Synthesis Lectures on
Engineering, Science, and Technology

SYNTHESIS
COLLECTION OF TECHNOLOGY

Horst R. Beyer

Introduction to Quantum Mechanics

With a Focus on Physics and Operator Theory

MOREMEDIA

Springer

Introduction

This book is a sequel to the author's "The Reasoning of Quantum Mechanics: Operator Theory and the Harmonic Oscillator," (RQM). RQM stresses the fundamental importance of the spectral theorems for (densely-defined, linear and) self-adjoint operators in Hilbert space, central results in the mathematical field of operator theory (OT), for the formulation and interpretation of the theory of quantum mechanics, including the description of the measurement process. This observation is complementary to the standard "Copenhagen" interpretation of quantum mechanics and due to von Neumann's insight, related to his generalization of the spectral theorem for bounded linear and self-adjoint operators on complex Hilbert spaces to the case of unbounded such operators in 1930, in connection with the development of the mathematical foundation of quantum mechanics, [53, 54]. Regrettably, von Neumann's insights are hardly visible in standard quantum mechanics textbooks, thereby obstructing a complete view of the theory.

RQM also details the treatment of a relevant physical system, the so-called "harmonic oscillator," consistently using the tools provided by OT. In short, RQM indicates the fact that OT "is" the natural language of quantum theory. Apart from its reference to geometric shapes, which is applicable only to classical physical theories, in essence, Galileo's statement still applies to the role of mathematics in the natural sciences,[1] on page 60 of his "Il Saggiatore," [32].

> La filosofia è scritta in questo grandissimo libro che continuamente ci sta aperto innanzi agli occhi (io dico l'universo), ma non si può intendere, se prima non s'impara a intender la lingua, e conoscer i caratteri ne' quali è scritto. Egli è scritto in lingua matematica, e i caratteri son triangoli, cerchi ed altre figure geometriche, senza i quali mezzi è impossibile intenderne umanamente parola; senza questi è un aggirarsi vanamente per un oscuro laberinto.

[1] Of course, the scientific method is of equal relevance to the natural sciences and cannot be replaced by mathematical reasoning. Without experiment and observation, the natural sciences would lose the authority to make statements about the natural world. Galileo is also among the founders of the scientific method. On the other hand, if the mathematical description of a class of physical systems, i.e., a physical theory, runs into mathematical contradictions, the theory would need correction.

On the other hand, it is also clear that ultimately physical understanding is an intuitive understanding that is more a world-view than language. After all, mathematics is a tool for physics to achieve physical understanding. A standard method in physics consists of the calculation of model systems, possibly using also numerical methods, with the goal of abstracting from the results physical intuition, i.e., features that generalize to more realistic situations. In this process of abstraction, of course, there is assumed a kind of stability of the features against perturbations that are in some sense "small." Therefore, once it has been established that OT "is" the natural language of quantum theory, the question remains of how to calculate using the methods of OT. This is the topic of the current book.

For this purpose, the book considers models that appear in standard introductions to quantum mechanics, but, unlike those standard introductions that try not to go beyond the, for this purpose inadequate, methods of calculus, consistently uses methods from OT. As a consequence, the results are mathematically rigorous, providing a reliable basis for the abstraction of physical intuition.

To mitigate the acquirement of the methods of OT, the book provides a substantial mathematical appendix, including proofs, thereby avoiding the necessity of a time-consuming search of the literature. In addition, the text contains 16 exercises.

Conventions

The symbols $\mathbb{N}$, $\mathbb{R}$, $\mathbb{C}$ denote the natural numbers (including zero), all real numbers, and all complex numbers, respectively. The symbols $\mathbb{N}^*$, $\mathbb{R}^*$, $\mathbb{C}^*$ denote the corresponding sets from which 0 has been excluded. We call $x \in \mathbb{R}$ positive (negative) if $x \geqslant 0$ ($x \leqslant 0$). In addition, we call $x \in \mathbb{R}$ strictly positive (strictly negative) if $x > 0$ ($x < 0$).

For every $n \in \mathbb{N}^*$, $e_1, \ldots, e_n$ denotes the canonical basis of $\mathbb{K}^n$, where $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, i.e., for every $i \in \{1, \ldots, n\}$ the i-th component of e_i has the value 1, whereas all other components of e_i vanish. For every $x = (x_1, \ldots, x_n) \in \mathbb{K}^n$, $|x|$ denotes the canonical norm of x given by

$$|x| := \sqrt{|x_1|^2 + \cdots + |x_n|^2}.$$

Also, we define the canonical scalar product of vectors $x = (x_1, \ldots, x_n)$, $y = (y_1, \ldots, y_n) \in \mathbb{K}^n$ by

$$x \cdot y := \begin{cases} x_1 y_1 + \cdots + x_n y_n & \text{if } \mathbb{K} = \mathbb{R} \\ x_1^* y_1 + \cdots + x_n^* y_n & \text{if } \mathbb{K} = \mathbb{C}, \end{cases}$$

where $*$ denotes complex conjugation. In addition, we define the open ball $U_\rho(x)$ of radius $\rho > 0$ around x by

$$U_\rho(x) := \{y \in \mathbb{R}^n : |y - x| < \rho\},$$

the closed ball $B_\rho(x)$ of radius $\rho \geqslant 0$ around x by

$$B_\rho(x) := \{y \in \mathbb{R}^n : |y - x| \leqslant \rho\}$$

and the n-sphere $S^n_\rho(x)$ of radius $\rho \geqslant 0$ around x by

$$S^n_\rho(x) := \{y \in \mathbb{R}^n : |y - x| = \rho\}.$$

In the latter symbol, the index ρ is omitted if $\rho = 1$ and the label x and the brackets are omitted if $x = 0$. In addition, for every $S \subset \mathbb{R}^n$, $\bar{S}$ denotes the closure of S in the Euclidean topology.

Further, in connection with matrices, for $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, the elements of $\mathbb{K}^n$ are considered as column vectors. In this connection, $M(n \times n, \mathbb{K})$ denotes the vector space of $n \times n$ matrices with entries from $\mathbb{K}$. For every $A \in M(n \times n, \mathbb{K})$, $\det A$ denotes its determinant and

$$\ker A := \{x \in \mathbb{K}^n : A \cdot x = 0\},$$

where the dot denotes matrix multiplication.

We always assume the composition of maps (which includes addition, multiplication, etc.) to be maximally defined. For instance, the addition of two maps is defined on the (possibly empty) intersection of their domains. For every non-empty set S, id_S denotes the identical map on S defined by $\mathrm{id}_S(p) := p$ for every $p \in S$.

For each $k \in \mathbb{N}$, $n \in \mathbb{N}^*$, $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and each non-empty open subset Ω of $\mathbb{R}^n$, the symbol $C^k(\Omega, \mathbb{K})$ denotes the linear space of continuous and k-times continuously partially differentiable $\mathbb{K}$-valued functions on Ω. Further, $C_0^k(\Omega, \mathbb{K})$ denotes the subspace of $C^k(\Omega, \mathbb{K})$ containing those elements that have a compact support in Ω. In addition, if $U \subset \mathbb{R}^n$ is non-open and such that $\Omega \subset U \subset \bar{\Omega}$, then $C^k(U, \mathbb{K})$ is defined as the *subspace* of $C^k(\Omega, \mathbb{K})$ consisting of those elements for which there is an extension to an element of $C^k(V, \mathbb{K})$ for some open subset V of $\mathbb{R}^n$ containing U. In the special case $k = 0$, the corresponding superscript is omitted.

A Short Summary of the Quantization Process

In the following, we give a short review of the process of quantization and the measuring process in quantum theory. For more details, we refer to [7].

The process of quantization associates with the observables of a classical mechanical system observables of the quantum system, i.e., densely-defined, linear, and self-adjoint operators (DLSO's) in a non-trivial complex Hilbert space X, in such a way that the operators corresponding to the components of position and momentum satisfy the canonical commutation rules (CCR) in its Weylian form. For instance, for a system in $\mathbb{R}^n$, $n \in \mathbb{N}^*$,

$$e^{i\tau(\hbar\kappa)^{-1}\hat{p}_k} e^{i\sigma\kappa\hat{q}_l} = e^{i\tau\sigma\delta_{kl}} e^{i\sigma\kappa\hat{q}_l} e^{i\tau(\hbar\kappa)^{-1}\hat{p}_k}, \tag{1}$$

where $\widehat{p}_k$ and $\widehat{q}_l$ are the operators corresponding to the k-th component of momentum and the l-th component of position, respectively, $k, l \in \{1, \dots, n\}$, $\kappa > 0$ is a scale of dimension l^{-1}, $\tau, \sigma \in \mathbb{R}$ and δ_{kl} is defined as 1 if $k = l$ and 0, otherwise.

The space X is a representation space. It is unique only up to a Hilbert space isomorphism. Theories related by such an isomorphism are called unitarily equivalent and are physically equivalent. Often, the representation space is chosen in such a way that a particular quantum observable is represented in a form that simplifies its further analysis. For instance, the so-called position representations and momentum representations are such representations for the operators corresponding to the components of position and momentum, respectively.

The pure states of the quantum system are given by rays in X, $\mathbb{C}^*.f$, where $f \in X\backslash\{0\}$. For a closed classical system, the operator $\hat{H}$ that is associated with the Hamiltonian of the classical system generates the time evolution of the quantum system. If the quantum system is in the state $\mathbb{C}^*.f$ at time $t = 0$, then the system is/was in the state

$$\mathbb{C}^*.e^{-i\frac{t}{\hbar}\hat{H}} f \tag{2}$$

at time $t > 0/t < 0$. We note that the unitary linear operator on X, $e^{-i\frac{t}{\hbar}\hat{H}}$ and the unitary linear operators on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ in (1) are defined via the functional calculus for $\hat{H}$ and for $\hat{p}_1, \dots, \hat{p}_n$ and $\hat{q}_1, \dots, \hat{q}_n$, respectively.

Classical observables have dimensions. So do corresponding observables in quantum theory, represented by DSLOs, including their spectra. The latter are the only possible outcomes of a measurement process and hence have a dimension. The elements of representation spaces have no dimension since they are not observable. As mentioned above, if Y is a complex Hilbert space and $U : X \to Y$ is a Hilbert space isomorphism, then Y is an equally valid representation space of the theory. If a DSLO A is the representation of a classical observable, then the DSLO UAU^{-1} is the representation of the same classical observable in the new representation. We note that, following our convention that the composition of maps is always maximally defined, the domain $D(UAU^{-1})$ of UAU^{-1} is given by $U(D(A))$, where $D(A)$ is the domain of A. We note that also probabilities are dimensionless.

Frequently, the representation space is given by the function space $L^2_{\mathbb{C}}(\Omega)$, where $\Omega \subset \mathbb{R}^n$ is some non-empty open subset of $\mathbb{R}^n$ and $n \in \mathbb{N}^*$. In this case, the coordinate projections of $\mathbb{R}^n$ need to be dimensionless. For instance, if $\Omega = \mathbb{R}^n$, then mathematically $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $f(x) := e^{-|x|^2}$, for every $x \in \mathbb{R}^n$, but physically this makes sense if and only if the coordinate projections of $\mathbb{R}^n$ are dimensionless. Of course, if the dimension of $\kappa > 0$ is equal to the inverse dimension of the coordinate projections of $\mathbb{R}^n$, then $e^{-\kappa^2||^2} \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, and this also makes physical sense. On the other hand, if the coordinate projections of $\mathbb{R}^n$ would be allowed to have a physical dimension, then spaces like $L^2_{\mathbb{C}}(\mathbb{R}^n)$ would contain a substantial amount of states that make no physical sense. Of course, this is physically unacceptable. In this case, what would the completeness of $L^2_{\mathbb{C}}(\mathbb{R}^n)$ mean? As a consequence, in this book, coordinate projections of spaces appearing in the definition of state spaces are dimensionless. This explains the frequent occurrence of a scale $\kappa > 0$ of dimension l^{-1} in the definition of observables in the book. Preferably, this scale should consist of physical constants required for the definition of the Hamiltonian of the quantum system. Only in cases like free motion, this is not possible, and the quantity has to be prescribed from "outside." The elements of the spectrum of an observable share the dimension of the observable. The application of theorems of OT to observables is easily possible by multiplying the observable by a constant with a dimension that is inverse to the dimension of the observable. In this way, observables are multiples of a dimensionless DLSO and, e.g., spectral theorems are applied to these dimensionless operators.

