On the uniqueness of the canonical commutation relations in quantum physics

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Certificate of Examination

This is to certify that the dissertation titled "**On the uniqueness of the canonical commutation relations in quantum physics**" submitted by **Satvik Singh (Reg. No. MS16075)** for the partial fulfilment of the BS-MS dual degree program of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

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Dated: May 26, 2021

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Prof. Arvind at the Indian Institute of Science Education and Research Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Satvik Singh
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In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

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Prof. Arvind
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Contents

Abstract

While quantum mechanics tells us that states of a given physical system reside in a Hilbert space and observables correspond to self-adjoint operators acting on that space, it doesn't provide a prescription to uniquely associate a Hilbert space and the relevant self-adjoint observables for any given system. Then, why is the dynamics of a free particle in one dimension always modelled by the space of complex square integrable functions with the position and momentum observables acting as the multiplication and differentiation operators, respectively? It is perfectly reasonable to expect that there may be other choices of the Hilbert space and of the self-adjoint operators linked with the position and momentum observables which serve equally as well to model the dynamics of the free particle. In this thesis, we aim to answer the aforementioned question by providing a self-contained account of the seminal Stone-von Neumann uniqueness theorem for the canonical commutation relation, which shows that it is the nature of the commutation relation between the position and momentum observables that (uniquely) fixes both the choice of the Hilbert space and of the self-adjoint operators linked with the position and momentum observables of the free particle.

Part I

1 | Introduction

During the early years of the 20th century, as the stark incapacity of the classical theory of mechanics to provide a full description of nature – especially at small length scales – was beginning to get exposed, a new and intriguing quantum theory of the universe was taking shape. Around the late 1920's, there were two competing models of quantum mechanics, both of which lacked a firm mathematical footing and were desperately in need of a unification: Schrödinger's wave mechanics [Sch26] and Heisenberg's matrix mechanics [Fla32]. One of the main challenges in this regard was to prove the existence of sufficiently nice realizations of the canonical commutation relations (CCR) between the position and momentum observables

$$QP - PQ = i\mathbb{1}, \tag{1.1}$$

and to tackle the question of their equivalence in both the models. It was not until the seminal work on the "Mathematical Foundations of Quantum Mechanics" by John von Neumann [vNBW18] was published in 1932 that the aforementioned problems acquired a satisfactory solution (after years of crucial efforts, especially by Weyl [Wey27], Stone [Sto30], and Von Neumann [vN31]). It was in this work where the ideas of formalizing the theory of quantum mechanics on a Hilbert space finally culminated into a mathematically precise shape and the stated commutation relations were rigorously and uniquely realized in terms of unbounded self-adjoint operators on a Hilbert space. The aim of the present thesis is to provide a self-contained introduction to the theory of linear operators on Hilbert spaces which is required to fully appreciate the significance of the hallmark equation of quantum physics as stated in Eq (1.1). We begin our journey in this chapter by laying out the basic formulation of quantum mechanics and by motivating the need to consider realizations of the CCR in Eq. (1.1).

For simplicity of exposition, we will mostly restrict ourselves to the case of a single free particle constrained to move in one dimension. Classically, we model the *phase space* of this system by using the cotangent bundle $T^*\mathscr{Q} \simeq \mathbb{R}^2$ of the configuration manifold $\mathscr{Q} = \mathbb{R}$. The physical observables then correspond to smooth real valued functions $f \in C^\infty(\mathbb{R}^2)$. By defining the Poisson bracket of $f, g \in C^\infty(\mathbb{R}^2)$ as follows

$$\{f, g\} = \partial_1 f \partial_2 g - \partial_2 f \partial_1 g, \tag{1.2}$$

the vector space $C^\infty(\mathbb{R}^2)$ endowed with the bracket $\{\cdot,\cdot\} : C^\infty(\mathbb{R}^2) \times C^\infty(\mathbb{R}^2) \to C^\infty(\mathbb{R}^2)$ can be easily shown to become a Lie algebra [1]. We now define the canonical *position* and *momentum* observables $Q, P \in C^\infty(\mathbb{R}^2)$, whose action on the phase space is to extract the position and momentum information from the given state $(x, p) \in \mathbb{R}^2$ of the system, respectively:

$$\forall (x, p) \in \mathbb{R}^2 : \quad Q(x, p) = x \quad \text{and} \quad P(x, p) = p. \tag{1.3}$$

[1] A Lie algebra is a vector space V equipped with a bilinear, anti-symmetric form $[\cdot,\cdot] : V \times V \to V$ which satisfies the Jacobi identity: $\forall x, y, z \in V : \quad [x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0$.

The Poisson bracket operation performed on the position and momentum observables gives us a first glimpse into the structure of the canonical commutation relation

$$\{Q,P\} = 1, \tag{1.4}$$

where the right hand side denotes the function which identically maps the entire phase space to one. The above commutation relation can be interpreted as a manifestation of the fact that the position and momentum observables are modelled as two fundamentally different and incompatible degrees of freedom in our theory.

Let us now transition into the realm of quantum mechanics, where the state space of the free particle constrained to move in one dimension is modelled by a separable complex Hilbert space $\mathscr{H}$, with the role of observables being acquired by self-adjoint linear operators $T : D(T) \to \mathscr{H}$ defined on suitable subspaces $D(T) \subseteq \mathscr{H}$. For now, we can think of self-adjointness of operators as some non-trivial generalization of the finite-dimensional notion of hermiticity of $d \times d$ complex matrices. Let us also, for the moment, restrict ourselves to the simpler space $\mathscr{B}(\mathscr{H})$ consisting of linear operators $T : \mathscr{H} \to \mathscr{H}$ that are bounded in the sense that for every non-zero $T \in \mathscr{B}(\mathscr{H})$, there exists a constant $c > 0$ such that

$$\forall x \in \mathscr{H} : \quad ||Tx|| \leq c||x||.$$ [2]

By defining the commutator bracket of two operators $A, B \in \mathscr{B}(\mathscr{H})$ as

$$[A,B] := AB - BA,$$

the space $\mathscr{B}(\mathscr{H})$ equipped with $[\cdot,\cdot] : \mathscr{B}(\mathscr{H}) \times \mathscr{B}(\mathscr{H}) \to \mathscr{B}(\mathscr{H})$ becomes a Lie algebra. At this point, the similarity of $\mathscr{B}(\mathscr{H})$ with the Lie algebra $C^\infty(\mathbb{R}^2)$ of classical observables on the phase space should start becoming apparant. Building upon this analogy, it is reasonable to demand that the position and momentum observables $Q, P \in \mathscr{B}(\mathscr{H})$ of the free particle should satisfy the following quantum analogue of Eq. (1.4):

$$[Q,P] = QP - PQ = c\mathbb{I}, \tag{1.5}$$

where $c \in \mathbb{C}$ is some complex number and $\mathbb{I} \in \mathscr{B}(\mathscr{H})$ is the identity operator. It is easy to see that since the operators Q, P are self-adjoint, $c \in \mathbb{C}$ must be purely imaginary, which we assume to be equal to the imaginary unit i. With the relevant background in place, we can now present a slight variant of our primary topic of investigation in the form of the following question.

Question 1.1. *Does there exist self-adjoint linear operators $Q, P \in \mathscr{B}(\mathscr{H})$ defined on some complex separable Hilbert space $\mathscr{H}$ such that*

$$QP - PQ = i\mathbb{I}\,?$$

Much of the complexity of quantum theory stems from the fact that the above question *cannot* be answered in the affirmative. In fact, a slightly weaker version of this fact can be proven with minimal effort, as we now show.

Proposition 1.2. *For a finite dimension Hilbert space $\mathscr{H} \simeq \mathbb{C}^d$, there are no self-adjoint linear operators $Q, P \in \mathscr{B}(\mathscr{H})$ which satisfy $[Q,P] = i\mathbb{I}$.*

[2] Here, $||\cdot||$ denotes the norm induced by the inner product on $\mathscr{H}$: $\forall x \in \mathscr{H} : \quad ||x|| = \sqrt{\langle x,x \rangle}$.

Proof. Assume on the contrary that there are such self-adjoint linear operators $Q, P \in \mathscr{B}(\mathscr{H})$ satisfying $[Q, P] = i\mathbb{I}$. Then, taking trace on both sides leads to a contradiction:

$$0 = \mathrm{Tr}(QP) - \mathrm{Tr}(PQ) = i\,\mathrm{Tr}(\mathbb{I}) \neq 0.$$

□

After reviewing the theory of bounded linear operators on Hilbert spaces, we will present a slightly trickier proof of the above proposition for infinite dimensional Hilbert spaces in Chapter 2. The natural next step would be to relax the boundedness assumption and consider a more general class of self-adjoint linear operators which can satisfy the required commutation relation. Fortunately, there do exist realizations of the canonical commutation relation in this setting. One such realization can be constructed on the Hilbert space of complex square integrable functions $L^2(\mathbb{R})$ by defining the following operators on suitable domains:

$$\begin{aligned} Q\psi(x) &= x\psi(x) \\ P\psi(x) &= -i\psi'(x). \end{aligned} \tag{1.6}$$

In Chapter 2, we will prove that Q, P as defined above are not bounded and cannot be defined on all of $L^2(\mathbb{R})$. However, there does exist a common dense domain $D \subseteq L^2(\mathbb{R})$ which stays invariant under both the operators such that $\forall \psi \in D$,

$$(QP - PQ)\psi(x) = i\psi(x). \tag{1.7}$$

What we have seen above is known as the *Schrödinger representation* of the canonical commutation relation, whose precise formulation forms the meat of Chapter 3. Fascinatingly, under some additional assumptions, this representation can be shown to be the only one! This is the content of the famous Stone-von Neumann uniqueness theorem, whose proof lies at the heart of the present thesis (Chapter 7) and will provide an apt conclusion to the theory that we are going to develop in the coming chapters. Unfortunately though, this means that the relatively easier theory of bounded operators is incapable of describing the quantum mechanical model of even the simplest possible physical systems. Thus, we inevitably need to get our hands dirty in the regime of unbounded operators, which is going to occupy us for a substantial part of this thesis (Chapters 3-6). In particular, the question of deciding whether the operators Q, P (or, for that matter, any unbounded operator) are self-adjoint is very subtle, which is why we have conveniently chosen to ignore it in our discussion above. We will get back to this issue later after developing the general theory of unbounded operators. Let us now conclude our introduction by briefly presenting an outline of this thesis.

- Chapter 2 reviews the basic background material on Hilbert spaces and bounded linear operators on Hilbert spaces, which forms the foundation upon which the following chapters are laid.

- Chapter 3 develops the theory of unbounded operators on Hilbert spaces and contains a precise description of the Schrödinger representation of the canonical commutation relation on $L^2(\mathbb{R})$.

- Chapter 4 motivates the study of the uniqueness of the Schrödinger representation of the canonical commutation relation, which forms the subject matter of the remaining chapters.

- Chapter 5 recalls the spectral theorem for bounded and unbounded self-adjoint operators on Hilbert spaces and hence lays the groundwork for the discussing the highlight theorems of Stone and Von Neumann in the next two chapters.

- Chapter 6 contains the proof of Stone's theorem on strongly continuous one-parameter unitary groups on Hilbert spaces.

- Chapter 7 forms the culmination of this thesis and contains the proof of the fundamental Stone-von Neumann uniquness theorem for the canonical commutation relation.

2 | Basic functional analysis

This chapter establishes the basic functional analytic background which will later prove to be essential in tackling the problems stated in the introductory chapter. In particular, we review the basic theory of Hilbert spaces and of bounded linear operators on Hilbert spaces. Since the material covered in this chapter is quite standard, we refrain from giving proofs for most of the results. Interested readers should refer to the classic texts [Rud91, Con85, RS12, Sun16, Sun96] for a more thorough study of these topics.

2.1 Hilbert spaces

Definition 2.1. *A Hilbert space $\mathscr{H}$ is a complex vector space endowed with an inner product $\langle\cdot,\cdot\rangle : \mathscr{H}\times\mathscr{H}\to\mathscr{H}$ such that $\mathscr{H}$ is* complete *with respect to the norm $||\cdot|| : \mathscr{H}\to[0,\infty)$ induced by the inner product: $||x|| = \sqrt{\langle x,x\rangle}$.*

A few remarks about the above definition are in order. Recall that a metric space is said to be *complete* if every cauchy sequence in that space converges within the space. We will follow the physicists' convention of the inner product being anti-linear in the first factor. Right at the onset, let us state one of the most useful inequalities in mathematics, the *Cauchy-Schwarz* inequality.

Proposition 2.2. *For a Hilbert space $\mathscr{H}$, the following inequality holds:*

$$\forall x,y\in\mathscr{H}: \qquad |\langle x,y\rangle| \le \|x\|\,\|y\|,$$

with equality occurring if and only if the set $\{x,y\}$ is linearly independent.

Recall that a closed subspace of any complete normed vector space (i.e., a *Banach* space) is itself complete. Hence, any closed subspace of a Hilbert space $S\subsetneq\mathscr{H}$ is itself a Hilbert space. Moreover, if we define the orthogonal complement of S as follows:

$$S^{\perp} := \{x\in\mathscr{H} : \forall y\in S : \langle x,y\rangle = 0\}, \tag{2.1}$$

then the Hilbert space splits up into a direct sum $\mathscr{H} = S\oplus S^{\perp}$, i.e., for every $x\in\mathscr{H}$, there exists unique $y\in S$ and $z\in S^{\perp}$ such that $x = y+z$. Now, we introduce the notion of the dual Hilbert space.

Definition 2.3. *Let $\mathscr{H}$ be a Hilbert space. Then, the collection $\mathscr{H}^*$ of all continuous linear functionals $\phi : \mathscr{H}\to\mathbb{C}$ is said to be the (topological) dual space of $\mathscr{H}$.*

A remarkable feature of Hilbert spaces is that their duals have the same structure as the original spaces themselves. This is the content of the *Riesz representation* theorem.

Theorem 2.4. *Consider a Hilbert space $\mathscr{H}$. Then, for every $\phi \in \mathscr{H}^*$, there exists a unique $y_\phi \in \mathscr{H}$ such that*

$$\forall x \in \mathscr{H}: \qquad \phi(x) = \langle y_\phi, x \rangle.$$

In other words, the correspondence $y_\phi \mapsto \phi$ sets up an anti-linear bijection between $\mathscr{H}$ and $\mathscr{H}^*$, which can be used to define the inner product $\langle \phi, \xi \rangle_* = \langle y_\xi, y_\phi \rangle$ on $\mathscr{H}^*$ so that $\mathscr{H}$ becomes canonically isomorphic to its dual $\mathscr{H}^*$.

