_\lambda} f_\lambda(x)\right| \quad (826)$$

$$= 0, \quad (827)$$

where (826) follows from Exercise 4.5. □

Therefore, we conclude the introduction of the pointwise integral on the space of ultrafunctions with the following Axiom.

Axiom 4: Integral axiom

For any $a \in \Gamma$, the pointwise integral fulfills the property:

$$d(a) := \oint \chi_a(x)dx > 0. \quad (828)$$

In particular, it allows us to equip the space of ultrafunctions $V^\circ(\Gamma)$ with the scalar product

$$\langle u, \tilde{u}\rangle_{V^\circ(\Gamma)} := \oint u(x)\tilde{u}(x)dx \quad (829)$$

$$= \sum_{a\in\Gamma} u(a)\tilde{u}(a)d(a), \quad (830)$$

and norm

$$\|u\|_{V^\circ(\Gamma)} := \sqrt{\oint |u(x)|^2 dx} \quad (831)$$

$$= \sqrt{\sum_{a\in\Gamma} |u(a)|^2 d(a)}, \quad (832)$$

respectively.

Exercise 4.7. *Prove that (830) and (832) fulfill the definitions of scalar product and norm.*

Importantly, we can define an ultrafunction that plays the role of the counterpart of (Dirac) δ-distribution and, in contrast to the latter, can undergo operations (e.g., product or square root) and generate an orthonormal basis of the space of ultrafunctions.

Definition 4.22. *Let $a \in \Gamma$. An ultrafunction $\delta_a \in V^\circ(\Gamma)$ such that*

$$\delta_a(x) = \frac{\chi_a(x)}{d(a)} \quad (833)$$

is called ***(Dirac) delta ultrafunction****.*

Indeed, it is straightforward to check that, for any $u \in V^\circ(\Gamma)$,

$$\oint u(x)\delta_a(x)dx = \sum_{x\in\Gamma} u(x)\frac{\chi_a(x)}{d(a)}d(x) \quad (834)$$

$$= u(a). \quad (835)$$

On the other hand, (Dirac) delta ultrafunctions are orthogonal with respect to the scalar product (830). For any $a, b \in \Gamma$, we have:

$$\begin{aligned}
\langle \delta_a, \delta_b \rangle_{V^\circ(\Gamma)} &= \oint \delta_a(x)\delta_b(x)dx && (836)\\
&= \frac{1}{d(a)d(b)} \oint \chi_a(x)\chi_b(x)dx && (837)\\
&= \frac{1}{d(a)d(b)} \sum_{x\in\Gamma} \chi_a(x)\chi_b(x)d(x) && (838)\\
&= \frac{\delta_{ab}}{d(a)}, && (839)
\end{aligned}$$

where $\delta_{ab} = 1$ if $a = b$, and $\delta_{ab} = 0$ otherwise. Therefore, it is possible to introduce an orthonormal basis $\{\sqrt{d(a)}\delta_a\}_{a\in\Gamma}$ on $V^\circ(\Gamma)$.

Lemma 4.4. *Let $a \in \Gamma$, $\{a_\lambda\}_{\lambda\in\mathfrak{L}}$ a net of elements $a_\lambda \in \Gamma_\lambda$ such that $a = \lim_{\lambda\uparrow\Lambda} a_\lambda$, and $\{\sigma_{a_\lambda}\}_{\lambda\in\mathfrak{L}}$ be a net of functions such that $\lim_{\lambda\uparrow\Lambda} \sigma_{a_\lambda}(x_\lambda) = \chi_a(x)$ and $d(a_\lambda) = \int_{-\omega_\lambda}^{\omega_\lambda} \sigma_{a_\lambda}(x)dx$. Then, for any $u \in V^\circ(\Gamma)$,*

$$u(a) = \lim_{\lambda\uparrow\Lambda} \int_{-\omega_\lambda}^{\omega_\lambda} u_\lambda(x)\delta_{a_\lambda}(x)dx, \tag{840}$$

where

$$\delta_{a_\lambda}(x) = \frac{\sigma_{a_\lambda}(x)}{d(a_\lambda)}. \tag{841}$$

Proof. First, we notice that

$$\begin{aligned}
u_\lambda(a_\lambda) &= \sum_{b_\lambda\in\Gamma_\lambda} u_\lambda(b_\lambda)\sigma_{b_\lambda}(a_\lambda) && (842)\\
&= \sum_{b_\lambda\in\Gamma_\lambda} u_\lambda(b_\lambda)\sigma_{a_\lambda}(b_\lambda) && (843)\\
&= \sum_{b_\lambda\in\Gamma_\lambda} u_\lambda(b_\lambda)\delta_{a_\lambda}(b_\lambda)d(b_\lambda) && (844)\\
&= \int_{-\omega_\lambda}^{\omega_\lambda} u_\lambda(b_\lambda)\delta_{a_\lambda}(x)dx, && (845)
\end{aligned}$$

where (842) and (842) follow from $\sigma_b(a) = \delta_{ab}$. Finally, taking the Λ-limit on both sided, we obtain (840). □

Finally, in order to equip $V^\circ(\Gamma)$ with a notion of derivative, we provide further restriction on the functional space $V(\mathbb{R})$, namely, we require $V(\mathbb{R}) \subset BV_{\text{loc}}(\mathbb{R})$, where the latter is the space of locally bounded functions. This allows us to include the notion of the weak derivative into it.