We conclude with a short summary of the measurement process in quantum theory. In 1930 and in connection with the development of the mathematical foundation of quantum mechanics, von Neumann proved the spectral theorem for densely-defined, linear, and self-adjoint operators in Hilbert spaces (DLSOs) [53]. Usually, this theorem comes in 3 forms. Most important for applications is the form that associates a "functional calculus" with every such operator. Adding the obtained insight to the standard ("Copenhagen") picture of quantum mechanics, it is obtained a complete picture. It reveals that, roughly speaking, every such operator is a "physical observable" and the other way around.[1] To every such operator and every element (or "physical state") of the Hilbert space, there corresponds a spectral measure, whose support is part of the spectrum[2] of the operator. These spectral measures are the principal observables of quantum theory; in particular, they can be measured by experiment.[3] The probability of a measurement of the observable A to find the measured value to belong to a Borel measurable subset of the spectrum[4] is given by the measure of this subset with respect to the spectral measure corresponding to (A and) the physical state, the latter assumed to have norm 1. In particular, the probability of a measurement of finding a value outside the spectrum $\sigma(A)$ of A is 0. If a measurement of A finds the a value inside a Borel measurable set, B, after the measurement, the physical state is given by the image of the state before the measurement under the operator $\big(\chi_B|_{\sigma(A)}\big)(A)$, where $\chi_B|_{\sigma(A)}$ denotes the restriction of the characteristic function corresponding to B to $\sigma(A)$, corresponding to B, according to the functional calculus that is associated with A. These operators are orthogonal projections. All states in the range of this operator have the property that the probability of finding the value of the observable to be inside the set B is 1, i.e., is absolutely certain.

[1] A common misconception in standard physics textbooks is to define observables as symmetric (or "Hermitian") linear operators. This condition is significantly weaker than self-adjointness. Now, there are no spectral theorems for the class of symmetric linear operators. Also, there are symmetric linear operators, (like the natural candidate for a momentum operator on the half-line, an operator that is maximally symmetric, but has no self-adjoint extensions), whose spectra include non-real values, thus excluding them as observables, e.g., see [8].

[2] Not just the eigenvalues.

[3] Every physicist learns that, unlike wave functions themselves, the spectral measures corresponding to the position operator, i.e., the squares of the absolute values of the wave functions, are observable. The same has to be true for other observables. Otherwise, the position operator would be singled out by the theory in an unnatural way. In this connection, it needs to be remembered that position operators are of no relevance in quantum field theory. Hence, the singling out of position operators in the development of quantum theory would be misleading, and actually was misleading in the precursor, "relativistic quantum mechanics," of quantum field theory.

[4] Which is a non-empty closed subset of the real numbers.

Constraints on Quantization

A natural question to ask is whether representation spaces can be finite-dimensional. Indeed, they cannot, if the quantization is required to satisfy the CCR. For the proof, we assume that the state space X is a finite-dimensional Hilbert space of dimension $n \in \mathbb{N}^*$, P, Q are linear operators on X[1] such that

$$[P, Q] = PQ - QP = \frac{\hbar}{i}. \tag{3}$$

For the proof that such P, Q do not exist, we use an orthonormal basis $f_1, \ldots, f_n$ of X. Then, it follows that

$$\begin{aligned}\sum_{k=1}^{n} \langle f_k | PQ f_k \rangle &= \sum_{k=1}^{n} \left\langle f_k | P \sum_{l=1}^{n} \langle f_l | Q f_k \rangle f_l \right\rangle = \sum_{k=1}^{n} \sum_{l=1}^{n} \langle f_l | Q f_k \rangle \cdot \langle f_k | P f_l \rangle \\ &= \sum_{k=1}^{n} \sum_{l=1}^{n} \langle f_l | P f_k \rangle \cdot \langle f_k | Q f_l \rangle = \sum_{k=1}^{n} \langle f_k | QP f_k \rangle,\end{aligned}$$

implying that

$$\sum_{k=1}^{n} \langle f_k | [P, Q] f_k \rangle = 0.$$

Since

$$\sum_{k=1}^{n} \langle f_k | \frac{\hbar}{i} f_k \rangle = \frac{n\hbar}{i},$$

---

[1] The reader might remember from Linear Algebra that every linear operator, defined on a finite-dimensional normed vector space, is also continuous. Further, it is easy to see that there are no proper dense subspaces of finite-dimensional normed vector spaces. Hence, every DSLO in X is defined on the whole of X and is continuous.

(3) leads to contradiction $0 = \frac{n\hbar}{i}$. ↯ Also, the CCR in their Weylian form cannot be satisfied, since these imply in the current case (3). Indeed, if

$$e^{i\tau(\hbar\kappa)^{-1}P}e^{i\sigma\kappa Q} = e^{i\tau\sigma}e^{i\sigma\kappa Q}e^{i\tau(\hbar\kappa)^{-1}P}, \tag{4}$$

for all $\tau, \sigma \in \mathbb{R}$, where $\kappa > 0$ is a scale factor of dimension l^{-1}, it follows by differentiation that

$$e^{i\tau(\hbar\kappa)^{-1}P}\kappa Q = \tau e^{i\tau(\hbar\kappa)^{-1}P} + \kappa Q e^{i\tau(\hbar\kappa)^{-1}P},$$

$$i\hbar^{-1}PQ = 1 + i\hbar^{-1}QP, [P, Q] = \frac{\hbar}{i}.$$

We note that, in this derivation, we used the fact that for every self-adjoint bounded linear operator S on X, we have that

$$e^{zS} = \sum_{k=0}^{\infty} \frac{z^k}{k!}.S^k,$$

for every $z \in \mathbb{C}$, where the convergence is in the operator norm on the space of linear maps on X. This fact is a consequence of the spectral theorem, Theorem 12.6.4 in the Appendix.[2] Also, we used in the derivation Theorem 12.9.14 from the Appendix.

In the sequel, the reader might wonder why the quantization process leads mostly to unbounded operators in quantum theory, i.e., to operators that are defined on proper dense subspaces of the state space X. In this connection, we note the following.

The spectrum of an observable A is bounded if and only if A is a bounded linear operator on the state space.

For the proof, we assume that $A : D(A) \to X$ is DLSO on a state space $X (\neq \{0\})$ and consider 2 cases. If the spectrum $(\phi \neq)\sigma(A)(\subset \mathbb{R})$ of A is bounded, it follows from the Spectral Theorem 12.6.2 that $D(A) = X$ and from the Spectral Theorem 12.6.4 in the Appendix (or the Hellinger-Toeplitz theorem, see Theorem 12.4.4 (ix)) in the Appendix that $A \in L(X, X)$. On the other hand, if A is a bounded linear operator on X, then it follows for complex λ satisfying $|\lambda| > \|A\|$ that $\|\lambda^{-1}A\| < 1$ and hence from Theorem 12.2.5 in the Appendix that $1 - \lambda^{-1}A$ is bijective. Hence $A - \lambda = -\lambda(1 - \lambda^{-1}A)$ is bijective, too. As a consequence, $\mathbb{C}\backslash B_{\|A\|}(0)$, where $B_{\|A\|}(0)$ is the closed ball in $\mathbb{C}$ of radius $\|A\|$ around 0, is contained in the resolvent set of A, and therefore, $\sigma(A) \subset B_{\|A\|}(0)$.

[2] We note this is true also if X is infinite-dimensional and S is a bounded self-adjoint operator on X.

The correspondence in quantum theory, of the range of possible values that a classical observable can assume, is the spectrum of the associated observable. There is no priori reason why the quantization should turn an unbounded range into a bounded spectrum or the other way around. Hence, if the range of possible values that a classical observable can assume is unbounded, as is often the case, we expect that the same is true for the spectrum of the associated observable in quantum theory. As a consequence, the majority[3] of observables in quantum theory are going to be only densely-defined, but not defined on the whole state space.

[3] Exceptions are position operators corresponding to physical systems that are confined to bounded subsets of space.

Contents

List of Symbols

OT	Operator theory
$\mathbb{N}$	The set of natural numbers
$\mathbb{R}$	The set of real numbers
$\mathbb{C}$	The set of complex numbers
$\mathbb{N}^*$	$\mathbb{N}\backslash\{0\}$
$\mathbb{R}^*$	$\mathbb{R}\backslash\{0\}$
$\mathbb{C}^*$	$\mathbb{C}\backslash\{0\}$
$\mathbb{K}$	$\in \{\mathbb{R}, \mathbb{C}\}$
$e_1, \ldots, e_n$	Canonical basis of $\mathbb{K}^n$
$\vert\,\vert$	Canonical norm on $\mathbb{K}^n$
$\cdot$	Canonical scalar product on $\mathbb{K}^n$
$U_\rho(x)$	Open ball of radius ρ around x in $\mathbb{R}^n$
$B_\rho(x)$	Closed ball of radius ρ around x in $\mathbb{R}^n$
$S^n_\rho(x)$	n-sphere of radius ρ around x
—	Closure
$M(n \times n, \mathbb{K})$	Real or complex $n \times n$ matrices
$\det A$	Determinant of a matrix A
$\ker A$	Null space of a matrix A
$\cdot$	Matrix multiplication
id_S	Identical map on S
$C^k(\Omega, \mathbb{K})$	k-times continuously partially differentiable $\mathbb{K}$-valued functions on Ω
$C^k_0(\Omega, \mathbb{K})$	k-times continuously partially differentiable $\mathbb{K}$-valued functions on Ω with compact support
$C^k(U, \mathbb{K})$	k-times continuously partially differentiable $\mathbb{K}$-valued functions on U
DLSO	Densely-defined, linear and self-adjoint operator
CCR	Canonical commutation rules
$\langle\vert\rangle$	Scalar product
$\Vert A\Vert$	Operator norm of A
$B_{\Vert A\Vert}(0)$	Closed ball of radius $\Vert A\Vert$ around 0
κ	Constant > 0 with dimension $1/\text{length}$

$\psi_{A,f}$	Spectral measure associated with the operator A and the state f
$\int_\Omega$	Lebesgue integral over the set Ω
dv^n	Lebesgue measure on $\mathbb{R}^n$
$f(A)$	Operator corresponding to the function f and the operator A
$\Vert\,\Vert_\infty$	L^∞-norm
$\Vert\,\Vert_1$	L^1-norm
$*$	Convolution product
$\Vert\,\Vert_2$	L^2-norm
$C_\infty(\mathbb{R}^n, \mathbb{C})$	Space of complex-valued continuous functions vanishing at infinity
Int	Integral operator
$[,]$	Commutator bracket
E^A	Spectral family corresponding to the operator A
$U^s_{\mathbb{C}}$	Universally measurable functions
DLO	Densely-defined, linear operator
$\perp$	Orthogonal complement
$\otimes$	Direct sum
Y_{lm}	Spherical harmonic
F	Gauss hypergeometric function
P^m_ℓ	Ferrers function
$\widehat{L}_3$	Component of angular momentum
$\widehat{L}^2$	Square of angular momentum
$(\mathbb{R}^n, +)$	Additive group of $\mathbb{R}^n$
$O(n)$	Orthogonal group
$\langle\vert\rangle_c$	Canonical scalar product for $\mathbb{K}^n$
$\overrightarrow{E}$	Electric field
$\overrightarrow{B}$	Magnetic field
$\ker A$	Kernel of A
$\mathrm{Ran} A$	Range of A
$U(n)$	Unitary group in n dimensions
$L^{(2\ell+1)}_{n-(\ell+1)}$	Generalized Laguerre polynomial
$L^{\vert m\vert}_n$	Generalized Laguerre polynomial