A Hilbert space $\mathscr{H}$ is said to be *separable* if it contains a countable dense subset. All Hilbert spaces in quantum physics (and in this thesis) are assumed to be separable. The upshot of this constraint is that it allows us to equip the Hilbert spaces with countable orthonormal bases.

Theorem 2.5. *A Hilbert space $\mathscr{H}$ is separable if and only if it admits a countable orthonormal basis, i.e., if and only if there exists a countable set $\{e_i\}_{i=1}^\infty$ such that*

$$\langle e_i, e_j \rangle = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}.$$

Moreover, every $x \in \mathscr{H}$ can be uniquely represented as $x = \sum_{i=1}^\infty \langle e_i, x \rangle e_i$, where the series converges unconditionally in $\mathscr{H}$ and $\|x\|^2 = \sum_{i=1}^\infty |\langle e_i, x \rangle|^2 < \infty$.

In the above theorem, it is important to note that the orthonormal basis of a separable Hilbert space $\mathscr{H}$ is not unique. However, the cardinality of the basis set is unique, which is defined to be the *dimension* of $\mathscr{H}$.

Let us conclude this section with a few examples of Hilbert spaces.

Example 2.6. Consider $\mathscr{H} = \mathbb{C}^n$ equipped with pointwise addition and scalar multiplication. Define the inner product $\langle x, y \rangle = \sum_{i=1}^n \bar{x}_i y_i$. Then, it is easy to see that $\mathscr{H}$ is a complex vector space which is complete with respect to the norm induced by the inner product, i.e., $\mathscr{H}$ is a Hilbert space with $\dim \mathscr{H} = n$.

Example 2.7. Consider the space of all square summable complex sequences

$$\mathscr{H} = l^2(\mathbb{N}) := \{(x_i)_{i \in \mathbb{N}} : \sum_{i=1}^\infty |x_i|^2 < \infty\}.$$

With addition and scalar multiplication defined pointwise, it is not too difficult to see that $\mathscr{H}$ is a complex vector space which turns into a separable Hilbert space with $\dim \mathscr{H} = \infty$ when equipped with the inner product

$$\langle (x_i)_{i \in \mathbb{N}}, (y_j)_{j \in \mathbb{N}} \rangle = \sum_{i=1}^\infty \bar{x}_i y_i.$$

Example 2.8. Consider the space $\mathscr{L}^2(\mathbb{R})$ of all square integrable Lebesgue measurable functions $\psi : \mathbb{R} \to \mathbb{C}$ with pointwise operations. Two functions $\psi, \phi \in \mathscr{H}$ are said to be equivalent (denoted $\psi \sim \phi$) if they are equal almost everywhere. Then $\sim$ can be shown to be an equivalence relation on $\mathscr{L}^2(\mathbb{R})$ and we define the quotient space $L^2(\mathbb{R}) := \mathscr{L}^2(\mathbb{R}) / \sim$. Then, $L^2(\mathbb{R})$ inherits all the pointwise operations from $\mathscr{L}^2(\mathbb{R})$ and becomes a Hilbert space with $\dim = \infty$ when equipped with the inner product:

$$\langle \psi, \phi \rangle = \int_{\mathbb{R}} \overline{\psi(x)} \phi(x) dx. \tag{2.2}$$

Notice that we've followed the usual convention of denoting an equivalence class of functions by some representative element within the class. It is easy to see that the above definition of inner product is independent of which elements are used to represent the given classes.

Remark 2.9. *It is perhaps worthwhile to emphasize that the relation in Eq.* (2.2) *does not represent a valid inner product on* $\mathscr{L}^2(\mathbb{R})$. *This is because for* $\psi \in \mathscr{L}^2(\mathbb{R})$, $\langle \psi, \psi \rangle = 0$ *does not imply that* ψ *is the zero function (it only implies that* ψ *is zero almost everywhere and hence lies in the equivalence class which contains the zero function).*

2.2 Bounded operators on Hilbert spaces

Definition 2.10. *An operator* $T : \mathscr{H} \to \mathscr{H}$ *is said to be* linear *if*

$$\forall \lambda \in \mathbb{C}, \forall x, y \in \mathscr{H} : \qquad T(\lambda x + y) = \lambda T(x) + T(y).$$

Recall that if $\mathscr{H} = \mathbb{C}^n$ is finite dimensional, then linearity of operators suffices to guarantee continuity as well. However, this is no longer true in infinite dimensions, as the following proposition illustrates.

Proposition 2.11. *For a linear map* $T : \mathscr{H} \to \mathscr{H}$ *defined on a Hilbert space* $\mathscr{H}$, *the following conditions are equivalent:*

- T *is continuous.*
- T *is continuous at* $0 \in \mathscr{H}$.
- T *is bounded in the sense that* $\sup_{\|x\| \leq 1} \|Tx\| = c < \infty$.

The final condition is equivalent to saying that T *maps bounded sets to bounded sets.*

We will denote the space of all bounded linear operators $T : \mathscr{H} \to \mathscr{H}$ on a Hilbert space $\mathscr{H}$ by $\mathscr{B}(\mathscr{H})$. It can be shown that $\mathscr{B}(\mathscr{H})$ turns into a Banach space when equipped with the the usual pointwise vector space operations and the *operator* norm

$$\begin{aligned} \|.\| : \mathscr{B}(\mathscr{H}) &\to [0, \infty) \\ T &\mapsto \sup_{\|x\| \leq 1} \|Tx\|. \end{aligned}$$

Moreover, the multiplicative structure on $\mathscr{B}(\mathscr{H})$ behaves nicely with respect to the operator norm, which turns $\mathscr{B}(\mathscr{H})$ into a *Banach algebra*, i.e.,

$$\forall T, S \in \mathscr{B}(\mathscr{H}) : \quad \|ST\| \leq \|S\| \, \|T\| \text{ and } \|TS\| \leq \|S\| \, \|T\|. \tag{2.3}$$

We now come to the very important notion of the *adjoint* of operators in $\mathscr{B}(\mathscr{H})$.

Proposition 2.12. *Let* $\mathscr{H}$ *be a Hilbert space. For every* $T \in \mathscr{B}(\mathscr{H})$, *there exists a unique* adjoint *operator* $T^* \in \mathscr{B}(\mathscr{H})$ *defined by the following relation*

$$\forall x, y \in \mathscr{H} : \quad \langle Tx, y \rangle = \langle x, T^* y \rangle.$$

It should be noted that if $\mathscr{H} = \mathbb{C}^n$ is finite dimensional, then the space $\mathscr{B}(\mathscr{H})$ can be naturally identified with the familiar space of $n \times n$ complex matrices $M_n(\mathbb{C})$, with the operation of conjugate transpose playing the role of the adjoint. We reiterate that in finite dimensions, the condition of continuity on linear operators is superfluous since every linear operator is automatically continuous/bounded. However, as we have seen above, continuity is an important constraint to impose for operators acting on infinite dimensional Hilbert spaces, which creates room for a rich interplay of techniques from linear algebra and analysis. We now list some important properties of the adjoint operation in $\mathscr{B}(\mathscr{H})$.

Proposition 2.13. *Let $\mathscr{H}$ be a Hilbert space. Then, for all $S, T \in \mathscr{B}(\mathscr{H})$ and $\lambda \in \mathbb{C}$, the following properties of the adjoint operation holds:*

- $(T^*)^* = T$, $(TS)^* = S^*T^*$ *and* $(\lambda T + S)^* = \bar{\lambda}T^* + S^*$
- $\|T\| = \|T^*\|$ *and* $\|T^*T\| = \|T\|^2$.

Remark 2.14. *A Banach algebra B equipped with an involution $* : B \to B$ which satisfies the properties listed in the above proposition is called a C^*-*algebra.

We now define the most important classes of operators in $\mathscr{B}(\mathscr{H})$.

Definition 2.15. *Let $\mathscr{H}$ be a Hilbert space. An operator $T \in \mathscr{B}(\mathscr{H})$ is said to be*

- self-adjoint *if* $T = T^*$.
- *an* orthogonal projection *if* $T = T^* = T^2$.
- unitary *if* $TT^* = T^*T = \mathbb{I}$.
- *an* isometry *if* $T^*T = \mathbb{I}$.
- normal *if* $T^*T = TT^*$.

A few remarks about the above definition are in order.

Remark 2.16. *There is a one-one correspondence between orthogonal projections in $\mathscr{B}(\mathscr{H})$ and closed subspaces of $\mathscr{H}$. Given any closed subspace $S \subseteq \mathscr{H}$, the mapping $\mathscr{H} \ni x \mapsto y \in S$, where $x = y + z$ is the unique splitting of x corresponding to the direct sum decomposition $\mathscr{H} = S \oplus S^\perp$, defines an orthogonal projection in $\mathscr{B}(\mathscr{H})$. Conversely, the range $P\mathscr{H}$ of any orthogonal projection $P \in \mathscr{B}(\mathscr{H})$ can be shown to be a closed subspace of $\mathscr{H}$ so that $\mathscr{H} = P\mathscr{H} \oplus (P\mathscr{H})^\perp$.*

Remark 2.17. *If $V \in \mathscr{B}(\mathscr{H})$ is an isometry, it follows that*

$$\forall x, y \in \mathscr{H} : \quad \langle Vx, Vy \rangle = \langle x, y \rangle.$$

One can easily show that the converse also holds. Notice that the property of preserving inner products implies that $\ker V = \{0\}$. *However, since the range of V may not cover the whole space $\mathscr{H}$, V is not necessarily invertible. Unitary operators in $\mathscr{B}(\mathscr{H})$ are precisely those isometries which can be inverted. Hence, it should be clear that unitary operators are the structure preserving operations on Hilbert spaces, i.e., they are linear bijections which preserve the inner products. In finite dimensions, there is no difference between an isometry and a unitary operator.*

Taking inspiration from the above remark, we say that two Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ are unitarily equivalent if there exists a linear bijection $U : \mathscr{H}_1 \to \mathscr{H}_2$ which preserves inner products. The following result can be thought of as the fundamental theorem on separable Hilbert spaces.

Theorem 2.18. *Every separable Hilbert space $\mathscr{H}$ is unitarily equivalent to either $\mathbb{C}^n$ (if $\dim \mathscr{H} = n < \infty$) or $l^2(\mathbb{N})$ (if $\dim \mathscr{H} = \infty$).*

Now that we have a basic understanding of bounded linear operators on Hilbert spaces, let us provide a definite answer to Question 1.1 from Chapter 1.

Theorem 2.19. *No bounded self-adjoint operators $P, Q \in \mathscr{B}(\mathscr{H})$ defined on some separable Hilbert space $\mathscr{H}$ can satisfy the canonical commutation relation*

$$QP - PQ = i\mathbb{I}.$$

Proof. Suppose there exist self-adjoint $P, Q \in \mathscr{B}(\mathscr{H})$ such that $QP - PQ = i\mathbb{I}$. Then, a simple inductive argument shows that $Q^nP - PQ^n = inQ^{n-1} \neq 0$ for all $n \in \mathbb{N}$. Now, since Q is self-adjoint, it is clear that $\|Q^n\| = \|Q\|^n$. Taking the operator norm on both sides of the above equation then yields

$$n\|Q\|^{n-1} = \|Q^nP - QP^n\| \leq 2\|Q\|^n\|P\|.$$

Since $Q \neq 0 \implies \|Q\| \neq 0$, we obtain $n \leq 2\|Q\|\|P\|$ for any $n \in \mathbb{N}$, which cannot be true since Q, P are bounded. □

Let us conclude this chapter by showing that the Schrödinger representation of the canonical commutation relation constructed in Chapter 1 consists of operators which are not bounded. Take $\mathscr{H} = L^2(\mathbb{R})$ and define Q, P as in Eq. 1.6. An immediate distinction from the setting of bounded operators can be noted by observing that Q, P cannot be defined on all of $\mathscr{H}$, since the derivatives of square integrable functions, for instance, are not guaranteed to be square integrable again. Let us consider the sequence of functions $(f_n)_{n\in\mathbb{N}}$ in $L^2(\mathbb{R})$ defined as $f_n(x) = \sqrt{n}e^{-n^2x^2}$. Then, one can easily show that the derivatives f_n' are again square integrable and the following equations hold:

$$\forall n \in \mathbb{N} : \quad \int_{\mathbb{R}} f_n(x)^2 dx = \sqrt{\pi/2} \qquad \text{and} \qquad \int_{\mathbb{R}} f_n'(x)^2 dx = n^2\sqrt{\pi/2}.$$

Hence, it is clear that P is not bounded on its domain. Similarly, it can be shown that Q is not bounded as well.

3 | Unbounded operators

We have now seen that bounded realizations of the canonical commutation relation on a separable Hilbert space do not exist. Thus, we expand our horizons in this chapter and lock horns with the theory of unbounded linear operators $T : D(T) \to \mathscr{H}$ which are typically only defined on linear subspaces $D(T) \subseteq \mathscr{H}$ within the Hilbert space $\mathscr{H}$. We will quickly see that in order for a sensible notion of adjoint to exist for unbounded operators, their domains $D(T)$ must at least be dense in $\mathscr{H}$. Moreover, we will impose some suitable continuity condition on these operators in order to bring some analytic flavour into an otherwise purely linear algebraic theory. Finally, we will see that the notion of self-adjointness for unbounded operators is very different and much more subtle than that for the bounded operators. Without further ado, let us now delve into the good stuff. The readers should refer to [Rud91, Chapter 13] and [Sun96, Chapter 5] for more elaborate discussions on unbounded operators on Hilbert spaces.

3.1 Fundamental concepts

Definition 3.1. *A densely defined linear operator T on a Hilbert space $\mathscr{H}$ is a linear mapping $T : D(T) \to \mathscr{H}$ defined on a dense linear subspace $D(T) \subseteq \mathscr{H}$.*

Since we will unanimously be concerned only with those linear operators on Hilbert spaces $T : D(T) \to \mathscr{H}$ which are densely defined, the denseness of the domains of all linear operators will be implicitly assumed to be true throughout this thesis.

Definition 3.2. *For linear operators $S : D(S) \to \mathscr{H}$ and $T : D(T) \to \mathscr{H}$, we say that T is an* extension *of S (denoted $S \subseteq T$) if $D(S) \subseteq D(T)$ and $\forall x \in D(S)$, $Sx = Tx$.*

If a linear operator $T : D(T) \to \mathscr{H}$ is bounded on its domain, then it can be uniquely extended to a bounded operator $\hat{T} \in \mathscr{B}(\mathscr{H})$ as follows. For every $x \in \mathscr{H}$, the denseness of $D(T)$ implies that there exists a sequence $(x_n)_{n\in\mathbb{N}}$ in $D(T)$ such that $\lim x_n = x$. Then, since T is bounded on $D(T)$, the sequence $(Tx_n)_{n\in\mathbb{N}}$ is cauchy in $\mathscr{H}$, which allows us to define $\hat{T}x := \lim Tx_n$. It is then straightforward to check that $\hat{T}$ is a well-defined operator in $\mathscr{B}(\mathscr{H})$. Since bounded operators are not useful from the point of view of realizing the canonical commutation relation, we will typically be interested in linear operators which are unbounded on their dense domains.