Definition 4.23. *Let $u \in V^\circ(\Gamma)$. The **generalized derivative** $D : V^\circ(\Gamma) \to V^\circ(\Gamma)$ is defined as follows:*

$$Du(a) = \lim_{\lambda\uparrow\Lambda} \langle \partial u_\lambda, \delta_{a_\lambda} \rangle_{V(\mathbb{R})}, \tag{846}$$

for any $a = \lim_{\lambda\uparrow\Lambda} a_\lambda$ with $a_\lambda \in \Gamma_\lambda$, where $\partial : V(\mathbb{R}) \to V(\mathbb{R})$ is a derivative on $V(\mathbb{R})$, and the net δ_{a_λ} is given by (841).

In particular, for any $f \in \mathcal{C}^1 \cap V(\mathbb{R})$ and $\partial f \in V(\mathbb{R})$,

$$\begin{aligned} Df^\circ(a) &= \lim_{\lambda\uparrow\Lambda} \langle \partial f, \delta_{a_\lambda} \rangle_{V(\mathbb{R})} && (847)\\ &= \lim_{\lambda\uparrow\Lambda} \int_{-\omega_\lambda}^{\omega_\lambda} \partial f(x) \delta_{a_\lambda}(x) dx && (848)\\ &= \lim_{\lambda\uparrow\Lambda} \partial f(a_\lambda) && (849)\\ &= (\partial f)^\circ(a), && (850)\end{aligned}$$

due to Lemma 4.4, so that the generalized derivative coincides with an extension of the usual derivative in this case. In order to guarantee locality of the generalized derivative, we conclude with the following Axiom.

Axiom 5: Generalized derivative axiom

For any $a \in \Gamma$ and $u \in V^\circ(\Gamma)$, the generalized derivative fulfills the properties:

$$\operatorname{supp}(D\chi_a(x)) \subset \mathfrak{mon}(a), \tag{851}$$

and, for some $c \in \mathbb{E}$,

$$Du = 0 \Leftrightarrow u = c\mathbb{1}^\circ. \tag{852}$$

This axiom weakens properties of usual derivative, first of all, Leibniz rule: indeed, for any $f, g \in \mathcal{C}^1(\mathbb{R})$, one has $\partial(f \cdot g) = \partial(f) \cdot g + f \cdot \partial(g)$. It is not necessarily fulfilled by the generalized derivative D, which is the price paid for having the algebra structure for the space of ultrafunctions and, as an important consequence, overcoming the Schwartz impossiblity result[18]. In order to show that Schwartz distributions are natually embedded into the space of ultrafunctions, first, we isolate ultrafunctions which can be associated to a distribution by introducing the following straightforward Definition.

Definition 4.24. *Let $u \in V^\circ(\Gamma)$ be an ultrafunction. It is called **distribution-like** if there exists a distribution $T \in \mathcal{D}^*(\mathbb{R})$ such that for any infinitely differentiable function $\varphi \in \mathcal{D}(\mathbb{R})$ with a compact support*[19]*,*

$$\oint u(x)\varphi^\circ(x)dx = T(\varphi). \tag{853}$$

Theorem 4.4. *For any $T \in \mathcal{D}^*(\mathbb{R})$, there exists an associated distribution-like ultrafunction $u_T \in V^\circ(\Gamma)$.*

Proof. Let $\mathcal{D}^\circ(\Gamma) \subset V^\circ(\Gamma)$ be the space of ultrafunctions constructed from $\mathcal{D}(\mathbb{R})$ via Definition 4.20, and $P_{\mathcal{D}^\circ(\Gamma)} : V^\circ(\Gamma) \to \mathcal{D}^\circ(\Gamma)$ be an orthogonal projector onto it. Then, for any $v \in V^\circ(\Gamma)$, we consider $v_\parallel = P_{\mathcal{D}^\circ(\Gamma)} v$. By Axiom 3, we can find a net $\{v_{\parallel,\lambda}\}_{\lambda\in\mathfrak{L}}$ of functions $v_{\parallel,\lambda} \in V_\lambda(\mathbb{R})$ such that $v_\parallel(x) = \lim_{\lambda\uparrow\Lambda} v_{\parallel,\lambda}(x_\lambda)$ for any $x = \lim_{\lambda\uparrow\Lambda} x_\lambda$, and we construct an ultrafunction $u_T \in V^\circ(\Gamma)$ such that

$$\oint u_T(x)v(x)dx = \lim_{\lambda\uparrow\Lambda} T(v_{\parallel,\lambda}). \tag{854}$$