1 Quantization of a Free Particle in N-Dimensional Space

A basic classical mechanical system in n space dimensions, $n \in \mathbb{N}^*$, is given by a point-particle of mass $m > 0$, solely interacting with an external potential V. The case of a vanishing potential, corresponds to a "free" particle. It is tempting to qualify the corresponding system as "simple," in the sense that not much can be learned from this system. According to classical mechanics, since there is no external force, such particles move uniformly in straight lines, i.e., perform geodesic motion in Euclidean space. So particles are somehow aware of the geometry of the surrounding space. This is not really simple. Similar is true for quantum mechanics. The Hamiltonian of the corresponding quantum system is a multiple of the Laplace operator that is also tied to Euclidean geometry, signaling the "awareness" of the quantum system of Euclidean geometry. More concretely, the quantum system is physically relevant, since it explains experiments, like the Davisson-Germer experiment from 1927 [20], by Clinton Davisson and Lester Germer at Western Electric, in which electrons, scattered by the surface of a crystal of nickel metal, displayed a diffraction pattern, confirming the hypothesis, advanced by Louis de Broglie in 1924, of wave-particle duality, an experimental milestone in the creation of quantum mechanics. In physics, such experiments are referred as "double-slit experiments," referring to Thomas Young's double-slit experiment from 1801 [78] that showed the wave character of light, in certain situations. Mathematically, it might surprise, as we shall see later, that the Hamiltonian corresponding to the motion of a charged particle in a Coulomb field can considered a "small" perturbation of the free Hamiltonian, i.e., is a relatively bounded perturbation of the free Hamiltonian, see Sect. 1.6.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_1.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_1

Although not difficult, we are not going to go through the quantization process for this particular system again, but give only the results. For more details about the process, we refer the reader to [7].

1.1 The Operators Corresponding to the Measurement of the Components of Position

In a *position representation,* the state space of the corresponding quantum system is given by $L^2_{\mathbb{C}}(\mathbb{R}^n)$ and *the operator* $\hat{q}_k$ *corresponding to the measurement of the* kth, $k \in \{1, \ldots, n\}$*, component of position* is given by the maximal multiplication operator $T_{u_k/\kappa}$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ with the kth coordinate projection $u_k : \mathbb{R}^n \to \mathbb{R}$ defined by $u_k(\bar{u}) := \bar{u}_k$ for all $\bar{u} = (\bar{u}_1, \ldots, \bar{u}_n) \in \mathbb{R}^n$, see Theorems 12.6.7, 12.6.8 and Corollary 12.6.9 in the Appendix. The quantity $\kappa > 0$ is a constant with dimension $1/\text{length}$ that is going to be left unspecified in the following, but is not going to affect the physical results.[1] Its spectrum consists of all real numbers and is purely absolutely continuous. Further, for any $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ with norm 1, the corresponding spectral measure $\psi_{\hat{q}_k, f}$ is given by

$$\psi_{\hat{q}_k, f}(I) = \int_{\{u \in \mathbb{R}^n : u_k \in \kappa I\}} |f|^2 \, dv^n \ ,$$

for every bounded interval I of $\mathbb{R}$. The quantity $\psi_{\hat{q}_k, f}(I)$ gives the probability in a position measurement of finding the k-th coordinate to be in the range I, if the particle is in the state $\mathbb{C}^*.f$. Further, for every bounded and universally measurable function $f : \mathbb{R} \to \mathbb{C}$:

$$f(\hat{q}_k) = T_{f \circ (u_k/\kappa)} \ , \tag{1.1}$$

where $T_{f \circ (u_k/\kappa)}$ is the maximal multiplication operator with the function $f \circ (u_k/\kappa)$, defined by

$$T_{f \circ (u_k/\kappa)} g := [f \circ (u_k/\kappa)] \cdot g \ ,$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$.

We expect that measurement of the k-th coordinate is independent of the measurement of the lth coordinate, if $k \neq l$. Indeed, this is true since the corresponding operators commute, see Sect. 2.1. Following the laws of probability for independent random variables, the probability of finding the position of the particle to belong to a "box" $I_1 \times \cdots \times I_n$, where $I_1, \ldots, I_n$ are intervals in $\mathbb{R}$, is given by the product of the probabilities of finding

[1] It is reasonable to use the inverse of the Compton wave length $\kappa := mc/h$, where c denotes the speed of light in vacuum. On the other hand, c is a foreign object in a non-relativistic theory, like Newtonian physics or quantum mechanics, where there is instantaneous propagation of any action. A natural de Broglie wave length h/mv does not exist for a free particle because there is no natural speed v for the system. This would be different if the particle would be confined to a finite space.

the components of the position of the particle to belong to the intervals $I_1, \ldots, I_n$, respectively. Hence, the probability of finding the position of the particle to belong to a Lebesgue measurable set $\Omega \subset \mathbb{R}^n$ is given by[2]

$$\int_{\kappa\Omega} |f|^2 \, dv^n \ , \tag{1.2}$$

if $\|f\| = 1$. For instance, the probability of finding the position of the particle to belong to the interval $I_1 \times \ldots \times I_n$ in physical space, where

$$I_k = [a_k \kappa^{-1}, b_k \kappa^{-1}] \ ,$$

$a_k \in \mathbb{R}$, $b_k \in \mathbb{R}$, $a_k \leqslant b_k$ are dimensionless, for every $k \in \{1, \ldots, n\}$, is given by

$$\begin{aligned} &\int_{[a_1,b_1]\times\ldots\times[a_n,b_n]} |f(\mathbf{u})|^2 \, du_1 \ldots du_n \\ &= \int_{I_1\times\ldots\times I_n} \kappa^n |f(\kappa^{-1}\mathbf{x})|^2 \, dx_1 \ldots dx_n \ , \end{aligned}$$

where $\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ are points in physical space. In a position representation, the coordinates $u_1, \ldots, u_n$ of points $\mathbf{u} = (u_1, \ldots, u_n)$ in the domains of functions belonging to the representation space can be interpreted as numbers whose multiplication by the unit of length κ^{-1} lead to a point $\kappa^{-1}\mathbf{u} = (\kappa^{-1}u_1, \ldots, \kappa^{-1}u_n, \kappa^{-1}u_n)$ in physical space. Of course, if Ω is a set of measure 0, e.g., like all countable sets, the corresponding probability is 0. In particular, the probability of finding the particle in an exact location ("point") is 0.[3]

Before giving these operators, we provide basic tools frequently applied in the proof of the essential self-adjointness of operators induced by formal partial differential operators, namely partial integration and mollification.

1.2 Partial Integration and an Auxiliary Sequence

Lemma 1.2.1 (Partial Integration) *Let $n \in \mathbb{N}^*$, $\Omega \subset \mathbb{R}^n$ a non-empty open subset and $f \in C^1(\Omega, \mathbb{C})$, $g \in C_0^1(\Omega, \mathbb{C})$. Then,*

$$\int_\Omega f(u) \cdot \partial_j g(u) \, du_1 \ldots du_n = -\int_\Omega (\partial_j f)(u) \cdot g(u) \, du_1 \ldots du_n \tag{1.3}$$

[2] We note that this reasoning is completely independent of the presence of any interaction potential. The Lebesgue measure v^n in n dimensions is essentially the product measure of the spectral measures corresponding to the operators associated with the measuring process of the components of the position.

[3] This is true also for finite space. Already in this aspect, quantum mechanics is more realistic than classical physics. In classical physics, particles are "point" particles that are hard to imagine. Quantum mechanics and later quantum field theory weaken this notion somewhat.

Proof For the proof, let $j \in \{1, \ldots, n\}$, $\tau_j : \mathbb{R}^n \to \mathbb{R}^n$ the linear C^1-diffeomorphism that exchanges the jth and the nth canonical basis vector of $\mathbb{R}^n$, $(\tau_j := \mathrm{id}_{\mathbb{R}^n}$ if $j = n)$. From the assumptions, it follows that $f \cdot \partial_j g, \big(\partial_j f\big) \cdot g, \partial_j(f \cdot g) = \big(\partial_j f\big) \cdot g + f \cdot \partial_j g \in C_0(\Omega, \mathbb{C})$ and hence that $(\partial_j f) \cdot g, \partial_j(f \cdot g)$ are integrable. Hence, it follows from the change of variable formula for Lebesgue integrals that

$$
\begin{aligned}
&\int_\Omega f(u) \cdot (\partial_j g)(u)\, du_1 \ldots du_n \qquad (1.4)\\
&= -\int_\Omega (\partial_j f)(u) \cdot g(u)\, du_1 \ldots du_n + \int_\Omega [\,\partial_j(f \cdot g)](u)\, du_1 \ldots du_n \\
&= -\int_\Omega (\partial_j f)(u) \cdot g(u)\, du_1 \ldots du_n + \int_{\tau_j(\Omega)} \{\partial_n\big[(f \cdot g) \circ \tau_j\big]\}(u)\, du_1 \ldots du_n \ ,
\end{aligned}
$$

where we used the idempotence of τ_j as well as that $|\det(\tau_j')| = 1$ We note that $-(f \cdot g) \circ \tau_j \in C_0^1(\tau_j(\Omega), \mathbb{C})$ an hence also that

$$\overset{\wedge}{\overline{(f \cdot g) \circ \tau_j}} \in C_0^1(\mathbb{R}^n, \mathbb{C})$$

as well as that

$$\overset{\wedge}{\overline{\partial_n \big[(f \cdot g) \circ \tau_j\big]}} = \partial_n \overset{\wedge}{\overline{(f \cdot g) \circ \tau_j}} \ ,$$

where the wedge symbol denotes the extension of a function to a function on $\mathbb{R}^n$, assuming the value 0 in the complement of the domain of the original function. Hence it follows from Fubini's theorem and the fundamental theorem of calculus that

$$
\begin{aligned}
&\int_{\tau_j(\Omega)} \{\partial_n \big[(f \cdot g) \circ \tau_j\big]\}(u)\, du_1 \ldots du_n \qquad (1.5)\\
&= \int_{\mathbb{R}^n} \Big[\partial_n \overset{\wedge}{\overline{(f \cdot g) \circ \tau_j}}\ \Big](u)\, du_1 \ldots du_n \\
&= \int_{\mathbb{R}^{n-1}} \left\{ \int_{\mathbb{R}} \Big[\ \overset{\wedge}{\overline{(f \cdot g) \circ \tau_j}}\ (u_1, \ldots, u_{n-1}, \cdot)\Big]'(u_n)\, du_n \right\} du_1 \ldots du_{n-1} = 0 \ .
\end{aligned}
$$

From (1.4), (1.5) follows (1.3). □

In the next step, we construct a sequence in $C_0^\infty(\mathbb{R}^n, \mathbb{C})$ that is used for extending minimal operators in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, induced by formal partial differential operators, to operators with the domain $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. The latter domain is appropriate for subsequent use of the Fourier transformation F_2, since F_2 maps $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ onto itself. For the definition, we use an auxiliary function $\rho \in C^\infty(\mathbb{R}, \mathbb{R})$, such that

$$\rho(u) \begin{cases} = 0 & \text{for } u \in (-\infty, -2) \\ \in [0,1] & \text{for } u \in [-2,-1] \\ = 1 & \text{for } u \in (-1, \infty) \end{cases} , \tag{1.6}$$

for every $u \in \mathbb{R}$, implying that

$$\rho' \in C_0^\infty(\mathbb{R}, \mathbb{R}) \text{ and } \operatorname{supp}(\rho') \subset [-2, -1] .$$