In general, linear (unbounded) operators on Hilbert spaces can be very strange. In order to get some analytic handle on these objects, we need to impose some sort of continuity on them. Before doing this, let us refresh our memory of continuity of operators in $\mathscr{B}(\mathscr{H})$. For every $T \in \mathscr{B}(\mathscr{H})$ and an arbitrary sequence (x_n) in $\mathscr{H}$ converging to x, the sequence (Tx_n) converges to Tx. Moreover, the limit Tx is independent of the sequence (x_n) and depends only on x. Now, for an unbounded operator $T : D(T) \to \mathscr{H}$, two things can go wrong. Firstly, the convergence of a sequence (x_n) in $\mathscr{H}$ does not guarantee the convergence of (Tx_n). Secondly, even if (Tx_n) is convergent, the limit may very well depend on the sequence (x_n) in the sense that a different sequence (x'_n) converging to the same x may exist such that $\lim Tx'_n \neq \lim Tx_n$.

We bypass the above difficulties by defining the following class of linear operators.

Definition 3.3. *The graph $G(T)$ of a linear operator $T : D(T) \to \mathscr{H}$ is defined to be the subspace $G(T) := \{(x, Tx) \in \mathscr{H} \times \mathscr{H} \mid x \in D(T)\}$. Then, T is said to be*

- closed *if $G(T)$ is closed as a subset of $\mathscr{H} \times \mathscr{H}$.*
- closable *if there exists a closed linear operator $S : D(S) \to \mathscr{H}$ such that $T \subseteq S$.*

Notice that for an arbitrary Hilbert space $\mathscr{H}$, in order for the usual topological notions to be well-defined in $\mathscr{H} \times \mathscr{H}$, we can equip it with pointwise vector space operations and the inner product $\langle (x_1, y_1), (x_2, y_2) \rangle = \langle x_1, y_1 \rangle + \langle x_2, y_2 \rangle$, so that it again becomes a Hilbert space.

Let us now try to understand Definition 3.3 in a bit more detail. What does it mean for the graph $G(T)$ of a linear operator $T : D(T) \to \mathscr{H}$ to be closed in $\mathscr{H} \times \mathscr{H}$? It means that for all sequences $(x_n)_{n \in \mathbb{N}}$ in $D(T)$ such that $\lim x_n = x$ and $\lim Tx_n = y$, it must be the case that $x \in D(T)$ and $y = Tx$. If T is not closed but closable, it just means that the domain $D(T)$ is not large enough to guarantee the aforementioned continuity property but it can be suitably extended so that there exists a closed extension $S : D(S) \to \mathscr{H}$ of T with the required continuity. For closable linear operators, it thus sounds reasonable to look for a minimal closed extension.

Definition 3.4. *For a closable linear operator $T : D(T) \to \mathscr{H}$, its* closure *is defined to be the closed linear extension $\overline{T} : D(\overline{T}) \to \mathscr{H}$ ($T \subseteq \overline{T}$) with the property that for all closed linear extensions $S : D(S) \to \mathscr{H}$ ($T \subseteq S$), it is the case that $\overline{T} \subseteq S$.*

Lemma 3.5. *Let $T : D(T) \to \mathscr{H}$ be a closable linear operator. Then, its closure $\overline{T}$ is the unique closed linear operator defined by the following property*

$$G(\overline{T}) = \overline{G(T)},$$

where $\overline{G(T)}$ denotes the topological closure of $G(T)$ in $\mathscr{H} \times \mathscr{H}$.

Proof. Notice that since T is closable, there exists a closed extension $T \subseteq S$ such that $G(T) \subseteq G(S)$ and $G(S)$ is a closed subspace of $\mathscr{H} \times \mathscr{H}$. Now, by definition of topological closure, $\overline{G(T)}$ is the minimal closed subset that contains $G(T)$. Hence, the following inclusion holds: $G(T) \subseteq \overline{G(T)} \subseteq G(S)$. Moreover, it is easy to check that $\overline{G(T)}$ is indeed a graph of some linear operator on $\mathscr{H}$, since it is a linear subspace of $\mathscr{H} \times \mathscr{H}$ which doesn't contain a point of the form $(0, y)$ for some $y \neq 0$. If such a point did belong in $\overline{G(T)}$ and hence in $G(S)$, it would imply that $S(0) = y \neq 0$, which is impossible since S is linear. We leave an easy proof of the fact that the only condition on a subspace $G \subseteq \mathscr{H} \times \mathscr{H}$ to represent the graph of some linear operator on $\mathscr{H}$ is that G must not contain a point of the form $(0, y)$, where $y \neq 0$. □

Let us now extend the notion of the adjoints to the realm of unbounded operators.

Definition 3.6. *For every linear operator $T : D(T) \to \mathscr{H}$, there exists a unique linear operator (called its* adjoint*) $T^* : D(T^*) \to \mathscr{H}$ with domain*

$$D(T^*) := \{y \in \mathscr{H} \mid \exists! z \in \mathscr{H} : \forall x \in D(T) : \langle y, Tx \rangle = \langle z, x \rangle\},$$

defined as $T^* y := z$, where $y \in D(T^*)$ and $z \in \mathscr{H}$ are as above.

Notice that the domain $D(T^*)$ of the adjoint of a linear operator $T : D(T) \to \mathscr{H}$ is defined to contain precisely those $y \in \mathscr{H}$ for which the linear mapping

$$D(T) \ni x \mapsto \langle y, Tx \rangle \in \mathbb{C}$$

is continuous. Now, if and only if the domain $D(T)$ is dense in $\mathscr{H}$, can we uniquely extend this mapping to the whole Hilbert space so as to obtain an element of the dual $\mathscr{H}^*$, see the discussion following Definition 3.2 for more details on how to obtain this extension. The Riesz representation theorem (Theorem 2.4) then guarantees the existence of a unique vector $T^* y := z \in \mathscr{H}$ for each $y \in D(T^*)$ with the property that $\forall x \in D(T) : \langle y, Tx \rangle = \langle z, x \rangle$. This is why it is essential to work with densely defined linear operators. Finally, observe that if T is bounded on its domain, then $D(T^*)$ is trivially seen to be equal to the entire Hilbert space $\mathscr{H}$, and Definition 3.6 reduces to the one in Proposition 2.12. We note some interesting properties of adjoints in the following propositions.

Proposition 3.7. *For linear operators $S : D(S) \to \mathscr{H}$ and $T : D(T) \to \mathscr{H}$,*

$$S \subseteq T \implies T^* \subseteq S^*.$$

Proof. Let us write down the definition of the domains of $D(S^*)$ and $D(T^*)$:

$$D(S^*) = \{y \in \mathscr{H} \mid \exists! z \in \mathscr{H} : \forall x \in D(S) : \langle y, Sx \rangle = \langle z, x \rangle\}$$
$$D(T^*) = \{y \in \mathscr{H} \mid \exists! z \in \mathscr{H} : \forall x \in D(T) : \langle y, Tx \rangle = \langle z, x \rangle\}$$

Now, since $D(S) \subseteq D(T)$ and $\forall x \in D(S) : Sx = Tx$, it is evident that a stricter condition needs to be checked in order to ensure membership of a given $y \in \mathscr{H}$ in $D(T^*)$ when compared to $D(S^*)$. Hence, $D(T^*) \subseteq D(S^*)$ and $\forall y \in D(T^*) : T^* y = S^* y$. ☐

Proposition 3.8. *For a linear operator $T : D(T) \to \mathscr{H}$, its adjoint T^* is always closed.*

Proof. We intend to show that the graph of T^* is the orthogonal complement of a subspace in $\mathscr{H} \times \mathscr{H}$, and is hence closed. Let $G = \{(Tx, -x) \in \mathscr{H} \times \mathscr{H} \,|\, x \in D(T)\}$. Then, for $y \in D(T^*)$, we have that $\forall x \in D(T) : \langle y, Tx \rangle = \langle T^* y, x \rangle \implies (y, T^* y) \in G^{\perp} \implies G(T^*) \subseteq G^{\perp}$. Conversely, if $(y, z) \in G^{\perp}$, then $\forall x \in D(T)$, we have that $\langle y, Tx \rangle - \langle z, x \rangle = 0$, which clearly implies that $y \in D(T^*)$ and $T^* y = z$. Thus, $(y, z) \in G(T^*)$ and $G^{\perp} \subseteq G(T^*)$. In other words, if we define the unitary operator $\mathscr{U} : \mathscr{H} \times \mathscr{H} \to \mathscr{H} \times \mathscr{H}$ as $\mathscr{U}(x, y) = (y, -x)$, the following equality holds

$$G(T^*) = [\mathscr{U} G(T)]^{\perp}.$$

☐

Remark 3.9. *For a densely defined linear operator $T : D(T) \to \mathscr{H}$, its adjoint may not necessarily be densely defined.*

It turns out that there is an intriguing connection between the adjoint of a linear operator $T : D(T) \to \mathscr{H}$ and the property of closability of T, as we now illustrate.

Proposition 3.10. *A linear operator $T : D(T) \to \mathscr{H}$ is closable if and only if its adjoint $T^* : D(T^*) \to \mathscr{H}$ is densely defined, in which case $\overline{T} = T^{**}$. Moreover, for a closable linear operator $T : D(T) \to \mathscr{H}$, the following relation holds: $T^* = (\overline{T})^*$.*

Proof. Assume first that T is closable. Then, if $y \in D(T^*)^\perp$, it is easy to see that $(y,0) \in G(T^*)^\perp$, which implies that $(0,y) \in \overline{G(T)} = G(\overline{T})$, see Proposition 3.8. This in turn implies that $y = 0$, see the closing discussion in the proof of Lemma 3.5. Hence $D(T^*)$ lies dense in $\mathscr{H}$. Conversely, if $D(T^*)$ is densely defined, one can define the closed operator T^{**} and quickly deduce that $T \subseteq T^{**}$. Moreover, if we take $\mathscr{U}$ to be the unitary operator from Proposition 3.8, we can write

$$G(T^{**}) = [\mathscr{U} G(T^*)]^\perp = [-\mathscr{U}^* G(T^*)]^\perp = [-\mathscr{U}^*(\mathscr{U} G(T))^\perp]^\perp = [G(T)^\perp]^\perp = \overline{G(T)},$$

so that we can exploit Lemma 3.5 to infer that $T^{**} = \overline{T}$.

Finally, if T is a closable operator, Proposition 3.7 informs us that $T \subseteq \overline{T} \implies (\overline{T})^* \subseteq T^*$. Hence, to obtain the equality $(\overline{T})^* = T^*$, we must show that $D(T^*) \subseteq D((\overline{T})^*)$. With this end in sight, assume that $x \in D(T^*)$. Then, by definition of the adjoint, we have

$$\forall y \in D(T) : \quad \langle x, Ty \rangle = \langle T^* x, y \rangle.$$

Consider now an arbitrary $z \in D(\overline{T})$. Then, there exists a sequence $(z_n)_{n \in \mathbb{N}}$ in $D(T)$ such that $z_n \to z$ and $T z_n \to \overline{T} z$. Hence, we have that

$$\langle x, \overline{T} z \rangle = \lim_{n \to \infty} \langle x . T z_n \rangle = \lim_{n \to \infty} \langle T^* x, z_n \rangle = \langle T^* x, z \rangle.$$

This is precisely the condition that $x \in D((\overline{T})^*)$, which is what we wanted to show. □

3.2 Symmetric and self-adjoint operators

Recall that a bounded operator $T \in \mathscr{B}(\mathscr{H})$ is said to be self-adjoint if it is equal to its adjoint, i.e. $T = T^*$. From Proposition 2.12, this is equivalent to saying that

$$\forall x, y \in \mathscr{H} : \quad \langle x, Ty \rangle = \langle Tx, y \rangle. \tag{3.1}$$

The situation is drastically different when the concerned operators are unbounded.

Definition 3.11. *A linear operator $T : D(T) \to \mathscr{H}$ is said to be*

- symmetric, *if $T \subseteq T^*$.*
- self-adjoint, *if $T = T^*$.*
- essentially self-adjoint, *if it is closable and its closure $\overline{T}$ is self-adjoint.*

Note that the symmetry condition for $T : D(T) \to \mathscr{H}$ in the above definition is equivalent to the following property

$$\forall x, y \in D(T) : \quad \langle x, Ty \rangle = \langle Tx, y \rangle, \tag{3.2}$$

which can be interpreted as a "naive" attempt towards generalizing the notion of self-adjointness from the bounded to the unbounded regime. The naivety here stems from the fact that Eq (3.2) only implies $T \subseteq T^*$, and *not* $T = T^*$, since although T and T^*

clearly agree on $D(T)$, the domain of T^* can be larger. Hence, we see that self-adjointness is a strictly stronger notion than symmetricity for unbounded operators. Also notice that Proposition 2.12 implies that a symmetric operator is closable while a self-adjoint operator is closed. Finally, essentially self-adjoint operators lie somewhere between the symmetric and self-adjoint operators, as we now exhibit.

Lemma 3.12. *Let $T : D(T) \to \mathscr{H}$ be a closable linear operator. Then,*

$$\begin{aligned} T \text{ is symmetric} &\iff T \subseteq \overline{T} \subseteq T^*. \\ T \text{ is essentially self-adjoint} &\iff T \subseteq \overline{T} = T^*. \\ T \text{ is self-adjoint} &\iff T = \overline{T} = T^*. \end{aligned}$$

Proof. If T is symmetric, we know by definition that $T \subseteq T^*$. Moreover, since the closure $\overline{T}$ is the minimal closed extension of T and T^* is always closed, we obtain

$$T \subseteq \overline{T} \subseteq T^*.$$

If T is essentially self-adjoint, we know that the closure $\overline{T}$ is self-adjoint. Moreover, since T is closable, Proposition 3.10 tells us that $T^* = (\overline{T})^*$, so that we obtain the desired result

$$T \subseteq \overline{T} = (\overline{T})^* = T^*.$$

If T is self-adjoint, the desired conclusion is trivial to deduce. □

Let us come back into the physical world for a moment and ask ourselves why only self-adjoint operators on Hilbert spaces are chosen to be the observables in quantum mechanics. A substantial part of the reason has to do with the fact that the *spectral theorem* only holds for self-adjoint operators on Hilbert spaces, see Chapter 5. Among other things, this theorem ensures that a unique subset of the real line can be associated with each observable, which acts as the set of possible outcomes that one encounters upon measuring the observable. For now, the important thing to note is that the physically constructed operators $T : D(T) \to \mathscr{H}$ are typically only known to be symmetric, since the condition in Eq. (3.2) is straightforward to check in practice. On the other hand, proving that a given symmetric operator is self-adjoint is a whole lot harder. One needs to explicitly compute the domain $D(T^*)$ of the adjoint operator and show that it is equal to the original domain $D(T)$, which is easier said than done. If the originally chosen domain $D(T)$ is not exactly right, the operator will not turn out to be self-adjoint. In such a scenario, it becomes meaningful to ask if there are any self-adjoint extensions of the given operator which can act as observables. Here, the following possibilities can arise:

- There may not exist any self-adjoint extensions of T.
- There may exist many self-adjoint extensions of T, in which case it is impossible to make a unique selection without additional physical insight.
- There may be only one unique self-adjoint extension of T. This is the desirable situation which occurs precisely when T is essentially self-adjoint. The closure $\overline{T}$ then acts as the unique self-adjoint extension. If we assume that S is another self-adjoint extension of T, i.e., $T \subseteq S$, we can easily deduce that $S \subseteq T^* = (\overline{T})^* = \overline{T}$ by taking adjoints. But, since S is closed and $\overline{T}$ is the minimal closed extension, it must also be the case that $\overline{T} \subseteq S$. Hence, $S = \overline{T}$.