Then, for any $\varphi \in \mathcal{D}(\mathbb{R})$, we have

$$\begin{aligned} \oint u_T(x)\varphi^\circ(x)dx &= \lim_{\lambda\uparrow\Lambda} T(\varphi) && (855)\\ &= T(\varphi). && (856)\end{aligned}$$

[18]Weakening Leibniz rule is not the only way to embed Schwartz distributions to a differential algebra: e.g., Colombeau's algebra achieve this by restricting agreement of the algebra's product with the pointwise product to $C^\infty(\mathbb{R})$ instead of continuous functions.

[19]Notice that $\mathcal{D}(\mathbb{R})$ is a dense subspace of Schwartz space (668), so that $\mathcal{D}^*(\mathbb{R})$ naturally includes the space $\mathcal{S}^*(\mathbb{R})$ introduced in Definition 669.

□

The association provided by Theorem 4.4 can be made into bijection by considering a quotient set of the set of distribution-like ultrafunctions with respect to equivalence classes

$$[u]_{\mathcal{D}^*} = \left\{ v \in V^\circ(\Gamma) \middle| \forall \varphi \in \mathcal{D}(\mathbb{R}) : \oint (u(x) - v(x))\varphi^\circ(x)dx = 0 \right\}, \tag{857}$$

and the resulting bijection associates a Schwartz distribution $T \in \mathcal{D}^*(\mathbb{R})$ to a unique equivalence class $[u]_{\mathcal{D}^*}$ such that $u \in V^\circ(\Gamma)$ fulfills (853). In turn, Definition 4.24 suggests embedding of L^2-functions into the space of ultrafunctions: given $f \in L^2(\mathbb{R})$, we associate to an ultrafunction f° such that

$$\oint f^\circ(x)v(x)dx = \lim_{\lambda\uparrow\Lambda} \int f(x)v_\lambda(x)dx, \tag{858}$$

for any $v \in V^\circ(\Gamma)$ with the corresponding net $\{v_\lambda\}_{\lambda\in\mathfrak{L}}$.

4.3 Operators on ultrafunctions and quantum mechanics

Having introduced the space of ultrafunctions $V^\circ(\Gamma)$ and analyzed some of its properties, we proceed by its applications to quantum mechanics. First, we provide the following useful definitions.

Definition 4.25. *A mathematical entity is called* ***internal*** *if it is a* Λ*-limit of some other entities.*

Our goal is to construct a system of axioms of non-relativistic quantum mechanics using the space of ultrafunctions instead of the Hilbert space $L^2(\mathbb{R})$. Therefore, we define a complex version of the former.

Definition 4.26. *The* ***space of complex-valued ultrafunctions*** $\mathcal{H}^\circ(\Gamma)$ *is defined as a complexification*

$$\mathcal{H}^\circ(\Gamma) = V^\circ(\Gamma) \oplus iV^\circ(\Gamma) \tag{859}$$

of the space of ultrafunctions $V^\circ(\Gamma)$*.*

Definition 4.26 implies that $\mathcal{H}^\circ(\Gamma)$ is constructed by considering a complexification $\mathcal{H}(\mathbb{R}) = V(\mathbb{R}) \oplus iV(\mathbb{R})$ of the original functional space $V(\mathbb{R})$ and constructing a family of finite-dimensional spaces $\{\mathcal{H}_\lambda(\mathbb{R})\}_{\lambda\in\mathfrak{L}} = \{V_\lambda(\mathbb{R}) \oplus iV_\lambda(\mathbb{R})\}_{\lambda\in\mathfrak{L}}$. Now, we can use the space $\mathcal{H}^\circ(\Gamma)$ as a configurational space of quantum mechanics, modifying thereby the first Axiom of quantum mechanics.

Axiom 1'

The configuration space of a physical system is a space of complex-valued ultrafunctions $\mathcal{H}^\circ(\mathbb{R})$, with physical state being represented by normalized elements $u \in \mathcal{H}^\circ(\mathbb{R})$, i.e., $\|u\|_{\mathcal{H}^\circ(\mathbb{R})} = 1$.