The function ρ is defined by

$$\rho(u) := \left(\int_{-\infty}^{\infty} h(-(\bar{u}+1)(\bar{u}+2))\, d\bar{u} \right)^{-1} \cdot \begin{cases} 0 & \text{for } u \leqslant -3 \\ \int_{-4}^{u} h(-(\bar{u}+1)(\bar{u}+2))\, d\bar{u} & \text{for } u > -3 \end{cases} ,$$

for every $u \in \mathbb{R}$, where the auxiliary function $h \in C^\infty(\mathbb{R}, \mathbb{R})$ is defined by

$$h(u) := \begin{cases} 0 & \text{for } u \leqslant 0 \\ \exp(-1/u) & \text{for } u > 0 \end{cases} ,$$

for every $u \in \mathbb{R}$, implying that

$$\operatorname{Ran} h \subset [0, 1) , \lim_{u \to +\infty} h(u) = 1 .$$

The auxiliary sequence $\rho_1, \rho_2, \ldots$ in $C_0^\infty(\mathbb{R}^n, \mathbb{C})$ is defined by

$$\rho_\nu := \rho \circ (-\nu^{-2} |\ |^2) ,$$

for every $\nu \in \mathbb{N}^*$. In particular,

$$\rho_\nu(u) = \begin{cases} 0 & \text{for } |u| \geqslant \sqrt{2}\,\nu \\ 1 & \text{for } |u| \leqslant \nu \end{cases} \text{ and } \operatorname{Ran}(\rho_\nu) \subset [0, 1] ,$$

for every $u \in \mathbb{R}^n$ and $\nu \in \mathbb{N}^*$. With the help of the sequence $\rho_1, \rho_2, \ldots$, we define for $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ a corresponding sequence $f_1, f_2, \ldots$ in $C_0^\infty(\mathbb{R}^n, \mathbb{R})$ by

$$f_\nu := \rho_\nu \cdot f ,$$

for every $\nu \in \mathbb{N}^*$. Then

$$|f_\nu - f|^2 = (1 - \rho_\nu)^2 \cdot |f|^2 \leqslant 2\,|f|^2 ,$$

for every $\nu \in \mathbb{N}^*$, and hence it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \| f_\nu - f \|_2 = 0 \ . \tag{1.7}$$

For use inside the Sect. 3.5 on the Hamiltonian of the harmonic oscillator, we note that for every complex polynomial p in n variables, it follows that

$$|pf_\nu - pf|^2 = (1-\rho_\nu)^2 \cdot |pf|^2 \leqslant 2\,|pf|^2 \ ,$$

for every $\nu \in \mathbb{N}^*$, and from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \| pf_\nu - pf \|_2 = 0 \ . \tag{1.8}$$

Further for $k \in \{1, \dots, n\}$,

$$\left| \frac{\partial \rho_\nu}{\partial u_k} \right| = \left| -\frac{2}{\nu^2}\, p_k \left(\rho' \circ (-\nu^{-2} \,|\ |^2) \right) \right| \leqslant \frac{C_1}{\nu} \ ,$$

where p_k denotes the coordinate projection of $\mathbb{R}^n$ onto the kth coordinate,

$$C_1 := 2\sqrt{2}\, \|\rho'\|_\infty$$

and

$$\left| \frac{\partial^2 \rho_\nu}{\partial u_k^2} \right| = \left| -\frac{2}{\nu^2} \left(\rho' \circ (-\nu^{-2}\,|\ |^2) \right) + \frac{4}{\nu^4}\, p_k^2 \cdot \left(\rho'' \circ (-\nu^{-2}\,|\ |^2) \right) \right| \leqslant \frac{C_2}{\nu^2} \ ,$$

where

$$C_2 := 2 \left(\|\rho'\|_\infty + 4\,\|\rho''\|_\infty \right) \ .$$

Hence,

$$\begin{aligned}
\left| \frac{\partial f_\nu}{\partial u_k} - \frac{\partial f}{\partial u_k} \right|^2 &= \left| \frac{\partial \rho_\nu}{\partial u_k} \cdot f + (\rho_\nu - 1) \cdot \frac{\partial f}{\partial u_k} \right|^2 \leqslant \left[\frac{C_1}{\nu}\, |f| + |1-\rho_\nu| \cdot \left| \frac{\partial f}{\partial u_k} \right| \right]^2 \\
&\leqslant 2 \left[\frac{C_1^2}{\nu^2}\, |f|^2 + (1-\rho_\nu)^2 \cdot \left| \frac{\partial f}{\partial u_k} \right|^2 \right] \leqslant 2 \left[C_1^2\, |f|^2 + 4 \cdot \left| \frac{\partial f}{\partial u_k} \right|^2 \right]
\end{aligned}$$

and

$$\begin{aligned}
&\left| \frac{\partial^2 f_\nu}{\partial u_k^2} - \frac{\partial^2 f}{\partial u_k^2} \right|^2 = \left| \frac{\partial^2 \rho_\nu}{\partial u_k^2} \cdot f + 2\, \frac{\partial \rho_\nu}{\partial u_k} \cdot \frac{\partial f}{\partial u_k} + (\rho_\nu - 1) \cdot \frac{\partial^2 f}{\partial u_k^2} \right|^2 \\
&\leqslant \left[\frac{C_2}{\nu^2}\, |f| + \frac{2C_1}{\nu} \left| \frac{\partial f}{\partial u_k} \right| + |1-\rho_\nu| \cdot \left| \frac{\partial^2 f}{\partial u_k^2} \right| \right]^2 \\
&\leqslant 3 \left[C_2^2\, |f|^2 + 4C_1^2 \left| \frac{\partial f}{\partial u_k} \right|^2 + 4 \cdot \left| \frac{\partial^2 f}{\partial u_k^2} \right|^2 \right] \ .
\end{aligned}$$

It follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu\to\infty}\left\|\frac{\partial f_\nu}{\partial u_k}-\frac{\partial f}{\partial u_k}\right\|_2=0 \tag{1.9}$$

and that

$$\lim_{\nu\to\infty}\left\|\frac{\partial^2 f_\nu}{\partial u_k^2}-\frac{\partial^2 f}{\partial u_k^2}\right\|_2=0\ .$$

The latter implies also that

$$\lim_{\nu\to\infty}\|\triangle f_\nu-\triangle f\|_2=0\ . \tag{1.10}$$

1.3 The Operators Corresponding to the Measurement of the Components of Momentum

The operator corresponding to the measurement of the kth, $k\in\{1,\dots,n\}$, *component of the momentum* is given by the closure $\hat{p}_k$ of the densely-defined, linear, symmetric and essentially self-adjoint operator

$$\hat{p}_{k0}: C_0^\infty(\mathbb{R}^n,\mathbb{C})\to L^2_{\mathbb{C}}(\mathbb{R}^n)\ ,$$

given by

$$\hat{p}_{k0}f:=\frac{\hbar\kappa}{i}\,\frac{\partial f}{\partial u_k}\ ,$$

for every $f\in C_0^\infty(\mathbb{R}^n,\mathbb{C})$.

In the following, we give corresponding details. We note that $\hat{p}_{k0}$ is densely-defined, since $C_0^\infty(\mathbb{R}^n,\mathbb{C})$ is a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Further, $\hat{p}_{k0}$ is well-defined, since $\hat{p}_{k0}f\in C_0^\infty(\mathbb{R}^n,\mathbb{C})$ for every $f\in C_0^\infty(\mathbb{R}^n,\mathbb{C})$. Also, as consequence of the linearity of differentiation and outer multiplication of complex-valued functions by complex numbers, $\hat{p}_{k0}$ is linear. As a consequence of "partial integration," $\hat{p}_{k0}$ is symmetric

$$\begin{aligned}\langle f|\hat{p}_{k0}g\rangle &= \frac{\hbar\kappa}{i}\int_{\mathbb{R}^n} f^*(u)\,\frac{\partial g}{\partial u_k}(u)\,du_1\dots du_n\\ &= -\frac{\hbar\kappa}{i}\int_{\mathbb{R}^n}\frac{\partial f^*}{\partial u_k}(u)\,g(u)\,du_1\dots du_n\\ &= \int_{\mathbb{R}^n}\left(\frac{\hbar\kappa}{i}\int_{\mathbb{R}^n}\frac{\partial f}{\partial u_k}\right)^*(u)\,g(u)\,du_1\dots du_n\\ &= \langle\hat{p}_{k0}f|g\rangle\ ,\end{aligned}$$

for all $f,g\in C_0^\infty(\mathbb{R}^n,\mathbb{C})$, where Lemma 1.2.1 has been used. Even further, from (1.7) and (1.9), it follows that $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ is part of the domain of the closure $\hat{p}_k$ of $\hat{p}_{k0}$ and that

$$\hat{p}_k f = \frac{\hbar\kappa}{i} \frac{\partial f}{\partial u_k} \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. We continue the analysis of $\hat{p}_k$ with the help of the unitary Fourier transformation F_2. First, we conclude from known properties of F_2 that

$$F_2\, \hat{p}_k f = \frac{\hbar\kappa}{i}\, F_2 \frac{\partial f}{\partial u_k} = \frac{\hbar\kappa}{i}\, i\, v_k F_2 f = \hbar\kappa\, T_{v_k} F_2 f \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$, where T_{v_k} denotes the maximal multiplication in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ with the kth coordinate projection $v_k : \mathbb{R}^n \to \mathbb{R}$ defined by $v_k(\bar{v}) := \bar{v}_k$ for all $\bar{v} = (\bar{v}_1, \dots, \bar{v}_n) \in \mathbb{R}^n$. Hence, it follows that

$$F_2\, \hat{p}_k F_2^{-1} f = \hbar\kappa\, T_{v_k} f \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. According to characterization of essential self-adjointness from Theorem 12.4.9, the restriction of T_{v_k} to $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ is essentially self-adjoint since

$$T_{v_k \pm i} \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

contain $C_0^\infty(\mathbb{R}^n, \mathbb{C})$ and are therefore dense in $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Since F_2 is unitary, this implies also the essential self-adjointness of the restriction of $\hat{p}_k$ to $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. Hence it follows the self-adjointness of $\hat{p}_k$ and the essential self-adjointness of $\hat{p}_{k0}$. We note that since F_2 is unitary and since $\hbar\kappa\, T_{v_k}$ is self-adjoint, it follows the relation (1.11) below.

The Hilbert space isomorphism to the momentum representation is given by the unitary Fourier transformation

$$F_2 : L^2_{\mathbb{C}}(\mathbb{R}^n) \to L^2_{\mathbb{C}}(\mathbb{R}^n) \ .$$

The operator in that representation corresponding to the measurement of the kth, $k \in \{1, \dots, n\}$, component of the momentum is given by the maximal multiplication operator $\hbar\kappa T_{v_k}$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $v_k : \mathbb{R}^n \to \mathbb{R}$ is the kth coordinate projection of $\mathbb{R}^n$, defined by $v_k(\bar{v}) := \bar{v}_k$ for all $\bar{v} = (\bar{v}_1, \dots, \bar{v}_n) \in \mathbb{R}^n$,

$$F_2\, \hat{p}_k F_2^{-1} = \hbar\kappa . T_{v_k} \ . \tag{1.11}$$

From the properties of maximal multiplication operators, Theorems 12.6.7, 12.6.8 and Corollary 12.6.9 in the Appendix, it follows that *the spectrum of $\hat{p}_k$ consists of all real numbers and is purely absolutely continuous*. Further, for any $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ with norm 1, the corresponding spectral measure $\psi_{\hat{p}_k, f}$ is given by

$$\psi_{\hat{p}_k, f}(I) = \int_{\{v \in \mathbb{R}^n : v_k \in (\hbar\kappa)^{-1} I\}} |F_2 f|^2 \, dv^n \ ,$$

for every bounded interval I of $\mathbb{R}$. The quantity $\psi_{\hat{p}_k, f}(I)$ gives the probability in a momentum measurement of finding the kth component of momentum to be in the range I, if the particle is in the state $\mathbb{C}^*.f$. Further, for every bounded and universally measurable function $f : \mathbb{R} \to \mathbb{C}$:

$$f(\hat{p}_k) = F_2^{-1} \circ T_{f \circ (\hbar\kappa v_k)} \circ F_2 \ , \tag{1.12}$$

where $T_{f \circ (\hbar\kappa v_k)}$ is the maximal multiplication operator with the function $f \circ (\hbar\kappa v_k)$, defined by

$$T_{f \circ (\hbar\kappa v_k)} g := [f \circ (\hbar\kappa v_k)] \cdot g \ ,$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$.
Again, we expect that the measurement of the kth component of momentum is independent of the measurement of the lth component, if $k \neq l$. Indeed, this true, due to commuting of the corresponding operators, see Sect. 2.1. Following the laws of probability for independent random variables, the probability of the momentum of the particle to belong to a "box" $I_1 \times \cdots \times I_n$, where $I_1, \ldots, I_n$ are intervals in $\mathbb{R}$, is given by the product of the probabilities of finding the components of the position of the particle to belong to the intervals $I_1, \ldots, I_n$, respectively. Hence, the probability of finding the momentum of the particle to belong to a Lebesgue measurable set $\Omega \subset \mathbb{R}^n$ is given by[4]

$$\int_{(\hbar\kappa)^{-1}\Omega} |F_2 f|^2 \, dv^n \ . \tag{1.13}$$

Of course, if Ω is a set of measure 0, e.g., like all countable sets, the corresponding probability is 0. In particular, the probability of finding the particle to have a precise momentum is 0.