The above discussion informs us that it is of utmost physical relevance to decide when a given symmetric operator is self-adjoint or essentially self-adjoint. The following theorems are important results in this direction. Let us first state an easy Lemma.

Lemma 3.13. *For a linear operator $T : D(T) \to \mathscr{H}$, $(\operatorname{range} T)^{\perp} = \ker T^*$. In addition, if T is closed, then $\ker T$ is a closed subspace of $\mathscr{H}$.*

Proof. Trivial, see [Sun96, Lemma 5.2.5]. □

Theorem 3.14. *For a symmetric operator $T : D(T) \to \mathscr{H}$, the following are equivalent:*

- *T is self-adjoint.*
- *T is closed and $\ker(T^* + i) = \ker(T^* - i) = \{0\}$.*
- $\operatorname{range}(T + i) = \operatorname{range}(T - i) = \mathscr{H}$.

Proof. Assume first that $T = T^*$. Then, T is automatically closed. Moreover, for a non-zero $\lambda \in \mathbb{C} \setminus \mathbb{R}$, if there exists $x \in D(T)$ such that $Tx = \lambda x$, then we can write

$$\lambda \langle x, x\rangle = \langle x, Tx\rangle = \langle Tx, x\rangle = \bar{\lambda} \langle x, x\rangle,$$

which clearly implies that $x = 0$, since $\lambda \neq \bar{\lambda}$. Hence, $\ker(T + \lambda) = 0$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

Now, assume that T is closed and $\ker(T^* \pm i) = \{0\}$. Then, $\operatorname{range}(T \pm i)^{\perp} = \ker(T^* \mp i) = \{0\}$ (see Lemma 3.13) so that both ranges are dense in $\mathscr{H}$. Moreover, since T is symmetric, it is easy to see that $\forall x \in D(T)$:

$$\begin{aligned} \|(T \mp i)x\|^2 = \langle (T \mp i)x, (T \mp i)x\rangle &= \langle Tx, Tx\rangle \pm i\langle x, Tx\rangle \mp i\langle Tx, x\rangle + \langle x, x\rangle \\ &= \|Tx\|^2 + \|x\|^2. \end{aligned}$$

Hence, the mapping $\operatorname{range}(T \pm i) \ni (T \pm i)x \mapsto (Tx, x) \in G(T)$ sets up an isometric correspondence between the given spaces. Since we already know that $G(T)$ is closed, the previous argument implies that $\operatorname{ran}(T \pm i) = \mathscr{H}$.

Finally, assume that $\operatorname{ran}(T \pm i) = \mathscr{H}$. Now, since $T - i$ is surjective, for every $x \in D(T^*)$, we can find $y \in D(T)$ such that $(T - i)y = (T^* - i)x$. Moreover, since T is symmetric ($T \subseteq T^*$), we have that y also lies in $D(T^*)$ and $(T - i)y = (T^* - i)y$, so that $(x - y) \in \ker(T^* - i) = \operatorname{ran}(T + i)^{\perp} = \{0\}$ (see Lemma 3.13). Hence, $x = y \in D(T)$ and we arrive at the conclusion that $D(T^*) \subseteq D(T) \implies T = T^*$. □

Theorem 3.15. *For a symmetric operator $T : D(T) \to \mathscr{H}$, the following are equivalent:*

- *T is essentially self-adjoint.*
- $\ker(T^* + i) = \ker(T^* - i) = \{0\}$.
- $\overline{\operatorname{range}(T + i)} = \overline{\operatorname{range}(T - i)} = \mathscr{H}$.

Proof. Similar to that of Theorem 3.14. □

Now that we are equipped with the basic theory of unbounded operators on Hilbert spaces, let us properly describe the Schrödinger representation of the canonical commutation relation which was introduced towards the end of Chapter 1.

Theorem 3.16 (Schrödinger representation)**.** *Let $\mathscr{H} = L^2(\mathbb{R})$ and $D = C_c^\infty(\mathbb{R}) \subseteq L^2(\mathbb{R})$ be the dense linear subspace of smooth functions with compact support. Let the position and momentum operators $Q, P : D \to \mathscr{H}$ be defined as follows*

$$\begin{aligned} Q\psi(x) &= x\psi(x) \\ P\psi(x) &= -i\psi'(x). \end{aligned} \tag{3.3}$$

Then, the following statements hold true:

- *$Q : D \to D$ and $P : D \to D$.*
- *$\forall \psi \in D: \ (QP - PQ)\psi = i\psi$.*
- *Q and P are essentially self-adjoint on D.*

Proof. From the definition Q, P, it is trivial to infer that the domain $C_c^\infty(\mathbb{R})$ stays invariant under both of them. The next implication can be obtained with similar ease:

$$\forall \psi \in C_c^\infty(\mathbb{R}): \quad (QP - PQ)\psi(x) = -ix\psi'(x) + i\psi(x) + ix\psi'(x) = i\psi(x).$$

Now, to show that Q, P are essentially self-adjoint on $C_c^\infty(\mathbb{R})$, we will exploit Theorem 3.15. First of all, just by checking the validity of Eq. (3.2), it is trivial to deduce that both Q and P are symmetric on $C_c^\infty(\mathbb{R})$, so that we know $Q \subseteq Q^*$ and $P \subseteq P^*$.

Now, let us first deal with the momentum operator P. We intend to show that $\ker(P^* + i) = \{0\}$. To this end, let us assume $\psi \in D(P^*)$ is such that $P^*\psi = -i\psi$. This is equivalent to saying that for all $\phi \in C_c^\infty(\mathbb{R})$:

$$\int_{\mathbb{R}} i\overline{\phi'(x)}\psi(x)\,dx = \langle P\phi, \psi\rangle = \langle \phi, P^*\psi\rangle = \langle \phi, -i\psi\rangle = \int_{\mathbb{R}} -i\overline{\phi(x)}\psi(x).$$

The above equation can be used to show that ψ must be the zero function in $L^2(\mathbb{R})$, see [Hal13, Proposition 9.29]. Thus, we have shown that $\ker(P^* + i) = \{0\}$. An identical argument can be deployed to show that $\ker(P^* - i) = \{0\}$ as well, so that Theorem 3.15 can be employed to conclude that P is essentially self-adjoint on $C_c^\infty(\mathbb{R})$.

We now replicate the above argument for Q. Assume that $\psi \in D(Q^*)$ is such that $Q^*\psi = -i\psi$, so that the following equation holds for all $\phi \in C_c^\infty(\mathbb{R})$:

$$\int_{\mathbb{R}} x\overline{\phi(x)}\psi(x)\,dx = \langle Q\phi, \psi\rangle = \langle \phi, Q^*\psi\rangle = \langle \phi, -i\psi\rangle = \int_{\mathbb{R}} -i\overline{\phi(x)}\psi(x),$$

which clearly implies that $\psi = 0$ in $L^2(\mathbb{R})$. Hence, $\ker(Q^* + i) = \{0\}$ and a similar argument shows that $\ker(Q^* - i) = \{0\}$ as well, so that according to Theorem 3.15, Q is essentially self-adjoint on $C_c^\infty(\mathbb{R})$.

□

Motivated by the above theorem, we now conclude this chapter by formally defining what it means for some self-adjoint operators to form a representation of the canonical commutation relation.

Definition 3.17. *Two self-adjoint linear operators $Q : D(Q) \to \mathscr{H}$ and $P : D(P) \to \mathscr{H}$ are said to form a representation of the canonical commutation relation if there exists a common dense domain $D \subseteq D(Q) \cap D(P)$ with the following properties:*

- *$Q : D \to D$ and $P : D \to D$.*
- $\forall \psi \in D : \ (QP - PQ)\psi = i\psi$.
- *Q and P are essentially self-adjoint on D.*

This marks the end of the first part of our exposition. We have now explicitly constructed and studied one concrete representation of the canonical commutation relation on the Hilbert space $L^2(\mathbb{R})$. From the next chapter onwards, we will question the uniqueness of this representation, which will lead us finally to the Stone-von Neumann uniqueness theorem in Chapter 7.

Part II

4 | What next?

Is the Schrödinger representation of the canonical commutation relation unique? In its full generality, the answer is a brutal no. In fact, there exist uncountably many representations of the CCR which are all inequivalent, see [Phi81] and references therein. However, it turns out that a closely related uniqueness question has an affirmative answer. This question is formulated entirely in terms of families of bounded operators, which can be uniquely constructed from the self-adjoint operators present in the given representation of the CCR. To elaborate on this, let us consider two self-adjoint operators Q,P that form a representation of the CCR in the sense of Definition 3.17. We now define the following one-parameter families of bounded operators:

$$\{e^{itQ} : t \in \mathbb{R}\} \subseteq \mathscr{B}(\mathscr{H}) \quad \text{and} \quad \{e^{isP} : s \in \mathbb{R}\} \subseteq \mathscr{B}(\mathscr{H}). \tag{4.1}$$

At this juncture, the reader should be terribly confused. How are we defining the exponential of an unbounded operator? Why should this exponential be bounded? If Q,P were in the Banach space $\mathscr{B}(\mathscr{H})$ of bounded operators, then the situation would have been much saner as we could have easily defined the above families through the usual exponential power series. However, this cannot be done for unbounded operators, as there is no norm (and hence no notion of convergence) on the space of unbounded operators! Our aim in Chapter 5 would be to rigorously define a large class of functions (including the exponentials) of unbounded self-adjoint operators in order to completely decimate the above confusion. For now, let us assume that a sensible definition of the exponentials exist which is somewhat similar to the usual power series definition. In that case, a heuristic application of the well-known Baker-Hausdorff-Campbell lemma[1] on the exponentials in Eq (4.1) yields the following equation

$$\forall s,t \in \mathbb{R}: \qquad e^{isP}e^{itQ} = e^{ist}e^{itQ}e^{isP}, \tag{4.2}$$

which is known as the *Weyl* relation and can be thought of as the exponential analogue of the canonical commutation relation

$$QP - PQ = i\mathbb{1}. \tag{4.3}$$

Before proceeding further, it is critical to point out that Equations (4.2) and (4.3) are not equivalent! In other words, if Q and P form a representation of the CCR as in Definition 3.17, it does not automatically imply that the corresponding exponential families satisfy Eq (4.2). This provides strong evidence in favour of the following fact:

Heuristic calculations performed in the realm of unbounded operators can lead to horribly wrong conclusions!

[1] For bounded operators $A,B \in \mathscr{B}(\mathscr{H})$, the BHC lemma says that $e^{A+B} = e^{-[A,B]/2}e^{A}e^{B}$.

That being said, for the special position and momentum operators Q,P forming the Schrödinger representation of the CCR on $L^2(\mathbb{R})$, the corresponding exponential families of operators $\{e^{itQ}\}_{t\in\mathbb{R}}$ and $\{e^{isP}\}_{s\in\mathbb{R}}$ will be rigorously shown to satisfy the Weyl relations in Chapter 6. In this case, we say that the families $\{e^{itQ}\}_{t\in\mathbb{R}}$ and $\{e^{isP}\}_{s\in\mathbb{R}}$ form the Schrödinger representation of the Weyl relation. Conversely, the Stone-von Neumann theorem tells us that any other representation of the Weyl relation is equivalent to the Schrödinger representation. Put differently, if Q,P are self-adjoint operators such that the corresponding families of bounded exponentials satisfy the Weyl relations, then Q,P are the same as the usual position and momentum operators!

In the next two chapters, our aim is to build enough theory in order to properly formulate and prove the stated uniqueness theorem, which will form the subject matter of the last chapter.

5 | Spectral theorem

To say that the spectral theorem is a foundational result in modern operator theory would be an understatement. The implications of this cornerstone result pervade a variety of realms in both physics and mathematics. In our case, the spectral theorem will enable us to rigorously define a huge family of functions of self-adjoint operators (including the exponentials, as in Eq (4.1)), which will prove to be instrumental in our discussion of the Stone-von Neumann theorem later. Since the proofs of most of the results in this chapter are fairly involved, we have decided not to include them explicitly. The interested readers should refer to the provided references for details on the proofs. We list some excellent references on the subject here: [Rud91, Chapters 12-13], [Sun16], [Con85, Chapters IX-X], [Bor20] and [Hal13, Chapters 6-10].

5.1 Spectrum of closed operators

Recall that if $\mathscr{H}$ is finite dimensional, then each $T \in \mathscr{B}(\mathscr{H})$ can be identified with a matrix and the spectrum of T consists of the eigenvalues of this matrix. More precisely, the spectrum $\sigma(T)$ consists of all $\lambda \in \mathbb{C}$ such that $\ker(T - \lambda \mathbb{I}) \neq \{0\}$, which is equivalent to saying that $T - \lambda \mathbb{I}$ is not invertible. We generalize this notion for arbitrary closed operators in infinite dimensions as follows.