In order to start, we focus on an internal operator $A : \mathcal{H}^\circ(\Gamma) \to \mathcal{H}^\circ(\Gamma)$. It can be constructed via the Λ-limit with respect to a family of operators $A_\lambda : \mathcal{H}_\lambda(\mathbb{R}) \to \mathcal{H}_\lambda(\mathbb{R})$, so that

$$Au = \lim_{\lambda\uparrow\Lambda} A_\lambda u_\lambda, \tag{860}$$

for any $u(x) = \lim_{\lambda\uparrow\Lambda} u_\lambda(x_\lambda)$ with $u_\lambda \in \mathcal{H}_\lambda$ and any $x = x_\lambda$. Since every $\mathcal{H}_\lambda$ is finite-dimensional, A_λ are self-adjoint operators if and only if they are symmetric. This property transfers to A as well as it acts on a hyperfinite-dimensional space. In particular, the spectrum of A consists in this case of eigenvalues only, and

$$\sigma(A) = \left\{ \lim_{\lambda\uparrow\Lambda} \mu_\lambda \in \mathbb{E} \middle| \forall \lambda \in \mathfrak{L} : \ \mu_\lambda \in \sigma(A_\lambda) \right\}, \tag{861}$$

being a discrete spectrum in the sense of NSA. Its corresponding eigenfunctions are given via Λ-limits with respect to the corresponding eigenfunctions of A_λ and form an orthonormal basis of $\mathcal{H}^\circ(\mathbb{R})$. Therefore, in contrast to the operator theory on Hilbert spaces, operator theory on space of ultrafunctions does not require distinction between symmetric and self-adjoint operators. We have proven the following Theorem for operators on space of ultrafunctions.

Theorem 4.5. *Let $A : \mathcal{H}^\circ \to \mathcal{H}^\circ$ be an internal symmetric operator. Then it is self-adjoint.*

This leads to the following modification of Axiom 2 of quantum mechanics.

Axiom 2'

An observable a corresponds to a symmetric operator $A : \mathcal{H}^\circ(\mathbb{R}) \to \mathcal{H}^\circ(\mathbb{R})$.

In particular, we can reintroduce Schrödinger operators by modifying Definition 3.1 in the following way.

Definition 4.27. *We call* ***Schrödinger operator*** *$H^\circ : \mathcal{H}^\circ(\Gamma) \to \mathcal{H}^\circ(\Gamma)$ an operator*

$$H^\circ = -\frac{\hbar^2}{2m} D^2 + \mathcal{V}, \tag{862}$$

where $\mathcal{V} : \mathcal{H}^\circ(\Gamma) \to \mathcal{H}^\circ(\Gamma)$ is a multiplication operator defined as

$$(\mathcal{V}u)(x) = V(x)u(x), \tag{863}$$

where $V : \Gamma \to \mathbb{E}$ is an internal function.

Schrödinger operators that are defined in this manner remain self-adjoint and carry a hyperfinite (hence, discrete in the sense of NSA) spectrum. Moreover, space of ultrafunctions allows one to define Schrödinger operators with a singular potential, for example, modeled by the (Dirac) delta ultrafunction

$$V(x) = \tau\delta_a(x), \tag{864}$$

with $\tau \in \mathbb{E}$ and $a \in \Gamma$, which does not have counterpart in the standard L^2-space.

Axiom 3 of quantum mechanics can be modified in the following way taking into account discreteness of the spectrum of the operators that correspond to observables.

Axiom 3'

The only possible outcomes of a measurement of a form a set $\{\mathrm{st}(\mu_j)\}$, where $\mu_j \in \sigma(A)$ are the eigenvalues of A. If the physical system is in the state $u \in \mathcal{H}^\circ(\mathbb{R})$, an outcome $\mathrm{st}(\mu_j)$ can be obtained with a probability

$$\mathbb{P}_j = |\langle u|u_j\rangle_{\mathcal{H}^\circ(\mathbb{R})}|^2, \tag{865}$$

where u_j is the eigenfunction corresponding to the eigenvalues μ_j.

For example, considering position operator $\mathfrak{x} : \mathcal{H}^\circ(\mathbb{R}) \to \mathcal{H}^\circ(\mathbb{R})$ that acts as

$$\mathfrak{x}u(x) = xu(x), \tag{866}$$

for any $\mathcal{H}^\circ(\mathbb{R})$, it is straightforward to show that its eigenfunctions with respect to the corresponding eigenvalue $x \in \sigma(\mathfrak{x})$ are (Dirac) delta ultrafunctions δ_x. In turn, Axiom 3' suggests that a measurement of position of a quantum particle reveals a value $\bar{x} \in \{\mathrm{st}(x) | x \in \sigma(\mathfrak{x})\} = \mathbb{R}$, recovering the result from the standard approach to quantum mechanics.

While the dynamical Axiom 4 remains unchanged up to substitution of the Hilbert space by $\mathcal{H}^\circ(\mathbb{R})$, quantum mechanics on ultrafunctions requires an extra Axiom, which separates physical states from non-physical ones.

Axiom 5'

In a laboratory, only the states associated to a finite expectation value of the physically relevant quantities can be realized. These states are called physical states, the rest of the states is called ideal states.

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