1.4 The Hamilton Operator Governing Free Motion in $\mathbb{R}^n$

The operator corresponding to the measurement of the energy in $n \in \mathbb{N}^*$ space dimensions is given by the closure $\hat{H}$ of the densely-defined, linear, symmetric and essentially self-adjoint operator

$$\hat{H}_0 : C_0^\infty(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

given by

$$\hat{H}_0 f := -\frac{\hbar^2\kappa^2}{2m} \triangle f = -\varepsilon_0 \triangle f \ ,$$

for every $f \in C_0^\infty(\mathbb{R}^n, \mathbb{C})$,

$$\varepsilon_0 := \frac{\hbar^2\kappa^2}{2m} \ . \tag{1.14}$$

In the following, we give corresponding details. We note that $\hat{H}_0$ is densely-defined, since $C_0^\infty(\mathbb{R}^n, \mathbb{C})$ is a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Further, $\hat{H}_0$ is well-defined, since $\hat{H}_0 f \in C_0^\infty(\mathbb{R}^n, \mathbb{C})$ for every $f \in C_0^\infty(\mathbb{R}^n, \mathbb{C})$. Also, as consequence of the linearity of

[4] Again, we note that this reasoning is completely independent of the presence of any interaction potential.

differentiation and outer multiplication of complex-valued functions by complex numbers, $\hat{H}_0$ is linear. As a consequence of "partial integration," $\hat{H}_0$ is symmetric

$$\begin{aligned}
\left\langle f|\hat{H}_0 g\right\rangle &= \langle f| - \varepsilon_0 \triangle g\rangle = -\varepsilon_0 \sum_{k=1}^{n} \int_{\mathbb{R}^n} f^*(u)\, \frac{\partial^2 g}{\partial u_k^2}(u)\, du_1 \dots du_n \\
&= -\varepsilon_0 \sum_{k=1}^{n} \int_{\mathbb{R}^n} \frac{\partial^2 f^*}{\partial u_k^2}(u)\, g(u)\, du_1 \dots du_n \\
&= \int_{\mathbb{R}^n} \left(-\varepsilon_0 \sum_{k=1}^{n} \frac{\partial^2 f}{\partial u_k^2}\right)^{*}(u)\, g(u)\, du_1 \dots du_n \\
&= \langle -\varepsilon_0 \triangle f|g\rangle = \left\langle \hat{H}_0 f|g\right\rangle \ ,
\end{aligned}$$

for all $f, g \in C_0^\infty(\mathbb{R}^n, \mathbb{C})$, where Lemma 1.2.1 has been used. Even further, from (1.7) and (1.10), it follows that $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ is part of the domain of the closure $\hat{H} := \bar{\hat{H}}_0$ of $\hat{H}_0$ and that

$$\hat{H} f = -\varepsilon_0 \triangle f \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. We continue the analysis of $\hat{H}$ with the help of the unitary Fourier transformation F_2. First, we conclude from known properties of F_2 that

$$F_2 \hat{H} f = \varepsilon_0\, T_{|\ |^2} F_2 f \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$, where $T_{|\ |^2}$ denotes the maximal multiplication in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ with $|\ |^2$. Hence, it follows that

$$F_2\, \hat{H}\, F_2^{-1} f = \varepsilon_0\, T_{|\ |^2} f \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. According to the characterization of essential self-adjointness from Theorem 12.4.9 in the Appendix, the restriction of $T_{|\ |^2}$ to $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ is essentially self-adjoint since

$$T_{|\ |^2 \pm i} \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

contain $C_0^\infty(\mathbb{R}^n, \mathbb{C})$ and are therefore dense in $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Since F_2 is unitary, this implies also the essential self-adjointness of the restriction of $\hat{H}$ to $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. Hence it follows the self-adjointness of $\hat{H}$ and the essential self-adjointness of $\hat{H}_0$. We note that since F_2 is unitary and since $\varepsilon_0\, T_{|\ |^2}$ is self-adjoint, it follows that

$$F_2\, \hat{H}\, F_2^{-1} = \varepsilon_0 . T_{|\ |^2} \ . \tag{1.15}$$

From the properties of maximal multiplication operators, Theorems 12.6.7, 12.6.8 and Corollary 12.6.9 in the Appendix, it follows that the spectrum of $\hat{H}$ consists of the interval $[0, \infty)$ and is purely absolutely continuous. In particular, there is no ground state, e.g., differently to the harmonic oscillator. The lowest possible energy of the system is 0, but 0 is no eigenvalue.

Further, for any $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ with norm 1, the corresponding spectral measure ψ_f is given by

$$\psi_{\hat{H},f}(I) = \int_{\left\{v \in \mathbb{R}^n : |v|^2 \in \varepsilon_0^{-1} I\right\}} |F_2 f|^2 \, dv^n \ ,$$

for every bounded interval I of $\mathbb{R}$. The quantity $\psi_{\hat{H},f}(I)$ gives the probability in a energy measurement of finding the energy to be in the range I, if the particle is in the state $\mathbb{C}^*.f$. In particular, the probability of finding the particle to have a precise energy is 0. Further, for every bounded and universally measurable function $f : [0,\infty) \to \mathbb{C}$:

$$f(\hat{H}) = F_2^{-1} \circ T_{f\circ(\varepsilon_0 .|\ |^2)} \circ F_2 \ , \tag{1.16}$$

where $T_{f\circ(\varepsilon_0 .|\ |^2)}$ is the maximal multiplication operator with the function $f \circ (\varepsilon_0 .|\ |^2)$, defined by

$$T_{f\circ(\varepsilon_0 .|\ |^2)} g := [f \circ (\varepsilon_0 .|\ |^2)] \cdot g \ ,$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. In particular, the one-parameter group of unitary linear operators governing the time evolution of the system are given by

$$e^{-i\frac{t}{\hbar}\hat{H}} = F_2^{-1} \circ T_{e^{-i\frac{\varepsilon_0 t}{\hbar}.|\ |^2}} \circ F_2 \ , \tag{1.17}$$

for every $t \in \mathbb{R}$. More generally,

$$e^{-\left(\frac{1}{\varepsilon}+i\frac{t}{\hbar}\right)\hat{H}} = F_2^{-1} \circ T_{e^{-\varepsilon_0\left(\frac{1}{\varepsilon}+i\frac{t}{\hbar}\right).|\ |^2}} \circ F_2 \ , \tag{1.18}$$

for every $t \in \mathbb{R}$ and $\varepsilon > 0$, where ε has the dimension of an energy. As a consequence of the spectral theorem, Theorem 12.6.4 in the Appendix,

$$\lim_{\varepsilon\to\infty} \| e^{-\left(\frac{1}{\varepsilon}+i\frac{t}{\hbar}\right)\hat{H}} f - e^{-i\frac{t}{\hbar}\hat{H}} f \|_2 = 0 \ ,$$

for every $t \in \mathbb{R}$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$.

For later use, we are going to show that $C_0^2(\mathbb{R}^n, \mathbb{C})$ is a core for $\hat{H}$. For this purpose, we are going to use the following Lemma on Friedrichs mollifiers. For the proof see the proof of the more general Lemma 12.9.13 in the Appendix.

Lemma 1.4.1 (Friedrichs mollifiers) *Let $n \in \mathbb{N}^*$ and $h \in C_0^\infty(\mathbb{R}^n)$ be positive with a support contained in $B_1(0)$ as well as such that $h(x) = h(-x)$ for all $x \in \mathbb{R}^n$ and $\|h\|_1 = 1$. For instance,*

$$h(x) := \begin{cases} C \exp\left(-\frac{1}{1-|x|^2}\right) & \text{if } |x| < 1 \\ 0 & \text{if } |x| \geqslant 1 \end{cases}$$

for every $x \in \mathbb{R}^n$, where

$$C := \left[\int_{U_1(0)} \exp\left(-\frac{1}{1 - |\ |^2} \right) dv^n \right]^{-1} \ .$$

In addition, define for every $\nu \in \mathbb{N}^*$ *the corresponding* $h_\nu \in C_0^\infty(\mathbb{R}^n)$ *by*

$$h_\nu(x) := \nu^n h(\nu x)$$

for all $x \in \mathbb{R}^n$*. Finally, define for every* $\nu \in \mathbb{N}^*$ *and every* $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$

$$H_\nu f := h_\nu * f \ ,$$

and '$*$' denotes the convolution product. Then

(i) for every $\nu \in \mathbb{N}^*$ *the corresponding* H_ν *defines a bounded self-adjoint linear operator on* $L^2_{\mathbb{C}}(\mathbb{R}^n)$ *with operator norm* $\|H_\nu\| \leqslant 1$*,*

(ii)

$$\lim_{\nu \to \infty} H_\nu f = f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$*.*

If $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$, and the sequence $H_1, H_2, \ldots$ is defined as in the previous lemma, it follows for $\nu \in \mathbb{N}^*$ that $H_\nu f \in C_0^\infty(\mathbb{R}^n, \mathbb{C})$,

$$\triangle H_\nu f = h_\nu * \triangle f = H_\nu \triangle f$$

and hence also that

$$\lim_{\nu \to \infty} \triangle H_\nu f = \triangle f \ .$$

As consequence,

$$\hat{H} f = -\varepsilon_0 \triangle f \ ,$$

for every $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$. Since

$$\hat{H}_0 \subset \hat{H}\big|_{C_0^2(\mathbb{R}^n, \mathbb{C})} \subset \hat{H} := \bar{\hat{H}}_0 \ ,$$

it follows that $C_0^2(\mathbb{R}^n, \mathbb{C})$ is a core for $\hat{H}$. For use inside the Sect. 3.5 on the Hamiltonian of the harmonic oscillator, we note that if $g \in C(\mathbb{R}^n, \mathbb{C})$, it follows for $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$ that

$$\lim_{\nu \to \infty} g \, H_\nu f = g f \ . \tag{1.19}$$

For the proof, we note that as consequence of

$$\mathrm{supp}(h_\nu) \subset B_{1/\nu}(0) \subset B_1(0)$$

we have

$$\mathrm{supp}(H_\nu f) \subset C := \mathrm{supp}(f) + B_1(0) \ .$$

Since C is compact and g is continuous, $g|_C$ is bounded. Hence, it follows from

$$\lim_{\nu\to\infty} H_\nu f = f \ ,$$

with the help of Lebesgue's dominated convergence theorem, the validity of (1.19).

1.5 Time Evolution Generated by the Free Hamilton Operator

The time evolution generated by $\hat{H}$ is given as follows.