Definition 5.1. *Let $T : D(T) \to \mathscr{H}$ be a closed linear operator. Then, the* resolvent *set $\rho(T)$ is defined as $\rho(T) := \{\lambda \in \mathbb{C} \,|\, \exists S \in \mathscr{B}(\mathscr{H}), S(T - \lambda \mathbb{I}) \subseteq (T - \lambda \mathbb{I})S = \mathbb{I}\}$, and the* spectrum *$\sigma(T)$ is defined as $\sigma(T) := \mathbb{C} \setminus \rho(T)$.*

There can be three distinct ways by which $\lambda \in \mathbb{C}$ can lie in the spectrum:

- $\ker(T - \lambda \mathbb{I}) \neq \{0\}$. The collection of all such $\lambda \in \mathbb{C}$ is called the *point* spectrum $\sigma_p(T)$, which is nothing but the set of all eigenvalues of T.
- $\ker(T - \lambda \mathbb{I}) = \{0\}$, $\mathrm{range}(T - \lambda \mathbb{I}) \subseteq \mathscr{H}$ is dense but $(T - \lambda \mathbb{I})^{-1} : \mathrm{range}(T - \lambda \mathbb{I}) \to D(T)$ is unbounded. Such $\lambda \in \mathbb{C}$ are collected in the *continuous* spectrum $\sigma_c(T)$.
- $\ker(T - \lambda \mathbb{I}) = \{0\}$ but $\mathrm{range}(T - \lambda \mathbb{I}) \subseteq \mathscr{H}$ is not dense. The collection of all such $\lambda \in \mathbb{C}$ is called the *residual* spectrum.

It is easy to see that the spectrum of any closed operator T can be decomposed into the disjoint union: $\sigma(T) = \sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T)$.

Remark 5.2. *The elements of the continuous spectrum of a closed operator T can be thought of as the* approximate *eigenvalues of T in the following sense. By definition, if*

$\lambda \in \sigma_c(T)$, then $(T-\lambda\mathbb{I})^{-1}$: range$(T-\lambda\mathbb{I}) \to D(T)$ is unbounded, i.e., there exists a sequence $(x_n)_{n\in\mathbb{N}}$ of unit vectors in range$(T-\lambda\mathbb{I})$ *such that $\|(T-\lambda\mathbb{I})^{-1}x_n\| \to \infty$ as $n \to \infty$. Now, if we define another sequence of unit vectors*

$$y_n := (T-\lambda\mathbb{I})^{-1}x_n/\|(T-\lambda\mathbb{I})^{-1}x_n\|,$$

it should be clear that $\|(T-\lambda\mathbb{I})y_n\| \to 0$ as $n \to \infty$.

Proposition 5.3. *[Con85, Chapter X, Proposition 1.17; Chapter VII, Theorem 3.6] The spectrum $\sigma(T)$ of a closed operator $T : D(T) \to \mathscr{H}$ is closed in $\mathbb{C}$. Moreover, if $T \in \mathscr{B}(\mathscr{H})$, then $\sigma(T)$ is bounded (hence compact) and non-empty.*

Let us now conclude this section by making some interesting observations on the spectrum of self-adjoint operators.

Proposition 5.4. *[Con85, Chapter X, Corollary 2.9] A closed symmetric operator $T : D(T) \to \mathscr{H}$ is self-adjoint if and only if $\sigma(T) \subseteq \mathbb{R}$. Moreover, the residual spectrum of a self-adjoint operator is empty.*

5.2 Projection-valued measures

For a set Δ, we denote its power set by $\mathscr{P}(\Delta)$. Given a choice of topology $\tau \subseteq \mathscr{P}(\Delta)$ on Δ, $\mathfrak{F}(\tau) \subseteq \mathscr{P}(\Delta)$ is used to denote the σ-algebra generated by τ, so that $(\Delta, \mathfrak{F}(\tau))$ becomes a *measurable* space. We will mostly consider $\Delta = \mathbb{R}$ (or $\Delta = \mathbb{C}$) and $\tau = \tau_{\mathbb{R}}$ (or $\tau = \tau_{\mathbb{C}}$) to be the standard topology, so that $\mathfrak{F}(\tau)$ becomes the *Borel* σ-algebra on $\mathbb{R}$ (or $\mathbb{C}$). For topological spaces (Δ, τ) and $(\mathbb{C}, \tau_{\mathbb{C}})$, a function $f : \Delta \to \mathbb{C}$ is said to be *measurable* if $\omega \in \mathfrak{F}(\tau_{\mathbb{C}}) \implies \{\lambda \in \Delta \,|\, f(\lambda) \in \omega\} \in \mathfrak{F}(\tau)$.

Definition 5.5. *A* projection-valued measure *(PVM) on a topological space (Δ, τ) is a map $E : \mathfrak{F}(\tau) \to \mathscr{B}(\mathscr{H})$ with the following properties:*

- *$E(\emptyset) = 0$ and $E(\Delta) = \mathbb{I}$.*
- *$\forall \omega \in \mathfrak{F}(\tau)$: $E(\omega)$ is an orthogonal projection.*
- *$\forall \omega_1, \omega_2 \in \mathfrak{F}(\tau)$: $E(\omega_1 \cap \omega_2) = E(\omega_1)E(\omega_2)$.*
- *$\forall$disjoint $\omega_1, \omega_2 \in \mathfrak{F}(\tau)$: $E(\omega_1 \cup \omega_2) = E(\omega_1) + E(\omega_2)$.*
- *$\forall x, y \in \mathscr{H}$: the function $E_{x,y} : \mathfrak{F}(\tau) \to \mathbb{C}$ defined by $E_{x,y}(\omega) = \langle x, E(\omega)y\rangle$ is a regular complex measure. Then $E_{x,x} := E_x$ is a regular, positive, and finite measure.*

Given a PVM $E : \mathfrak{F}(\tau) \to \mathscr{B}(\mathscr{H})$ on a topological space (Δ, τ), we define $L^\infty(E)$ as the space of all bounded measurable functions $f : \Delta \to \mathbb{C}$, where any two almost everywhere agreeing functions are identified with each other like in Example 2.8. This space can be equipped with all the usual pointwise operations (scalar multiplication and vector addition/multiplication), including an involution defined by pointwise complex conjugation (denoted $\bar{f}$). We also equip this space with the *essential supremum* norm $\|\cdot\|_\infty$, which, for a given $f \in L^\infty(E)$, is defined to be the minimal $M \geq 0$ such that $|f(\lambda)| \leq M$ almost everywhere. The next theorem identifies this space with a special type of subalgebra of $\mathscr{B}(\mathscr{H})$.

Theorem 5.6. *[Rud91, Theorem 12.21]*
*Let $E : \mathfrak{F}(\tau) \to \mathscr{B}(\mathscr{H})$ define a PVM on a topological space (Δ, τ). Then, $L^\infty(E)$ is isometrically *-isomorphic to a closed, commutative, *-subalgebra of $\mathscr{B}(\mathscr{H})$. The mapping $f \mapsto \int_\Delta f dE$ sets up the required isomorphism, where the integral is uniquely defined by the following relation*

$$\forall x, y \in \mathscr{H} : \quad \langle x, \int_\Delta f dE\, y\rangle = \int_\Delta f dE_{x,y}.$$

By a closed, commutative, *-subalgebra of $\mathscr{B}(\mathscr{H})$, we mean a (topologically) closed subspace of $\mathscr{B}(\mathscr{H})$ in which operator multiplication is commutative and the subspace is closed under this multiplication and the adjoint operation. If we denote $\int_\Delta f dE$ by $\Psi(f)$, then Ψ is an isometric *-isomorphism is equivalent to saying that Ψ is one-one and for all $f, g \in L^\infty(E)$,

- $\Psi(f+g) = \Psi(f) + \Psi(g)$ and $\Psi(fg) = \Psi(f)\Psi(g)$.
- $\Psi(\bar{f}) = \Psi(f)^*$ and $\|\Psi(f)\| = \|f\|_\infty$.

Notice that if f is real valued, then the above property implies that $\Psi(f)$ is self-adjoint. Finally, it can be shown that

$$\forall x \in \mathscr{H} : \quad \|\Psi(f)x\|^2 = \int_\Delta |f|^2 dE_x.$$

Now, let us see if we can extend the above integration procedure to work even for unbounded functions $f : \Delta \to \mathbb{C}$. In this case, it is natural to expect that the integrals $\int_\Delta f dE$ will be also be unbounded.

Theorem 5.7. *[Rud91, Theorem 13.24]*
Let $E : \mathfrak{F}(\tau) \to \mathscr{B}(\mathscr{H})$ define a PVM on a topological space (Δ, τ) and let $f : \Delta \to \mathbb{C}$ be a measurable function. Then, there exists a (densely defined) closed linear operator

$$\int_\Delta f dE : D_f \to \mathscr{H} \quad \text{with} \quad D_f = \left\{ x \in \mathscr{H} \mid \int_\Delta |f|^2 dE_x < \infty \right\},$$

which is uniquely defined by the following relation

$$\forall x \in \mathscr{H}, \forall y \in D_f : \quad \langle x, \int_\Delta f dE\, y\rangle = \int_\Delta f dE_{x,y}.$$

Moreover, if $f \in L^\infty(E)$, then $\Psi(f) \in \mathscr{B}(\mathscr{H})$ and the construction in Theorem 5.6 is recovered.

If we denote $\int_\Delta f dE$ by $\Psi(f)$ again, the following properties of the integral hold:

- $\Psi(f) + \Psi(g) \subseteq \Psi(f+g)$ and $\Psi(f)\Psi(g) \subseteq \Psi(fg)$.
- $\Psi(\bar{f}) = \Psi(f)^*$ and $\forall x \in D_f : \|\Psi(f)x\| = \int_\Delta |f|^2 dE_x$.

Notice that in the first property above, we do not have equality of operators (as was the case with integrals of bounded functions) since the domains of the concerned operators may not necessarily be equal. At this point, we should perhaps a common notational convention regarding integrals. Often, instead of using the function name f inside the integrals, people use the function values $f(\lambda)$ and change the measure symbol to $E(d\lambda)$, so as to obtain an expression of the following form:

$$\int_\Delta f(\lambda) E(d\lambda) = \int_\Delta f dE$$

5.3 The main theorem

Let $E : \mathfrak{F}(\tau_{\mathbb{R}}) \to \mathscr{B}(\mathscr{H})$ define a PVM on the topological space $(\mathbb{R}, \tau_{\mathbb{R}})$. Then,

$$T = \int_{\mathbb{R}} \mathrm{id}_{\mathbb{R}}\, dE = \int_{\mathbb{R}} \lambda E(d\lambda)$$

defined on D_{id} as in Theorem 5.7 is self-adjoint, where $\mathrm{id}_{\mathbb{R}} : \mathbb{R} \to \mathbb{R}$ is the identity mapping. The celebrated spectral theorem for self-adjoint operators can be interpreted as a converse to the above statement, as we now see.

Theorem 5.8. *[Rud91, Theorem 13.30]*
Let $T : D(T) \to \mathscr{H}$ be a self-adjoint operator. Then, there exists a unique PVM $E : \mathfrak{F}(\tau_{\sigma(T)}) \to \mathscr{B}(\mathscr{H})$ on the topological space $(\sigma(T), \tau_{\sigma(T)})$ such that

$$T = \int_{\sigma(T)} \mathrm{id}_{\sigma(T)}\, dE = \int_{\sigma(T)} \lambda E(d\lambda),$$

where $\tau_{\sigma(T)}$ denotes the subset topology that $\sigma(T) \subseteq \mathbb{R}$ inherits from $(\mathbb{R}, \tau_{\mathbb{R}})$.

Out of the many significant applications of the spectral theorem, we will be interested in the following one.

Definition 5.9. *Let $T : D(T) \to \mathscr{H}$ be a self-adjoint operator and $E : \mathfrak{F}(\tau_{\sigma(T)}) \to \mathscr{B}(\mathscr{H})$ be the associated PVM. Then, for a measurable $f : \sigma(T) \to \mathbb{C}$, we define*

$$f(T) := \int_{\sigma(T)} f dE : D_f \to \mathscr{H} \quad \text{with} \quad D_f = \left\{ x \in \mathscr{H} \mid \int_{\sigma(T)} |f|^2 dE_x < \infty \right\}$$

as a densely defined closed linear operator using Theorem 5.7.

In the next chapter, we will use families of exponential functions $f_t(\lambda) = e^{it\lambda}$ (which are obviously bounded) in Definition 5.9 above to define and study the one-parameter family of bounded operators $\{e^{itT}\}_{t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ for any given self-adjoint operator T.

6 | One parameter unitary groups

In this chapter, we aim to place the introductory discussion of Chapter 4 within a rigorous mathematical framework by employing the spectral theorem. In order to do so, we must introduce the concept of one-parameter unitary groups, which form the main topic of investigation in the present chapter.

6.1 Setting the stage

Definition 6.1. *A family of unitary operators $\{U_t\}_{t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ forms a strongly continuous one-parameter unitary group (OPUG) if the following statements hold true:*

- $U_0 = \mathbb{1}$.
- $\forall s,t \in \mathbb{R}:\ U_s U_t = U_{s+t} = U_t U_s$.
- $\forall x \in \mathscr{H}:\ \|U_t x - x\| \to 0$ *as* $t \to 0$.

For any such family $\{U_t\}_{t\in\mathbb{R}}$, we define its infinitesimal generator as a linear operator $A : D(A) \to \mathscr{H}$ with $D(A) := \{x \in \mathscr{H} \mid \lim_{t\to 0} \frac{1}{i}\frac{U_t x - x}{t}$ exsits$\}$, and

$$\forall x \in D(A): \quad Ax := \lim_{t\to 0} \frac{1}{i}\frac{U_t x - x}{t}.$$

Note that the continuity condition in the above definition is equivalent to saying that $\forall x \in \mathscr{H}:\ \|U_s x - U_t x\| \to 0$ as $s \to t$. Moreover, this strong continuity of the family $\{U_t\}_{t\in\mathbb{R}}$ is weaker than demanding continuity in the operator norm, i.e.,

$$\|U_t - \mathbb{1}\| \to 0 \text{ as } t \to 0 \implies \forall x \in \mathscr{H}:\ \|U_t x - x\| \to 0 \text{ as } t \to 0,$$

but the reverse implication does not hold. An incisive reader would have also observed that the definition of the infinitesimal generator above mimics that of the derivative of the operator-valued mapping $\mathbb{R} \ni t \mapsto U_t \in \mathscr{B}(\mathscr{H})$ at $t = 0$.

In light of Definition 6.1, the families of operators defined in Eq (4.1) for arbitrary self-adjoint operators Q, P acting on $\mathscr{H}$ can be shown to form strongly continuous OPUGs, as we now prove.

Theorem 6.2. *For a self-adjoint operator $T : D(T) \to \mathscr{H}$, the family $\{e^{itT}\}_{t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ forms a strongly continuous OPUG with T as its infinitesimal generator.*

Proof. Spectrally decompose $T = \int_{\sigma(T)} \lambda E(d\lambda)$ as in Theorem 5.8. Then, it is clear that $\{e^{itT}\}_{t\in\mathbb{R}}$ forms a unitary group, since $\forall s,t \in \mathbb{R}$:

$$(e^{itT})^* e^{itT} = \int_{\sigma(T)} e^{-it\lambda} e^{it\lambda} E(d\lambda) = \int_{\sigma(T)} E(d\lambda) = \mathbb{1}_{\mathscr{H}} = (e^{itT})(e^{itT})^*,$$

and

$$e^{isT}e^{itT} = \int_{\sigma(T)} e^{i(s+t)\lambda}E(d\lambda) = e^{i(s+t)T}.$$

Strong continuity of the group follows by noting that $\forall x \in \mathscr{H}, \forall t \in \mathbb{R}$:

$$\|U_t x - x\|^2 = \left\| \int_{\sigma(T)} (e^{it\lambda} - 1)E(d\lambda)\, x \right\|^2 = \int_{\sigma(T)} |e^{it\lambda} - 1|^2 E_x(d\lambda),$$

where, since $f_t(\lambda) = e^{it\lambda} - 1 \to 0$ pointwise as $t \to 0$ and $\forall t, \lambda \in \mathbb{R} : |f_t(\lambda)|^2 \leq 4$, we can apply the dominated convergence theorem ([Rud87, Theorem 1.34]) to conclude that $\|U_t x - x\|^2 \to 0$ as $t \to 0$. Now, let $A : D(A) \to \mathscr{H}$ be the infinitesimal generator of the group and let $x \in D(T)$. Then,

$$\left\| \frac{U_t x - x}{it} - Tx \right\|^2 = \int_{\sigma(T)} \left| \frac{e^{it\lambda} - 1}{it} - \lambda \right|^2 E_x(d\lambda),$$

and it is straightforward to show that

$$f_t(\lambda) = \frac{e^{it\lambda} - 1}{it} - \lambda \to 0 \text{ pointwise as } t \to 0 \text{ and } \forall t, \lambda \in \mathbb{R} : |f_t(\lambda)|^2 \leq 4\lambda^2.$$

Moreover, since $x \in D(T)$, we have $\int_{\sigma(T)} \lambda^2 E(d\lambda) < \infty$ (see Definition 5.9), which allows us to apply the dominated convergence theorem again to conclude that

$$\left\| \frac{U_t x - x}{it} - Tx \right\|^2 \to 0 \text{ as } t \to 0.$$

In other words, we have shown that $\forall x \in D(T) : Ax = Tx \implies T \subseteq A$ and $A^* \subseteq T^*$. Finally, since T is self-adjoint and A is symmetric:

$$\forall x, y \in D(A) : \quad \langle x, Ay \rangle = \lim_{t \to 0} \left\langle x, \frac{U_t y - y}{it} \right\rangle = \lim_{t \to 0} \left\langle \frac{U_{-t} x - x}{-it}, y \right\rangle = \langle Ax, y \rangle,$$

we obtain $A \subseteq A^* \subseteq T^* = T$, which when combined with $T \subseteq A$ implies $A = T$. □

6.2 Stone's theorem

In the last section, we saw that every self-adjoint operator can be used to define a strongly continuous OPUG via the functional calculus provided by the spectral theorem. We now explore the converse of this statement, and actually prove that it holds!

Theorem 6.3 (Stone's theorem)**.** *Given a strongly continuous OPUG $\{U_t\}_{t \in \mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$, its infinitesimal generator $A : D(A) \to \mathscr{H}$ is densely defined and self-adjoint such that*

$$\forall t \in \mathbb{R} : \quad U_t = e^{itA}.$$

Proof. We present the proof as a sequence of claims.
Claim 1. $\forall x \in D(A), \forall t \in \mathbb{R} : U_t x \in D(A)$.
Proof. Observe that

$$\lim_{s \to 0} \frac{U_s U_t x - U_t x}{is} = U_t \left(\lim_{s \to 0} \frac{U_s x - x}{is} \right) = U_t A x.$$

Hence, $U_t x \in D(A)$ and $A(U_t x) = U_t(Ax)$. Put differently, for a fixed $x_0 \in D(A)$, the function $x(t) = U_t x_0$ is the solution to the differential equation $x'(t) = iAx(t)$ with the initial condition $x(0) = x_0$.

Claim 2. $D(A) \subseteq \mathscr{H}$ is dense.

Proof. For an arbitrary $f \in C_c^\infty(\mathbb{R})$, define $B_f = \int_{\mathbb{R}} f(t) U_t dt \in \mathscr{B}(\mathscr{H})$ as follows:

$$\forall x, y \in \mathscr{H}: \quad \langle x, B_f y \rangle = \int_{\mathbb{R}} f(t) \langle x, U_t y \rangle dt.$$

It should be clear that the above equation defines a bounded functional on $\mathscr{H} \times \mathscr{H}$ which is anti-linear in the first argument and linear in the second. A simple application of the Theorem 2.4 then implies that $B_f \in \mathscr{B}(\mathscr{H})$ is well-defined. Now, consider an arbitrary $x \in \mathscr{H}$. Then,

$$\begin{aligned} U_s B_f x - B_f x = \int_{\mathbb{R}} [f(t) U_s U_t - f(t) U_t] x dt &= \int_{\mathbb{R}} [f(t-s) U_t - f(t) U_t] x dt \\ &= \int_{\mathbb{R}} [f(t-s) - f(t)] U_t x dt. \end{aligned}$$

Hence, $\forall f \in C_c^\infty(\mathbb{R}), \forall x \in \mathscr{H} : B_f x \in D(A)$, since the following limit exists

$$\lim_{s \to 0} \frac{U_s B_f x - B_f x}{s} = -\int_{\mathbb{R}} \lim_{s \to 0} \frac{f(t-s-f(t)}{-s} U_t x dt = \int_{\mathbb{R}} f'(t) U_t x dt$$

Notice that the first equality above was obtained by using the dominated convergence theorem. Finally, consider a sequence of non-negative functions $(f_n)_{n \in \mathbb{N}}$ in $C_c^\infty(\mathbb{R})$ such that for each n, $\operatorname{supp} f_n = [-1/n, 1/n]$ and $\int_{\mathbb{R}} f_n(t) dt = 1$. Then, the denseness of $D(A)$ in $\mathscr{H}$ follows by observing that every $x \in \mathscr{H}$ can be approximated by elements in $D(A)$ to an arbitrary degree of closeness

$$\|B_{f_n} x - x\| = \left\| \int_{\mathbb{R}} f_n(t) [U_t x - x] dt \right\| \leq \sup_{-1/n \leq t \leq 1/n} \|U_t x - x\| \int_{\mathbb{R}} f_n(t) \to 0 \text{ as } n \to \infty,$$

where the strong continuity of $\{U_t\}_{t \in \mathbb{R}}$ is used to obtain the limit.

Claim 3. $A : D(A) \to \mathscr{H}$ is self-adjoint.

Proof. We already know that A is symmetric from Theorem 6.2, i.e. $A \subseteq A^*$. Now, let $y \in D(A^*)$. Then, $\forall x \in D(A) : \langle y, Ax \rangle = \langle z, x \rangle$, where $z = A^* y$. But,

$$\forall x \in D(A): \quad \langle y, Ax \rangle = \lim_{t \to 0} \left\langle y, \frac{U_t x - x}{it} \right\rangle = \lim_{t \to 0} \left\langle \frac{U_{-t} y - y}{-it}, x \right\rangle = \langle z, x \rangle \tag{6.1}$$

$$\implies \left\langle \left(\lim_{t \to 0} \frac{U_t y - y}{it} \right) - z, x \right\rangle = 0 \tag{6.2}$$

Since the above implication holds for all $x \in D(A)$ and $D(A) \subseteq \mathscr{H}$ is dense, we conclude that for each $y \in D(A^*)$, the aforementioned limit $\lim_{t \to 0} \frac{U_t y - y}{it} = Ay$ exists and equals $z = A^* y$. Therefore, $A^* \subseteq A$, and we arrive at the desired result $A = A^*$.

Claim 4. $\forall t \in \mathbb{R} : U_t = e^{itA}$.

Proof. Let $\{V_t\}_{t \in \mathbb{R}}$ be the strongly continuous OPUG generated by the self-adjoint operator A as in Theorem 6.2. For an arbitrary $x \in D(A)$, define $w(t) = U_t x - V_t x$. Then, from Claim 1 and Theorem 6.2, we have that $\forall t \in \mathbb{R} : w(t) \in D(A)$ and

$$w'(t) = iAU_t x - iAV_t x = iAw(t).$$

Moreover, if we define the real valued function $\mathfrak{w}(t) = \|w(t)\|^2 = \langle w(t), w(t) \rangle$, it is clear that

$$\begin{aligned} \forall t \in \mathbb{R}: \quad \mathfrak{w}'(t) = \langle w'(t), w(t) \rangle + \langle w(t), w'(t) \rangle &= \langle iAw(t), w(t) \rangle + \langle w(t), iAw(t) \rangle \\ &= -i\langle w(t), Aw(t) \rangle + i\langle w(t), Aw(t) \rangle \\ &= 0 \end{aligned}$$

Since $w(0) = 0$, the above equation implies that $w(t) = 0 = U_t x - V_t x$ for all $t \in \mathbb{R}$. As $x \in D(A)$ was arbitrary, we infer that $\forall t \in \mathbb{R}, \forall x \in D(A) : U_t x = V_t x$. Finally, the equality of U_t and V_t for all $t \in \mathbb{R}$ follows from the denseness of $D(A)$ in $\mathscr{H}$.

□

Remark 6.4. *It would be insightful for the reader to show that for a given strongly continuous OPUGs, its infinitesimal generator is a* bounded *self-adjoint operator if and only if the group is continuous in the operator norm.*

Combing the results of Theorems 6.2 and 6.3, we can now say that there is a one-one correspondence between strongly continuous OPUGs and self-adjoint linear operators.

6.3 Examples

We end this chapter by giving two examples of strongly continuous OPUGs and their corresponding self-adjoint generators, which will turn out to be the familiar position and momentum operators from the Schrödinger representation of the canonical commutation relation, see Theorem 3.16.

Example 6.5 (The translation group in $L^2(\mathbb{R})$)**.**
Consider $\mathscr{H} = L^2(\mathbb{R})$ and for each $s \in \mathbb{R}$, define $U_s \in \mathscr{B}(\mathscr{H})$ as follows:

$$\forall \psi \in L^2(\mathbb{R}) : \quad U_s \psi(x) = \psi(x+s). \tag{6.3}$$

It should be evident that $\{U_s\}_{s\in\mathbb{R}}$ forms a OPUG. To show its strong continuity, observe that for every $\psi \in C_c^\infty(\mathbb{R}) \subseteq L^2(\mathbb{R})$, $\psi(x+s)$ converges uniformly to $\psi(x)$ as $s \to 0$ [This is because each $\psi \in C_c^\infty(\mathbb{R})$ is continuous with a compact support and thus is also uniformly continuous]. Moreover, since the compact supports of these functions are of finite measure, it is easy to show that $\psi(x+s)$ actually converges to $\psi(x)$ in the L^2 norm as $s \to 0$. Now, since $C_c^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, for every $\varepsilon > 0$ and $\phi \in L^2(\mathbb{R})$, there exists a $\delta > 0$ and $\psi \in C_c^\infty(\mathbb{R})$ such that

$$\forall s \in \mathbb{R}: \ \|\phi - \psi\| < \varepsilon/3 \implies \|U_s\phi - U_s\psi\| < \varepsilon/3 \text{ and } |s| < \delta \implies \|U_s\psi - \psi\| < \varepsilon/3.$$

Hence, for every $\varepsilon > 0$, there exists a $\delta > 0$ such that for $|s| < \delta$, we obtain

$$\|U_s\phi - \phi\| \leq \|U_s\phi - U_s\psi\| + \|U_s\psi - \psi\| + \|\psi - \phi\| < \varepsilon.$$

Finally, let us investigate how the infinitesimal generator $A : D(A) \to \mathscr{H}$ of $\{U_s\}_{s\in\mathbb{R}}$ looks like. Its action is defined as

$$A\psi := \lim_{s\to 0} \frac{U_s\psi - \psi}{is},$$

wherever the limit exists in $L^2(\mathbb{R})$. If we restrict ourselves to the dense domain $C_c^\infty(\mathbb{R}) \subseteq L^2(\mathbb{R})$, it is not too difficult to prove that the above limit converges in $L^2(\mathbb{R})$ to the derivative $-i\psi'$. Thus, on $D = C_c^\infty(\mathbb{R})$, the infinitesimal generator is defined precisely like the momentum operator from the Schrödinger representation (see Theorem 3.16) and is hence essentially self-adjoint on D. The actual self-adjoint generator is then obtained by taking the unique closure.

Example 6.6 (The phase multiplication group in $L^2(\mathbb{R})$)**.**
Consider $\mathscr{H} = L^2(\mathbb{R})$ and for each $t \in \mathbb{R}$, define $V_t \in \mathscr{B}(\mathscr{H})$ as follows:

$$\forall \psi \in L^2(\mathbb{R}) : \quad V_t\psi(x) = e^{itx}\psi(x). \tag{6.4}$$

It is easy to see that $\{V_t\}_{t\in\mathbb{R}}$ forms a strongly continuous OPUG. Notice that for proving strong continuity, it suffices to show that $e^{itx}\psi(x) - \psi(x)$ converges to 0 pointwise as $t \to 0$, since we can bound $|e^{itx}\psi(x) - \psi(x)|^2 \leq 4|\psi(x)|^2$ to show convergence in the L^2 norm by exploiting the dominated convergence theorem. Now, observe that for each $\psi \in C_c^\infty(\mathbb{R})$ and $x \in \mathbb{R}$:

$$\lim_{t\to 0} \frac{e^{itx}\psi(x) - \psi(x)}{it} = \lim_{t\to 0} \frac{e^{itx} - 1}{t} \frac{\psi(x)}{i} = x\psi(x). \tag{6.5}$$

In addition, since for all $x, t \in \mathbb{R}$:

$$\left| \frac{e^{itx}\psi(x) - \psi(x)}{it} - x\psi(x) \right|^2 \leq 4|x\psi(x)|^2,$$

and ψ has compact support so that the RHS above is integrable, the dominated convergence theorem tells us that the limit in Eq (6.5) converges in the L^2 norm. Hence, the infinitesimal generator A of $\{V_t\}_{t\in\mathbb{R}}$ acts on $C_c^\infty(\mathbb{R})$ as the position operator from the Schrödinger representation, see Theorem 3.16. The same theorem tells us that A is essentially self-adjoint on $C_c^\infty(\mathbb{R})$ and therefore can be closed to obtain the unique self-adjoint generator of $\{V_t\}_{t\in\mathbb{R}}$.