Time Evolution for a free Particle in n-Dimensional Space I

For $t \in \mathbb{R}^*$, we have[a]

$$e^{-i\,\frac{t}{\hbar}\bar{H}_0} f = \left(\pi i\,\frac{4\varepsilon_0 t}{\hbar}\right)^{-n/2} \cdot \left(e^{i\,\frac{\hbar}{4\varepsilon_0 t}\cdot|\ |^2} * f\right) \ , \tag{1.20}$$

for $f \in L^1_{\mathbb{C}}(\mathbb{R}^n) \cap L^2_{\mathbb{C}}(\mathbb{R}^n)$, and for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$

$$e^{-i\,\frac{t}{\hbar}\bar{H}_0} f = \lim_{\nu\to\infty} \left(\pi i\,\frac{4\varepsilon_0 t}{\hbar}\right)^{-n/2} \cdot \left[e^{i\,\frac{\hbar}{4\varepsilon_0 t}\cdot|\ |^2} * (\chi_{[-\nu,\nu]^n}\, g)\right] \ , \tag{1.21}$$

almost everywhere pointwise on $\mathbb{R}^n$, where $*$ denotes the convolution product.

[a] We note that since the first factor is in $L^\infty_{\mathbb{C}}(\mathbb{R}^n)$, in addition to leading to an element of $L^2_{\mathbb{C}}(\mathbb{R}^n)$, the following convolution results in a bounded uniformly continuous function.

For the proof, see Theorem 12.7.1 in the Appendix. In addition, the proof of the latter theorem shows that

Time Evolution for a free Particle in n-Dimensional Space II

$$e^{-\left(\frac{1}{\varepsilon}+i\,\frac{t}{\hbar}\right)\bar{H}_0} f = (4\pi\,\varepsilon_0\,\sigma_\varepsilon)^{-n/2}\, e^{-\frac{1}{4\,\varepsilon_0\,\sigma_\varepsilon}\cdot|\ |^2} * f \ , \tag{1.22}$$

for every $t \in \mathbb{R}$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where

$$\sigma_\varepsilon := \frac{1}{\varepsilon} + i\,\frac{t}{\hbar}\ ,$$

and $\varepsilon > 0$ has the dimension of an energy.

1.5.1 Large Time Asymptotics of the Evolution

As a first application of the previous explicit representation in the position representation, of the time evolution generated by the free Hamilton operator, we study the large time asymptotic of $e^{-i\,(t/\hbar)\hat{H}} f$, for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, which is also of relevance in scattering theory. For this purpose, let $t \in \mathbb{R}^*$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. We define $U_t f, V_t f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ by

$$U_t f := \left(2\,\frac{\varepsilon_0 t}{\hbar}\,i\right)^{-n/2} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|\ |^2} \cdot \left[(F_2 f)\circ\left(\frac{\hbar}{2\varepsilon_0 t}\,\mathrm{id}_{\mathbb{R}^n}\right)\right],$$
$$V_t f := \left(2\,\frac{\varepsilon_0 t}{\hbar}\,i\right)^{n/2} F_2^{-1}\left\{e^{-i\,\frac{\varepsilon_0 t}{\hbar}|\ |^2} \cdot \left[f\circ\left(2\,\frac{\varepsilon_0 t}{\hbar}\,\mathrm{id}_{\mathbb{R}^n}\right)\right]\right\}\ .$$

Then

$$\|U_t f\|_2^2 = \left(2\,\frac{\varepsilon_0 |t|}{\hbar}\right)^{-n}\left\|(F_2 f)\circ\left(\frac{\hbar}{2\varepsilon_0 t}\,\mathrm{id}_{\mathbb{R}^n}\right)\right\|_2^2$$
$$= \left(\frac{\hbar}{2\varepsilon_0|t|}\right)^{n}\left\|(F_2 f)\circ\left(\frac{\hbar}{2\varepsilon_0 t}\,\mathrm{id}_{\mathbb{R}^n}\right)\right\|_2^2 = \|F_2 f\|_2^2 = \|f\|_2^2\ ,$$
$$\|V_t f\|_2^2 = \left(2\,\frac{\varepsilon_0 |t|}{\hbar}\right)^{n}\left\|e^{-i\,\frac{\varepsilon_0 t}{\hbar}|\ |^2}\cdot\left[f\circ\left(2\,\frac{\varepsilon_0 t}{\hbar}\,\mathrm{id}_{\mathbb{R}^n}\right)\right]\right\|_2^2$$
$$= \left(2\,\frac{\varepsilon_0 |t|}{\hbar}\right)^{n}\left\|f\circ\left(2\,\frac{\varepsilon_0 t}{\hbar}\,\mathrm{id}_{\mathbb{R}^n}\right)\right\|_2^2 = \|f\|_2^2\ .$$

Since $U_t : (L^2_{\mathbb{C}}(\mathbb{R}^n) \to L^2_{\mathbb{C}}(\mathbb{R}^n),\ f \mapsto U_t f)$ and $V_t : (L^2_{\mathbb{C}}(\mathbb{R}^n) \to L^2_{\mathbb{C}}(\mathbb{R}^n),\ f \mapsto V_t f)$ are obviously linear, the latter implies that U_t and V_t are linear isometries and hence in particular injective. Further, a short calculation shows that $V_t U_t f = f$, for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and hence that V_t is also surjective and hence as a whole bijective. The latter implies that $U_t f = V_t^{-1} f$, for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, and hence that U_t is bijective, too. Finally, from the polarization identities for $\mathbb{C}$-Sesquilinear forms on complex vector spaces, see Theorem 12.3.3 (ii) in the Appendix, it follows that U_t and V_t are unitary linear operators and that $V_t = U_t^*$. Further for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, it follows that

$$
\begin{aligned}
&\left[\left(e^{-i\,\frac{t}{\hbar}\bar{H}_0} - U_t\right) f\right](u) \\
&= \left(4\,\frac{\varepsilon_0 t}{\hbar}\,\pi i\right)^{-n/2} \cdot \int_{\mathbb{R}^n} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|u-\bar{u}|^2} f(\bar{u})\,dv^n \\
&\quad - \left(4\,\frac{\varepsilon_0 t}{\hbar}\,\pi i\right)^{-n/2} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|u|^2} \cdot \int_{\mathbb{R}^n} e^{-i\,\frac{\hbar}{2\varepsilon_0 t}\,u\cdot\bar{u}} f(\bar{u})\,dv^n \\
&= \left(4\,\frac{\varepsilon_0 t}{\hbar}\,\pi i\right)^{-n/2} \cdot \int_{\mathbb{R}^n} e^{i\,\frac{\hbar}{4\varepsilon_0 t}(\,|u|^2+|\bar{u}|^2-2u\cdot\bar{u}\,)} f(\bar{u})\,dv^n \\
&\quad - \left(4\,\frac{\varepsilon_0 t}{\hbar}\,\pi i\right)^{-n/2} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|u|^2} \cdot \int_{\mathbb{R}^n} e^{-i\,\frac{\hbar}{2\varepsilon_0 t}\,u\cdot\bar{u}} f(\bar{u})\,dv^n \\
&= \left(4\,\frac{\varepsilon_0 t}{\hbar}\,\pi i\right)^{-n/2} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|u|^2} \cdot \int_{\mathbb{R}^n} e^{-i\,\frac{\hbar}{2\varepsilon_0 t}\,u\cdot\bar{u}} \left(e^{i\,\frac{\hbar}{4\varepsilon_0 t}|\bar{u}|^2} - 1\right) f(\bar{u})\,dv^n \\
&= \left(2\,\frac{\varepsilon_0 t}{\hbar}\,i\right)^{-n/2} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|u|^2} \cdot \left\{F_2\left[\left(e^{i\,\frac{\hbar}{4\varepsilon_0 t}|\ |^2} - 1\right) f\right]\right\}\left(\frac{\hbar}{2\varepsilon_0 t}\,u\right) ,
\end{aligned}
$$

for every $u \in \mathbb{R}^n$. Hence

$$
\begin{aligned}
&\|(e^{-i\,\frac{t}{\hbar}\bar{H}_0} - U_t)f\|_2^2 \leqslant \left\|\left(e^{i\,\frac{\hbar}{4\varepsilon_0 t}|\ |^2} - 1\right) f\right\|_2^2 = 4\left\|\sin\left(\frac{\hbar}{8\varepsilon_0|t|}\,|\ |^2\right)\cdot f\right\|_2^2 \\
&= 4\int_{\mathbb{R}^n} \sin^2\left(\frac{\hbar}{8\varepsilon_0|t|}\,|\ |^2\right)|f|^2\,dv^n ,
\end{aligned}
$$

and it follows from Lebesgue's dominated convergence theorem that

$$
\lim_{t\to\pm\infty} \|(e^{-i\,\frac{t}{\hbar}\bar{H}_0} - U_t) f\|_2 = 0 .
$$

Summarizing the previous, we arrive at the following result.

Large Time Asymptotics of $e^{-i\,(t/\hbar)\hat{H}} f$, for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$

For every $t \in \mathbb{R}^*$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$,

$$
\|(e^{-i\,\frac{t}{\hbar}\bar{H}_0} - U_t)f\|_2^2 \leqslant 4\int_{\mathbb{R}^n} \sin^2\left(\frac{\hbar}{8\varepsilon_0|t|}\,|\ |^2\right)|f|^2\,dv^n ,
$$

and hence

$$
\lim_{t\to\pm\infty} \|(e^{-i\,\frac{t}{\hbar}\bar{H}_0} - U_t) f\|_2 = 0 ,
$$

where for every $t \in \mathbb{R}^*$, the unitary linear operator U_t on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ is defined by

$$U_t g := \left(2\,\frac{\varepsilon_0 t}{\hbar}\,i\right)^{-n/2} e^{i\,\frac{\hbar}{4\varepsilon_0 t}|\;|^2}\cdot\left[(F_2 g)\circ\left(\frac{\hbar}{2\varepsilon_0 t}\,\mathrm{id}_{\mathbb{R}^n}\right)\right],$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$.

We note that for every $t \in \mathbb{R}^*$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$

$$|U_t f|^2 = \left(\frac{\hbar}{2\varepsilon_0|t|}\right)^n \left|(F_2 f)\circ\left(\frac{\hbar}{2\varepsilon_0 t}\,\mathrm{id}_{\mathbb{R}^n}\right)\right|^2 .$$

If $\|f\|_2 = 1$ and $\Omega \subset \mathbb{R}^n$ is a Lebesgue measurable subset of "momentum space," then

$$\int_{(\hbar\kappa)^{-1}\,\Omega} |F_2 f|^2\,dv^n\ ,$$

see (1.13), is the probability of finding the momentum of the particle at time 0 to belong to the Lebesgue measurable set Ω. After "a sufficiently large time $t > 0$ of evolution" or "for a sufficiently large negative time $t < 0$," the probability of finding the position of the particle to belong to the Lebesgue measurable set $\frac{t}{m}\,\Omega \subset \mathbb{R}^n$ "in position space," see (1.2), is or has been, respectively, approximately given by,

$$\begin{aligned}\int_{\kappa\,\frac{t}{m}\Omega} |U_t f|^2\,dv^n &= \int_{\kappa\,\frac{t}{m}\Omega}\left(\frac{\hbar}{2\varepsilon_0|t|}\right)^n \left|(F_2 f)\circ\left(\frac{\hbar}{2\varepsilon_0 t}\,\mathrm{id}_{\mathbb{R}^n}\right)\right|^2 dv^n\\ &= \int_{(\hbar\kappa)^{-1}\,\Omega} |F_2 f|^2\,dv^n\ ,\end{aligned}$$

i.e., asymptotically for $t \to +\infty$ or $t \to -\infty$, the particle moves increasingly or moved, respectively, like a flow of free classical particles of mass m, with momentum density $|F_2 f|^2$.