To conclude this chapter, let us consider the OPUGs $\{U_s\}_{s\in\mathbb{R}}$ and $\{V_t\}_{t\in\mathbb{R}}$ from the aforementioned examples and show that they satisfy the Weyl relations as in Eq (4.2). For an arbitrary $\psi \in L^2(\mathbb{R})$, we have

$$(U_sV_t\psi)(x) = (V_t\psi)(x+s) = e^{ist}e^{itx}\psi(x+s) \tag{6.6}$$
$$(V_tU_s\psi)(x) = e^{itx}(U_s\psi)(x) = e^{itx}\psi(x+s). \tag{6.7}$$

We know that the self-adjoint infinitesimal generators of $\{U_s\}_{s\in\mathbb{R}}$ and $\{V_t\}_{t\in\mathbb{R}}$ are the familiar momentum and position operators P and Q (uniquely extended from their common domain of essential self-adjointness $C_c^\infty(\mathbb{R})$ by taking closures), respectively. Hence, we can write $U_s = e^{isP}$ and $V_t = e^{itQ}$ so that Eqs. (6.6) and (6.7) can be recast in the desired form

$$\forall s, t \in \mathbb{R} : \quad e^{isP}e^{itQ} = e^{ist}e^{itQ}e^{isP}.$$

7 | Stone-von Neumann theorem

We have come a long way since we first hinted at the existence of the Schrödinger representation of the CCR in Chapter 1. Let us summarize what we have learnt about this representation so far. By fixing the dense domain $D = C_c^\infty(\mathbb{R}) \subseteq L^2(\mathbb{R})$, the position and momentum operators $Q, P : D \to L^2(\mathbb{R})$ are defined as

$$\begin{aligned} Q\psi(x) &= x\psi(x) \\ P\psi(x) &= -i\psi'(x). \end{aligned} \tag{7.1}$$

D serves as a domain of essential self-adjointness for both the operators while also staying invariant under their actions, see Theorem 3.16. Then, we have

$$\forall \psi \in D: \qquad (QP - PQ)\psi = i\psi, \tag{7.2}$$

and we say that the operators $Q, P : D \to D$ form the Schrödinger representation of the CCR on $L^2(\mathbb{R})$ (see Definition 3.17). Denoting the unique self-adjoint closures of the aforementioned operators by the same letters Q and P, we can construct the corresponding strongly continuous OPUGs $\{e^{isP}\}_{s\in\mathbb{R}}$ and $\{e^{itQ}\}_{t\in\mathbb{R}}$, which have been shown to satisfy the Weyl relations:

$$\forall s, t \in \mathbb{R}: \qquad e^{isP} e^{itQ} = e^{ist} e^{itQ} e^{isP}. \tag{7.3}$$

We say that $\{e^{isP}\}_{s\in\mathbb{R}}$ and $\{e^{itQ}\}_{t\in\mathbb{R}}$ form the Schrödinger representation of the Weyl relations on $L^2(\mathbb{R})$. Now, before proceeding further, let us quickly collect a few key definitions regarding the representations of the Weyl relations below.

Definition 7.1. *Two strongly continuous OPUGs $\{U_s\}_{s\in\mathbb{R}}, \{V_t\}_{t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ are said to form a representation of the Weyl relations if*

$$\forall s, t \in \mathbb{R}: \qquad U_s V_t = e^{ist} V_t U_s.$$

Definition 7.2. *A representation $\{U_s\}_{s\in\mathbb{R}}, \{V_t\}_{t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ of the Weyl relations is said to be irreducible if $\forall s, t \in \mathbb{R}$, there is no non-trivial subspace of $\mathscr{H}$ (i.e., a subspace which is neither $\{0\}$ nor $\mathscr{H}$) that stays invariant under the operators U_s and V_t.*

Definition 7.3. *Two representations $\{U_s, V_t\}_{s,t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ and $\{U'_s, V'_t\}_{s,t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H}')$ of the Weyl relations are said to be unitarily equivalent if there exists a unitary bijection $\mathscr{U} : \mathscr{H} \to \mathscr{H}'$ such that*

$$\forall s, t \in \mathbb{R}: \qquad \mathscr{U} U_s \mathscr{U}^* = U'_s \quad \textit{and} \quad \mathscr{U} V_t \mathscr{U}^* = V'_t$$

We already saw in Chapter 4 that there exist many inequivalent representations of the CCR in the sense of Definition 3.17. In contrast, all irreducible representations of the Weyl relations can be shown to be equivalent to one another! We prove this fundamental result in the present chapter, which singles out the Schrödinger representation of the Weyl relations as the unique one.

7.1 Why is the Schrödinger representation special?

This short section examines some key properties of the Schrödinger representation of the Weyl relations, which will prove to be instrumental in our discussion of the main uniqueness theorem in the next section.

Lemma 7.4. *The Schrödinger representation of the Weyl relations is irreducible, i.e., $\forall s,t \in \mathbb{R}$, there is no non-trivial subspace of $L^2(\mathbb{R})$ that stays invariant under the unitary operators e^{isP} and e^{itQ}.*

Proof. Suppose that there exists such a non-trivial invariant subspace $K \subseteq L^2(\mathbb{R})$. Let $0 \neq f \in K$ and $0 \neq g \in K^{\perp}$. Then, the invariance condition implies that

$$\forall s,t \in \mathbb{R}: \quad 0 = \langle g, e^{itQ}e^{isP}f \rangle = \int_{\mathbb{R}} \overline{g(x)}e^{itx}f(x+s)dx.$$

If we define $h_s(x) = \overline{g(x)}f(x+s)$, then the above equation implies that the fourier transform $\hat{h}_s$ is identically zero, which inturn implies that h_s is identically zero for all $s \in \mathbb{R}$, since the fourier transfrom is injective. Thus, we have that for all $x,s \in \mathbb{R}$, $\overline{g(x)}f(x+s) = 0$, so that either f or g is identically zero, leading to a contradiction. □

Let us now look at another special property of the Schrödinger representation, namely the existence of a vacuum state. To this end, let us fix a new domain $D = \mathscr{S}(\mathbb{R}) = \{f \in L^2(\mathbb{R}) \,|\, \forall n,m \in \mathbb{N}: \sup_{x\in\mathbb{R}} |x^n f^{(m)}(x)| < \infty\}$ of rapidly decaying functions on $\mathbb{R}$. $\mathscr{S}(\mathbb{R})$ is also called the *Schwarz* space. It is straightforward to verify that the position and momentum operators Q,P as defined in Eq (7.1) keep $\mathscr{S}(\mathbb{R})$ invariant. Moreover, since Q,P are known to be essentially self-adjoint on $C_c^\infty(\mathbb{R})$ and $C_c^\infty(\mathbb{R}) \subseteq \mathscr{S}(\mathbb{R})$, the Schwarz space $\mathscr{S}(\mathbb{R})$ also acts as a domain of essential self-adjointness for Q,P and lies dense in $L^2(\mathbb{R})$, see Theorem 3.16. Finally, it is clear that on $\mathscr{S}(\mathbb{R})$, we have $QP - PQ = i\mathbb{I}$, so that we obtain a proper representation of the CCR in the sense of Definition 3.17. Now, let us define the creation and annihilation operators as follows:

$$a^* := \frac{Q - iP}{\sqrt{2}} : \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R}) \quad \text{and} \quad a := \frac{Q + iP}{\sqrt{2}} : \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R}). \tag{7.4}$$

Notice that a^* acts as the adjoint of a atleast on the domain $\mathscr{S}(\mathbb{R})$, since $\forall \psi, \phi \in \mathscr{S}(\mathbb{R})$:

$$\langle a\psi, \phi \rangle = \int_{\mathbb{R}} \frac{x\overline{\psi(x)}\phi(x) + \overline{\psi'(x)}\phi(x)}{\sqrt{2}}dx = \int_{\mathbb{R}} \frac{x\overline{\psi(x)}\phi(x) - \overline{\psi(x)}}{\sqrt{2}}\phi'(x)dx = \langle \psi, a^*\phi \rangle,$$

where integration by parts was used to obtain the second equality above and the boundary term didn't contribute as ψ, ϕ decay rapidly as $|x| \to \infty$. It is crucial to note that the CCR gets translated into the relation $[a, a^*] = \mathbb{I}$ for a and a^*, i.e.,

$$\forall \psi \in \mathscr{S}(\mathbb{R}): \quad aa^*\psi - a^*a\psi = \psi \tag{7.5}$$

Now, we define the vacuum state $\Omega \in \mathscr{S}(\mathbb{R})$ as follows

$$a\Omega = 0 \implies x\Omega(x) + \Omega'(x) = 0 \implies \Omega(x) = ce^{-x^2/2}, \tag{7.6}$$

for some $c = 1/\pi^{1/4}$ so that $\|\Omega\| = 1$. Observe that Ω does not have a compact support, which is precisely why we extended our domain from $C_c^\infty(\mathbb{R})$ to $\mathscr{S}(\mathbb{R})$. Let us now define the following ladder (or sequence) of functions:

$$e_0 = \Omega \quad \text{and} \quad e_n = (a^*)^n e_0 \text{ for } n \in \mathbb{N}, \tag{7.7}$$

so that a^* and a do indeed act as creation and annihilation operators on this ladder:

$$\forall n \in \mathbb{N} \cup \{0\} : \quad a^* e_n = e_{n+1} \quad \text{and} \quad a e_n = n e_{n-1}. \tag{7.8}$$

The first relation above is trivial to prove and the second can be shown by using an induction argument along with Eq (7.5). Moreover, $\operatorname{span}\{e_n : n \in \mathbb{N} \cup \{0\}\} \subseteq L^2(\mathbb{R})$ must be dense, because otherwise its closure would be a non-trivial invariant subspace for the operators e^{isP} and e^{itQ}, which is prohibited by Lemma 7.4. Finally, for $n \geq m$:

$$\langle e_n, e_m \rangle = \langle (a^*)^n e_0, e_m \rangle = \langle e_0, a^n e_m \rangle = \langle e_0, a^{n-m} a^m e_m \rangle = \begin{cases} 0 & \text{if } n > m \\ n! & \text{if } n = m \end{cases},$$

so that $\{e_n/\sqrt{n!}\}_{n \in \mathbb{N} \cup \{0\}}$ forms an orthonormal basis of $L^2(\mathbb{R})$.

Let us pause for a moment to appreciate the importance of the above construction. The properties of the Schrödinger representation of the CCR guarantee the existence of a special vacuum state $\Omega \in \mathscr{S}(\mathbb{R})$, from which we have cleverly recreated the entire structure of our Hilbert space $L^2(\mathbb{R})$! In general, if we have an irreducible representation of the CCR with vacuum, i.e., operators $a, a^* : D \to D$ satisfying $[a, a^*] = \mathbb{I}$ on a dense domain $D \subseteq \mathscr{H}$ and there exists $\Omega \in D$ such that $a\Omega = 0$, then we can follow the above steps to recover the entire Hilbert space as the closure of $\operatorname{span}\{(a^*)^n \Omega : n \in \mathbb{N} \cup \{0\}\}$ with inner product defined as $\langle (a^*)^n, (a^*)^m \rangle = n! \delta_{nm}$. Hence, we can easily show that the given representation is unitarily equivalent to the Schrödinger representation by setting up the mapping $\mathscr{H} \ni (a^*)^n \Omega \mapsto e_n \in L^2(\mathbb{R})$, where the e_n are defined for the Schrödinger representation as in Eq (7.7). Thus, the equivalence between a given irreducible representation of the CCR and the Schrödinger representation hinges on the existence of the vacuum state in the given representation. This fact will prove to be instrumental in our proof of the Stone-von Neumann uniqueness theorem in the next section.

7.2 The main theorem

We are now finally ready to state and prove the Stone-von Neumann uniqueness theorem for the canonical commutation relation.

Theorem 7.5 (Stone-von Neumann uniqueness theorem)**.**
Every representation $\{U_s, V_t\}_{s,t \in \mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ of the Weyl relations is unitarily equivalent to a countable direct sum of Schrödinger representations. More precisely, there exists a countable family of closed invariant subspaces $\{\mathscr{H}_i\}_{i \in \mathbb{N}}$ and unitary bijections $\mathscr{U}_i : \mathscr{H}_i \to L^2(\mathbb{R})$ such that $\mathscr{H} = \oplus_{i \in \mathbb{N}} \mathscr{H}_i$ and

$$\forall i \in \mathbb{N}, \forall s,t \in \mathbb{R} : \qquad \mathscr{U}_i U_s \mathscr{U}_i^* = e^{isP} \quad \text{and} \quad \mathscr{U}_i V_t \mathscr{U}_i^* = e^{itQ},$$

where $\{e^{isP}\}_{s \in \mathbb{R}}$ and $\{e^{itQ}\}_{t \in \mathbb{R}}$ are the translation and multiplication groups on $L^2(\mathbb{R})$, respectively (see Examples 6.5 and 6.6).

In particular, every irreducible representation of the Weyl relations is unitarily equivalent to the Schrödinger representation.

Proof. The proof proceeds in several steps.

Step 1: Studying properties of the Weyl *operators* $W(s,t) = e^{-ist/2}U_sV_t$.
Let us begin by combining the given representation into the following two-parameter family of Weyl operators defined for $s,t \in \mathbb{R}:\ W(s,t) = e^{-ist/2}U_sV_t$. Then,

$$
\begin{aligned}
W(s_1,t_1)W(s_2,t_2) &= e^{-is_1t_1}U_{s_1}V_{t_1}e^{-is_2t_2}U_{s_2}V_{t_2} \\
&= e^{-is_1t_1}e^{-s_2t_2}e^{-is_2t_1}U_{s_1+s_2}V_{t_1+t_2} \qquad (7.9) \\
&= e^{-i/2(s_1t_2-s_2t_1)}W(s_1+s_2,t_1+t_2) \qquad (7.10)
\end{aligned}
$$

Now, given any integrable function $h \in L^1(\mathbb{R}^2)$, we associate a bounded operator $W_h = \int_{\mathbb{R}^2} h(s,t)W(s,t)dsdt \in \mathscr{B}(\mathscr{H})$ to it by the following relation:

$$
\forall x,y \in \mathscr{H}: \quad \langle x, W_h y\rangle = \int_{\mathbb{R}^2} h(s,t)\langle x, W(s,t)y\rangle dsdt.
$$

We now intend to show that the mapping $h \mapsto W_h$ is injective, i.e., $W_h = 0 \implies h = 0$. To this end, observe that if $W_h = 0$, then for all $p,q \in \mathbb{R}$, we have

$$
\begin{aligned}
\int h(s,t)W(-p,-q)W(s,t)W(p,q)dsdt = 0 &\implies \int h(s,t)e^{i(pt-qs)}W(s,t)dsdt = 0 \\
&\implies \forall x,y \in \mathscr{H}: \int h(s,t)e^{i(pt-qs)}\langle x, W(s,t)y\rangle dsdt = 0
\end{aligned}
$$

In other words, the fourier transform of the mapping $(s,t) \mapsto h(s,t)\langle x, W(s,t)y\rangle$ is zero for all $x,y \in \mathscr{H}$, which implies that the mapping itself must be zero in $L^1(\mathbb{R}^2)$, from which it is straightforward to deduce that $h = 0$ in $L^1(\mathbb{R}^2)$.

Before proceeding further, let us collect a crucial convolution like property of the mapping $h \mapsto W_h$. We claim that $\forall h_1,h_2 \in L^1(\mathbb{R}^2)$:

$$
W_{h_1}W_{h_2} = W_h, \quad \text{where} \quad h(s,t) = \int_{\mathbb{R}^2} h_1(s-\mathfrak{s}',t-\mathfrak{t}')h_2(\mathfrak{s}',\mathfrak{t}')e^{i/2(s\mathfrak{t}'-\mathfrak{s}'t)}d\mathfrak{s}'d\mathfrak{t}'
$$

We leave an easy (but tedious) proof of the above identity to the reader.

Step 2: Defining the projector onto the vacuum subspace.
Let us dive back into our familiar Schrödinger representation, so that $W(s,t) = e^{-ist}e^{isP}e^{itQ}$, where Q,P are the usual position and momentum operators on $L^2(\mathbb{R})$. Let us investigate how the operator

$$
P = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-(s^2+t^2)/4}W(s,t)dsdt
$$

acts on $L^2(\mathbb{R})$. For $\psi \in L^2(\mathbb{R})$, we have

$$
\begin{aligned}
P\psi(x) &= \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-(s^2+t^2)/4}[W(s,t)\psi(x)]\,dsdt \\
&= \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-(s^2+t^2)/4} e^{ist/2} e^{itx}\psi(x+s)\,dsdt \\
&= \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-((y-x)^2+t^2)/4} e^{i(y-x)t/2} e^{itx}\psi(y)\,dydt \\
&= \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-((y-x)^2+t^2)/4} e^{i(y+x)t/2}\psi(y)\,dydt \\
&= \frac{1}{2\pi}\int_{\mathbb{R}} e^{-(y-x)^2/4}\psi(y)\left\{\int_{\mathbb{R}} e^{-t^2/4} e^{i(y+x)t/2}\,dt\right\}dy \\
&= \frac{1}{2\pi}\int_{\mathbb{R}} e^{-(y-x)^2/4}\psi(y)\left\{2\sqrt{\pi}e^{-(x+y)^2/4}\right\}dy \\
&= \frac{1}{\sqrt{\pi}}\int_{\mathbb{R}} e^{-(x^2+y^2)/2}\psi(y)\,dy = \left\{\int_{\mathbb{R}} \frac{e^{-y^2/2}}{\pi^{1/4}}\psi(y)\,dy\right\}\frac{e^{-x^2/2}}{\pi^{1/4}},
\end{aligned}
$$

so that $P\psi = \langle\Omega,\psi\rangle\Omega$, where $\Omega(x) = e^{-x^2/2}/\pi^{1/4}$ is the vacuum state from Section 7.1. Hence, P acts as the orthogonal projection onto the one-dimensional subspace spanned by the vacuum state. Motivated by this calculation, we define the vacuum projection in the given representation $\{U_s, V_t\}_{s,t\in\mathbb{R}}$ of the Weyl relations in an identical way

$$
P = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-(s^2+t^2)/4} W(s,t)\,dsdt.
$$

It can be easily verified that P satisfies all the properties of an orthogonal projection, see Definition 2.15. Firstly, note that since $e^{-(s^2+t^2)/4}$ stays invariant as $(s,t)\to(-s,-t)$, we have

$$
P^* = \int_{\mathbb{R}^2} e^{-(s^2+t^2)/4} W(-s,-t)\,dsdt = P.
$$

Moreover, it is not too difficult to establish the following identity:

$$
\forall s,t\in\mathbb{R}: \quad PW(s,t)P = e^{-(s^2+t^2)/4}P,
$$

which, for $s=t=0$, yields $P^2 = P$. Finally, since the mapping $h\mapsto W_h$ is injective, and $h(s,t) = e^{-(s^2+t^2)/4}$ is not zero in $L^1(\mathbb{R}^2)$, $P = W_h$ is a non-zero projection.

Step 3: Reconstructing the Hilbert space from vacuum.
Since we know that $P\neq 0$, we can construct the non-zero closed vacuum subspace $P\mathscr{H}$, see Remark 2.16. Let $\{\Omega_n\}_{n\in\mathbb{N}}$ be an (at most countable) orthonormal basis of $P\mathscr{H}$. Now, for each $n\in\mathbb{N}$, we define $\mathscr{H}_n := \overline{\operatorname{span}}\{W(s,t)\Omega_n \,|\, s,t\in\mathbb{R}\}$.

- It is easy to see that each $\mathscr{H}_n$ is invariant under $W(s,t)$ for all $s,t\in\mathbb{R}$.
- For $n\neq m$ and $x,y,s,t\in\mathbb{R}$, we have

$$
\begin{aligned}
\langle W(x,y)\Omega_n, W(s,t)\Omega_m\rangle &= \langle\Omega_n, e^{-i/2(ys-xt)}W(s-x,t-y)\Omega_m\rangle \\
&= \langle P\Omega_n, e^{-i/2(ys-xt)}W(s-x,t-y)P\Omega_m\rangle \\
&= \langle\Omega_n, e^{-i/2(ys-xt)}PW(s-x,t-y)P\Omega_m\rangle \\
&= \langle\Omega_n, e^{-i/2(ys-xt)}e^{-[(s-x)^2+(t-y)^2]/4}\Omega_m\rangle \\
&= 0.
\end{aligned}
$$

Hence, for $n \neq m$, $\mathscr{H}_n \perp \mathscr{H}_m$.

- If $\mathscr{H} \neq \oplus_{n\in\mathbb{N}}\mathscr{H}_n = \mathscr{K}$, then the orthogonal complement $\mathscr{K}^\perp$ becomes a non-trivial invariant subspace for all the Weyl operators $W(s,t)$. Hence, $\{U_s|_{\mathscr{K}^\perp}, V_t|_{\mathscr{K}^\perp}\}_{s,t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{K}^\perp)$ gives another representation of the Weyl relations on the Hilbert space $\mathscr{K}^\perp$. Going through the same motions as above, we can construct another non-zero vacuum projector P so that there exists a non-zero $\psi \in \mathscr{K}^\perp$ such that

$$\mathscr{K} \supseteq P\mathscr{H} \ni P\psi = \psi \in \mathscr{K}^\perp \implies \psi = 0 \implies \mathscr{K}^\perp = \{0\} \implies \mathscr{H} = \bigoplus_{n\in\mathbb{N}} \mathscr{H}_n.$$

Step 4: Showing equivalence of the representations $\{U_s|_{\mathscr{H}_n}, V_t|_{\mathscr{H}_n}\}_{s,t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H}_n)$.
In this final step, our aim is to show that the representations of the Weyl relations obtained by restricting the original representation to the invariant subspaces $\{\mathscr{H}_n\}_{n\in\mathbb{N}}$ are all equivalent to one another. To prove this, we will reconstruct the entire representation on each $\mathscr{H}_n$ just by using the corresponding vacuum state Ω_n and the Weyl relations. To this end, we fix $n \in \mathbb{N}$ and define $f_{s,t}^{(n)} := W(s,t)\Omega_n$ for $s,t \in \mathbb{R}$. Then, it is easy to recover the action of the Weyl operators as follows:

$$\forall x,y,s,t \in \mathbb{R}: \quad W(x,y)f_{s,t}^{(n)} = e^{-i/2(xt-ys)} f_{s+x,y+t}.$$

It is equally easy to construct explicit formulas for the inner products:

$$\begin{aligned}\langle f_{x,y}^{(n)}, f_{s,t}^{(n)}\rangle &= \langle \Omega_n, W(-x,-y)W(s,t)\Omega_n\rangle \\ &= \langle \Omega_n, PW(s-x,t-y)P\Omega_n\rangle e^{-i/2(ys-xt)} \\ &= e^{-[(s-x)^2+(t-y)^2]/4} e^{-i/2(ys-xt)}\end{aligned}$$

Now, given $\{U_s|_{\mathscr{H}_n}, V_t|_{\mathscr{H}_n}\}_{s,t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H}_n)$ and $\{U_s|_{\mathscr{H}_m}, V_t|_{\mathscr{H}_m}\}_{s,t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H}_m)$ for $n \neq m$, the above computations show that the mapping $f_{s,t}^{(n)} \mapsto f_{s,t}^{(m)}$ can be extended to a unitary bijection U between $\mathscr{H}_n$ and $\mathscr{H}_m$ such that

$$\forall s,t \in \mathbb{R}: \qquad UW(s,t)|_{\mathscr{H}_n}U^* = W(s,t)|_{\mathscr{H}_m}.$$

Therefore, all restricted representations are unitarily equivalent to each other. In particular, for two irreducible representations of the Weyl relations, the direct sum $\oplus_{n\in\mathbb{N}}\mathscr{H}_n$ has just one term for each irreducible representation and the above constructed U then serves as the unitary map that implements their equivalence. This finally shows that all irreducible representations of the Weyl relations are unitarily equivalent to the Schrödinger representation and any given representation of the Weyl relations splits up into a direct sum of Schrödinger representations, which is what we wanted to prove. □

The following corollary is a trivial consequence (or rather, a reformulation) of the Stone-von Neumann uniquness theorem.

Corollary 7.6. *Let $\mathscr{Q} : D(\mathscr{Q}) \to \mathscr{H}$ and $\mathscr{P} : D(\mathscr{P}) \to \mathscr{H}$ be self-adjoint operators such that the corresponding exponential families $\{e^{is\mathscr{P}}\}_{s\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ and $\{e^{it\mathscr{Q}}\}_{t\in\mathbb{R}} \subseteq \mathscr{B}(\mathscr{H})$ form an irreducible representation of the Weyl relations:*

$$\forall s,t \in \mathbb{R}: \qquad e^{is\mathscr{P}}e^{it\mathscr{Q}} = e^{ist}e^{it\mathscr{Q}}e^{is\mathscr{P}}.$$

Then, there exists a unitary bijection $\mathscr{U}: \mathscr{H} \to L^2(\mathbb{R})$ *such that*

$$\forall s,t \in \mathbb{R}: \qquad \mathscr{U} e^{is\mathscr{P}} \mathscr{U}^* = e^{isP} \quad \text{and} \quad \mathscr{U} e^{it\mathscr{Q}} \mathscr{U}^* = e^{itQ},$$

where $\{e^{isP}\}_{s\in\mathbb{R}}$ *and* $\{e^{itQ}\}_{t\in\mathbb{R}}$ *are the translation and multiplication groups on* $L^2(\mathbb{R})$*, respectively (see Examples 6.5 and 6.6). Thus,* $\mathscr{Q}$ *and* $\mathscr{P}$ *are unitarily equivalent to the position and momentum operators, respectively. In particular, there exists a dense domain* $D \subseteq D(\mathscr{Q}) \cap D(\mathscr{P}) \subseteq \mathscr{H}$ *such that*

- $\mathscr{Q}: D \to D$ *and* $\mathscr{P}: D \to D$.
- $\forall \psi \in D: \ (\mathscr{Q}\mathscr{P} - \mathscr{P}\mathscr{Q})\psi = i\psi$.
- $\mathscr{Q}$ *and* $\mathscr{P}$ *are essentially self-adjoint on* D.

Recall that in Chapter 4, we mentioned that the CCR and the Weyl relations

$$QP - PQ = i\mathbb{1} \qquad \text{and} \qquad e^{isP}e^{itQ} = e^{ist}e^{itQ}e^{isP},$$

respectively, are not equivalent to each other. However, we have just seen that if two OPUGs form an irreducible representation of the Weyl relations, then the corresponding infinitesimal generators form a representation of the CCR. Hence, it is the reverse implication which is not true, i.e., if two self-adjoint operators form a representation of the CCR, the associated OPUGs need not satisfy the Weyl relations, see [RS12, p. 275].

7.3 Conclusion

Quantum mechanics tells us that there is an associated complex Hilbert space with every physical system. States of the system are unit vectors in this space, while self-adjoint (or hermitian) operators play the role of observables. However, the theory *does not* give a prescription of uniquely assigning a Hilbert space to any given system. It is purely a modelling question! Then, why is it that the dynamics of a single particle constrained to move on a line, for instance, is always modelled on the Hilbert space of complex square integrable functions $L^2(\mathbb{R})$, with the position and momentum operators acting as follows:

$$\begin{aligned} Q\psi(x) &= x\psi(x), \\ P\psi(x) &= -i\psi'(x)? \end{aligned} \tag{7.11}$$

Why can't we choose to model this system on a different Hilbert space, with different kinds of position and momentum operators? After all, the list of possible choices is so huge that it is not even countable! If the reader is now able to answer this fundamental question, then this thesis would have served its purpose. In any case, let us conclude this thesis by providing a succinct answer to the above question. It is the structure of the commutation relation: $[Q,P] = i\mathbb{1}$, that is imposed on the prospective position and momentum operators which fixes both the Hilbert space and the action of the operators as stated in Eq. (7.11), see Theorem 7.5 and Corollary 7.6. This aptly summarizes the content of the Stone-von Neumann uniqueness theorem, whose proof serves as the centerpiece of this thesis.

Going forward, there are a lot of directions that one can pursue. The Stone-von Neumann theorem can be immediately generalizes to work for finitely many particles moving freely in three-dimensional space, see [Hal13, Theorem 14.8]. In that case, there will be a finite set $\{Q_j, P_j\}_{j=1}^n$ of position and momentum operators acting on their common domain of essential self-adjointness $C_c^\infty(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n)$ as follows:

$$\begin{aligned} Q_j \psi(x) &= x_j \psi(x), \\ P_j \psi(x) &= -i\partial_j \psi(x), \end{aligned} \tag{7.12}$$

and satisfying the following generalization of the CCR and the Weyl relations:

$$[Q_i, P_j] = i\delta_{ij} \qquad \text{and} \qquad e^{isP_i} e^{itQ_j} = e^{ist\delta_{ij}} e^{itQ_j} e^{isP_i}. \tag{7.13}$$

However, the Stone-von Neumann theorem breaks down rather dramatically in the realm of infinitely many degrees of freedom (i.e. when $n \to \infty$ in the above discussion), where one can show that there are infinitely many *inequivalent* representations of the Weyl relations. This is where quantum mechanics and quantum field theory part ways, and the reader is referred to [Der06, BR03] for introductory expositions on this topic.

One can also undertake a rigorous study of the so-called Gaussian continuous variable quantum systems, whose theory relies heavily on the uniqueness theorem discussed in this thesis along with a healthy serving of symplectic geometry and has immense applications in the rapidly progressing domain of quantum information, see [Par10, Par13, dG06, Ser17].

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