1.5.2 Time Evolution and Causality

Another important application concerns the support properties of the elements in the paths in Hilbert space described by (1.20). If $|f|^2$ has a compact support for an $f \in X \setminus \{0\}$, then (1.20) indicates that, for each $t \in \mathbb{R}^*$, the corresponding support of $|e^{-i\,\frac{t}{\hbar}\hat{H}} f|^2$, is not compact, since the result of a convolution of a function that has no compact support with a function of compact support. This is consistent with a theory using Newtonian ideas of space and time, where there is instantaneous propagation of any action, but inconsistent with a theory that is compatible with the theory of special relativity, where the speed of light c sets a limit for the speed of propagation of any action. On the other hand, this is of course not surprising because we are quantizing a Newtonian mechanical system. We note that the solutions of the heat equation display the same behavior, and indeed we are going to see in a later chapter a connection between the solutions of the Schrödinger equation and the solutions of the heat equation. Again, on the other hand, the above observation, concerning the the support properties of the functions involved in the convolution, although very plausible, does not provide a proof.

In the following, we are going to sketch a proof, using methods from the area of Paley-Wiener theorems. If $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ has a (representative) with compact support contained in a closed ball of radius $r > 0$, then, for the unique analytic extension $\widehat{F_2 f}$ of $F_2 f$ to an entire holomorphic function, there is $C > 0$ such that

$$|\widehat{F_2 f}(k)| \leqslant C e^{r\,|\mathrm{Im}(k)|} \ , \tag{1.23}$$

for every $k \in \mathbb{C}^n$, where $\mathrm{Im}(k) := {}^t(\mathrm{Im}(k_1), \ldots, \mathrm{Im}(k_n))$ for every $k = {}^t(k_1, \ldots, k_n) \in \mathbb{C}^n$. According to (1.17), for $t \in \mathbb{R}^*$,

$$(F_2\, e^{-i\frac{t}{\hbar}\hat{H}} f)(k) = e^{-i\frac{\varepsilon_0 t}{\hbar}(k_1^2+\cdots+k_n^2)} \cdot (F_2 f)(k) \ ,$$

for every $k = {}^t(k_1, \ldots, k_n) \in \mathbb{R}^n$. Hence, the unique analytic extension $F_2\, \widehat{e^{-i\frac{t}{\hbar}\hat{H}}} f$ of $F_2\, e^{-i\frac{t}{\hbar}\hat{H}} f$ to an entire holomorphic function is given by

$$(F_2\, \widehat{e^{-i\frac{t}{\hbar}\hat{H}}} f)(k) = e^{-i\frac{\varepsilon_0 t}{\hbar}(k_1^2+\cdots+k_n^2)} \cdot (\widehat{F_2 f})(k) \ ,$$

for every $k = {}^t(k_1, \ldots, k_n) \in \mathbb{C}^n$, which does not satisfy an estimate of the form (1.23). Hence, $F_2\, e^{-i\frac{t}{\hbar}\hat{H}} f$ is not a Fourier transform of a function with compact support, i.e., the support of $e^{-i\frac{t}{\hbar}\hat{H}} f$ is not compact.

1.5.3 Free Propagation of Gaussians

Since for $\sigma, \tau \in (0, \infty) \times \mathbb{R}$ and $u_0, v_0 \in \mathbb{R}^n$

$$\begin{aligned} &\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) * \exp(-\tau|\mathrm{id}_{\mathbb{R}^n} - v_0|^2) \\ &= \left(\frac{\pi}{\sigma+\tau}\right)^{n/2} \exp\left(-\frac{\sigma\tau}{\sigma+\tau}\,|\mathrm{id}_{\mathbb{R}^n} - u_0 - v_0|^2\right) \ , \end{aligned}$$

we have for every $t \in \mathbb{R}$,

$$
\begin{aligned}
&\lim_{\varepsilon\to\infty} (4\pi\,\varepsilon_0\,\sigma_\varepsilon)^{-n/2}\exp\left(-\frac{1}{4\varepsilon_0\sigma_\varepsilon}|\ |^2\right) * \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\\
&=\left(4\pi i\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2}\left(\frac{\pi}{\sigma-i\,\frac{\hbar}{4\varepsilon_0 t}}\right)^{n/2}\ \exp\left(i\,\frac{\sigma\,\frac{\hbar}{4\varepsilon_0 t}}{\sigma-i\,\frac{\hbar}{4\varepsilon_0 t}}\,|\mathrm{id}_{\mathbb{R}^n}-u_0|^2\right)\\
&=\left(\frac{-i\,\frac{\hbar}{4\varepsilon_0 t}}{\sigma-i\,\frac{2}{i}\,\frac{\hbar\kappa^2}{m}\,\sigma t\hbar 4\varepsilon_0 t}\right)^{n/2}\ \exp\left(i\,\frac{\sigma\,\frac{\hbar}{4\varepsilon_0 t}}{\sigma-i\,\frac{\hbar}{4\varepsilon_0 t}}\,|\mathrm{id}_{\mathbb{R}^n}-u_0|^2\right)\\
&=\left(1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2}\ \exp\left(-\frac{\sigma}{1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\,|\mathrm{id}_{\mathbb{R}^n}-u_0|^2\right)\ ,
\end{aligned}
$$

where we used

$$\tau=\frac{1}{4\varepsilon_0\sigma_\varepsilon}\ .$$

Hence,

Propagation of Gaussians I

$$
\begin{aligned}
&e^{-i\,\frac{t}{\hbar}\hat{H}}\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\\
&=\left(1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2}\exp\left(-\frac{\sigma}{1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\,|\mathrm{id}_{\mathbb{R}^n}-u_0|^2\right)\ ,
\end{aligned}
$$

for every $t\in\mathbb{R}$, $\sigma\in(0,\infty)\times\mathbb{R}$ and $u_0\in\mathbb{R}^n$.

For normalization, we note for $\sigma>0$ that

$$
\begin{aligned}
&\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\|_2=\|\exp(-\sigma|\ |^2)\|_2\\
&=\left(\int_{\mathbb{R}^n} e^{-2\sigma|\ |^2}\,dv^n\right)^{1/2}=\left(\frac{\pi}{2\sigma}\right)^{n/4}
\end{aligned}
$$

and hence that

$$\left\|\left(\frac{2\sigma}{\pi}\right)^{n/4}\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\right\|_2=1\ .$$

As a consequence, we arrive at the following result.

Propagation of Gaussians II

For every $t \in \mathbb{R}$, $\sigma > 0$ and $u_0 \in \mathbb{R}^n$

$$e^{-i\,\frac{t}{\hbar}\hat{H}}\,\frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\|_2}$$
$$= \left(\frac{1}{\sqrt{\pi}}\,\frac{\sqrt{2\sigma}}{1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\right)^{n/2} \exp\left(-\frac{\sigma}{1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\,|\mathrm{id}_{\mathbb{R}^n}-u_0|^2\right)\,,$$

and the corresponding observable probability distributions

$$\left|e^{-i\,\frac{t}{\hbar}\hat{H}}\,\frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\|_2}\right|^2 \tag{1.24}$$
$$= \left[\frac{1}{\pi}\,\frac{2\sigma}{1+16\sigma^2\left(\frac{\varepsilon_0 t}{\hbar}\right)^2}\right]^{n/2} \exp\left[-\frac{2\sigma}{1+16\sigma^2\left(\frac{\varepsilon_0 t}{\hbar}\right)^2}\,|\mathrm{id}_{\mathbb{R}^n}-u_0|^2\right]\,,$$

for every $t \in \mathbb{R}$, $\sigma > 0$ and $u_0 \in \mathbb{R}^n$, where $\varepsilon_0 = \frac{\hbar^2\kappa^2}{2m}$.

We note that for $t \in \mathbb{R}$, (1.24) coincides with the normal distribution of a random variable with mean u_0 and standard deviation

$$\sqrt{\frac{1}{4\sigma} + 4\sigma\cdot\left(\frac{\varepsilon_0 t}{\hbar}\right)^2}\,.$$

Time evolution keeps the mean unchanged, but increases the standard deviation, the latter asymptotically proportionally to $|t|$, for $t \to \pm\infty$. Further, it follows for every $v \in \mathbb{R}^n$ that

$$\left[F_2\,\frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\|_2}\right](v) = \left(\frac{2\sigma}{\pi}\right)^{n/4}[F_2\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)](v)$$
$$= \left(\frac{2\sigma}{\pi}\right)^{n/4} e^{-ivu_0}\,(F_2 e^{-\sigma.\mathrm{id}^2_{\mathbb{R}^n}})(v) = \left(\frac{2\sigma}{\pi}\right)^{n/4} e^{-ivu_0}\,(2\sigma)^{-n/2}\,e^{-v^2/(4\sigma)}$$
$$= (2\pi\sigma)^{-n/4} e^{-ivu_0}\,e^{-v^2/(4\sigma)}$$

and hence that

$$\boxed{\left|F_2\,\frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n}-u_0|^2)\|_2}\right|^2 = (2\pi\sigma)^{-n/2}\exp\left(-\frac{1}{2\sigma}\,|\ |^2\right)\,,}$$

which coincides with the normal distribution of a random variable with mean 0 and standard deviation $\sqrt{\sigma}$. We remark that this probability distribution is preserved by the time evolution, since as a consequence of (1.17)[5]

$$\begin{aligned}
&\left| F_2 e^{-i\frac{t}{\hbar}\hat{H}} \frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2)\|_2} \right|^2 \\
&= \left| e^{-i\frac{\varepsilon_0 t}{\hbar}.|\ |^2} F_2 \frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2)\|_2} \right\|^2 = \left| F_2 \frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2)\|_2} \right\|^2 \\
&= (2\pi\sigma)^{-n/2} \exp\left(-\frac{1}{2\sigma}|\ |^2\right) .
\end{aligned}$$

The reader might wonder, whether there are "moving Gaussians," i.e., a sort of Gaussians whose means changes with time. Indeed, such exist. For the derivation, we use the momentum representation, and data $\tilde{f} \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ at time 0 given by

$$\tilde{f}(v) := (2\pi\sigma)^{-n/4} e^{-[v-(\hbar\kappa)^{-1} p_0]^2/(4\sigma)} ,$$

for every $v \in \mathbb{R}^n$, where $p_0 = (p_{01}, \dots, p_{0n}) \in \mathbb{R}^n$ has the dimension of momentum. Hence,

$$|\tilde{f}|^2 = (2\pi\sigma)^{-n/2} \exp\left(-\frac{1}{2\sigma}|\mathrm{id}_{\mathbb{R}^n} - (\hbar\kappa)^{-1} p_0|^2\right)$$

describes a normal distribution with mean $(\hbar\kappa)^{-1} p_0$ and and standard deviation $\sqrt{\sigma}$. Since for every $t \in \mathbb{R}$, as a consequence of (1.17),

$$\begin{aligned}
&[F_2 e^{-i\frac{t}{\hbar}\hat{H}} F_2^{-1} \tilde{f}\,](v) = (2\pi\sigma)^{-n/4} e^{-i\frac{\varepsilon_0 t}{\hbar}.v^2} e^{-[v-(\hbar\kappa)^{-1} p_0]^2/(4\sigma)} \\
&= (2\pi\sigma)^{-n/4} e^{-i\frac{\varepsilon_0 t}{\hbar}.[2(\hbar\kappa)^{-1} p_0\cdot v-(\hbar\kappa)^{-2}|p_0|^2]} e^{-\left(\frac{1}{4\sigma}+i\frac{\varepsilon_0 t}{\hbar}\right).[v-(\hbar\kappa)^{-1} p_0]^2} \\
&= (2\pi\sigma)^{-n/4} e^{-i\frac{\varepsilon_0 t}{\hbar}.[2(\hbar\kappa)^{-1} p_0\cdot v-(\hbar\kappa)^{-2}|p_0|^2]} e^{-[v-(\hbar\kappa)^{-1} p_0]^2/[4(\frac{1}{\sigma}+4i\frac{\varepsilon_0 t}{\hbar})^{-1}]} \\
&= (2\pi\sigma)^{-n/4} e^{-i\frac{t}{\hbar}.(\frac{\hbar\kappa}{m} p_0\cdot v-\frac{|p_0|^2}{2m})} e^{-[v-(\hbar\kappa)^{-1} p_0]^2/[4(\frac{1}{\sigma}+4i\frac{\varepsilon_0 t}{\hbar})^{-1}]} \\
&= (2\pi\sigma)^{-n/4}\left(\frac{1}{2\sigma}+2i\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2} e^{i\frac{|p_0|^2}{2m}\cdot\frac{t}{\hbar}} \\
&\quad\cdot e^{-i\frac{\kappa t}{m} p_0\cdot v} \cdot [F_2 e^{i(\hbar\kappa)^{-1} p_0\cdot \mathrm{id}_{\mathbb{R}^n}} e^{-(\frac{1}{\sigma}+4i\frac{\varepsilon_0 t}{\hbar})^{-1}.|\ |^2}](v) \\
&= \left(\frac{2\sigma}{\pi}\right)^{n/4}\cdot\left(1+4i\sigma\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2} e^{i\frac{|p_0|^2}{2m}\cdot\frac{t}{\hbar}} \\
&\quad\cdot [F_2 e^{i(\hbar\kappa)^{-1} p_0\cdot(\mathrm{id}_{\mathbb{R}^n}-\frac{\kappa t}{m} p_0)} e^{-(\frac{1}{\sigma}+4i\frac{\varepsilon_0 t}{\hbar})^{-1}.|\mathrm{id}_{\mathbb{R}^n}-\frac{\kappa t}{m} p_0|^2}](v)
\end{aligned}$$

[5] More generally, as a consequence of (1.17), we have $|F_2 e^{-i\frac{t}{\hbar}\hat{H}} f|^2 = |F_2 f|^2$, for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$.

$$= \left(\frac{2\sigma}{\pi}\right)^{n/4} \cdot \left(1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2} e^{-i\,\frac{|p_0|^2}{2m}\cdot\frac{t}{\hbar}}$$
$$\cdot\, [F_2\, e^{i(\hbar\kappa)^{-1}\,p_0\cdot\mathrm{id}_{\mathbb{R}^n}}\, e^{-(\frac{1}{\sigma}+4i\,\frac{\varepsilon_0 t}{\hbar})^{-1}.|\mathrm{id}_{\mathbb{R}^n}-\frac{\kappa t}{m}\,p_0|^2}](v)\ ,$$

where $\varepsilon_0 = \frac{\hbar^2\kappa^2}{2m}$, and we used Lemma 12.9.24 from the Appendix, we have

$$f := F_2^{-1}\tilde{f} = \left(\frac{2\sigma}{\pi}\right)^{n/4} \cdot e^{i\,(\hbar\kappa)^{-1}\,p_0\cdot\mathrm{id}_{\mathbb{R}^n}}\, e^{-\sigma|\ |^2}\ ,$$

and

$$e^{-i\,\frac{t}{\hbar}\hat{H}}\,F_2^{-1}f = \left(\frac{2\sigma}{\pi}\right)^{n/4} \cdot \left(1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2} e^{-i\,\frac{|p_0|^2}{2m}\cdot\frac{t}{\hbar}}$$
$$\cdot\, e^{i(\hbar\kappa)^{-1}\,p_0\cdot\mathrm{id}_{\mathbb{R}^n}}\, e^{-\frac{\sigma}{1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}.|\mathrm{id}_{\mathbb{R}^n}-\frac{\kappa t}{m}\,p_0|^2}\ ,$$

for every $t \in \mathbb{R}$. As a consequence, we arrive at the following result.

Propagation of Gaussians III

For every $t \in \mathbb{R}, \sigma > 0$ and $p_0 = (p_{01}, \ldots, p_{0n}) \in \mathbb{R}^n$ with the dimension of momentum, $|F_2 f|^2$, where

$$f := \left(\frac{2\sigma}{\pi}\right)^{n/4} \cdot \exp[\,i\,(\hbar\kappa)^{-1}\,p_0\cdot\mathrm{id}_{\mathbb{R}^n}]\exp(-\sigma|\ |^2)\ ,$$

describes a normal distribution with mean $(\hbar\kappa)^{-1}\,p_0$ and standard deviation $\sqrt{\sigma}$. Further,

$$e^{-i\,\frac{t}{\hbar}\hat{H}}f = \left(\frac{2\sigma}{\pi}\right)^{n/4} \cdot \left(1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2} \exp\left(-i\,\frac{|p_0|^2}{2m}\cdot\frac{t}{\hbar}\right)$$
$$\cdot\,\exp[\,i\,(\hbar\kappa)^{-1}\,p_0\cdot\mathrm{id}_{\mathbb{R}^n}]\cdot\exp\left(-\frac{\sigma}{1+4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\,|\mathrm{id}_{\mathbb{R}^n}-\frac{\kappa t}{m}\,p_0|^2\right)\ ,$$

where $\varepsilon_0 = \frac{\hbar^2\kappa^2}{2m}$, and

$$\left|e^{-i\,\frac{t}{\hbar}\hat{H}}f\right|^2 = \left[\frac{1}{2\pi}\,\frac{4\sigma}{1+16\sigma^2\left(\frac{\varepsilon_0 t}{\hbar}\right)^2}\right]^{n/2} \tag{1.25}$$
$$\cdot\,\exp\left(-\frac{1}{2}\,\frac{4\sigma}{1+16\sigma^2\left(\frac{\varepsilon_0 t}{\hbar}\right)^2}\,|\mathrm{id}_{\mathbb{R}^n}-\frac{\kappa t}{m}\,p_0|^2\right)$$

describes a normal distribution with mean $\frac{\kappa t}{m}\, p_0$ and standard deviation

$$\sqrt{\frac{1}{4\sigma} + 4\sigma \cdot \left(\frac{\varepsilon_0 t}{\hbar}\right)^2}\ .$$

If $n = 1$, the mean is right moving if $p_0 > 0$ and left moving if $p_0 < 0$.

In the following, we study the evolution of a superposition of 2 Gaussians with different means, but equal standard deviations. We are going to see that the time evolution of the superposition shows an interference pattern for $t \approx m/(2\hbar\kappa^2)$. For this purpose, we note for $\sigma > 0$ that

$$\begin{aligned}
& e^{-i\,\frac{t}{\hbar}\hat{H}} \left(\frac{2\sigma}{\pi}\right)^{n/4} \left[\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\right] \\
&= \left(\frac{1}{\sqrt{\pi}}\,\frac{\sqrt{2\sigma}}{1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\right)^{n/2} \left[\exp\left(-\frac{\sigma}{1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\,|\mathrm{id}_{\mathbb{R}^n} - u_0|^2\right)\right. \\
&\quad \left. + \exp\left(-\frac{\sigma}{1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\,|\mathrm{id}_{\mathbb{R}^n} - v_0|^2\right)\right]\ .
\end{aligned}$$

For normalization, we note that

$$\begin{aligned}
& \|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\|_2^2 \\
&= \int_{\mathbb{R}^n} \big[\exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + 2\exp(-\sigma[\,|\mathrm{id}_{\mathbb{R}^n} - u_0|^2 + |\mathrm{id}_{\mathbb{R}^n} - v_0|^2]) \\
&\qquad + \exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\big]dv^n \\
&= \int_{\mathbb{R}^n} \Bigg[\exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2) \\
&\qquad + 2\exp\left\{-2\sigma\left[\,|\ |^2 - (u_0 + v_0)\cdot \mathrm{id}_{\mathbb{R}^n} + \frac{|u_0|^2 + |v_0|^2}{2}\right]\right\}\Bigg]dv^n \\
&= \int_{\mathbb{R}^n} \Bigg[\exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2) \\
&\qquad + 2\exp\left\{-2\sigma\left[\left|\mathrm{id}_{\mathbb{R}^n} - \frac{1}{2}\,(u_0 + v_0)\right|^2 + \frac{|u_0 - v_0|^2}{4}\right]\right\}\Bigg]dv^n
\end{aligned}$$

$$= \int_{\mathbb{R}^n} \Bigg\{ \exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-2\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)$$
$$+ 2\exp\left(-\frac{\sigma\,|u_0 - v_0|^2}{2}\right) \exp\left[-2\sigma \left|\mathrm{id}_{\mathbb{R}^n} - \frac{1}{2}(u_0 + v_0)\right|^2\right] \Bigg\} dv^n$$
$$= 2\left(\frac{\pi}{2\sigma}\right)^{n/2} \left[1 + \exp\left(-\frac{\sigma\,|u_0 - v_0|^2}{2}\right)\right]$$
$$= 4\left(\frac{\pi}{2\sigma}\right)^{n/2} e^{-\sigma\,|u_0 - v_0|^2/4} \cosh\left(\frac{\sigma\,|u_0 - v_0|^2}{4}\right) .$$

Hence,

$$\left(\frac{2\sigma}{\pi}\right)^{n/4} \|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\|_2$$
$$= 2e^{-\sigma\,|u_0 - v_0|^2/8} \cosh^{1/2}\left(\frac{\sigma\,|u_0 - v_0|^2}{4}\right) ,$$

and

Superposition of Gaussians

$$e^{-i\,\frac{t}{\hbar}\hat{H}}\, \frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\|_2}$$
$$= \frac{1}{2}\left(\frac{1}{\sqrt{\pi}}\,\frac{\sqrt{2\sigma}}{1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\right)^{n/2} \frac{e^{\sigma\,|u_0 - v_0|^2/8}}{\cosh^{1/2}\left(\frac{\sigma\,|u_0 - v_0|^2}{4}\right)}$$
$$\cdot \left[\exp\left(-\frac{\sigma\,|\mathrm{id}_{\mathbb{R}^n} - u_0|^2}{1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\right) + \exp\left(-\frac{\sigma\,|\mathrm{id}_{\mathbb{R}^n} - v_0|^2}{1 + 4i\sigma\,\frac{\varepsilon_0 t}{\hbar}}\right)\right],$$

and the corresponding observable probability distribution

$$\left| e^{-i\,\frac{t}{\hbar}\hat{H}}\, \frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\|_2} \right|^2$$
$$= \frac{e^{\sigma\,|u_0 - v_0|^2/4}}{\cosh\left(\frac{\sigma\,|u_0 - v_0|^2}{4}\right)} \left[\frac{1}{\pi}\,\frac{2\sigma}{1 + \left(4\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^2}\right]^{n/2}$$
$$\cdot \left\{ \sinh^2\left[\frac{\sigma\,(u_0 - v_0)\cdot(u_0 + v_0 - 2\cdot\mathrm{id}_{\mathbb{R}^n})}{2\left[1 + \left(4\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^2\right]}\right]\right.$$

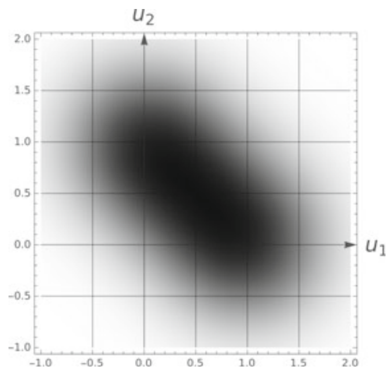


Fig. 1.1 Density plot of the probability distribution for the position of the particle at time 0 in the u_1, u_2-plane, of the superposed Gaussians, for $n = 3$, $\sigma = 1$, $u_0 = (1, 0, 0)$, $v_0 = (0, 1, 0)$. Relative darker colors indicate relative higher probabilities

$$+\cos^2\left[\frac{\sigma\,(u_0 - v_0)\cdot(u_0 + v_0 - 2\cdot \mathrm{id}_{\mathbb{R}^n})\,\frac{\hbar\kappa^2}{m}\,\sigma t}{1 + \left(4\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^2}\right]\Bigg\}$$

$$\cdot \exp\left[-\frac{\sigma\,\left(|\mathrm{id}_{\mathbb{R}^n} - u_0|^2 + |\mathrm{id}_{\mathbb{R}^n} - v_0|^2\right)}{1 + \left(4\sigma\,\frac{\varepsilon_0 t}{\hbar}\right)^2}\right], \tag{1.26}$$

for every $t \in \mathbb{R}$, $\sigma > 0$, $u_0 \in \mathbb{R}^n$ and $v_0 \in \mathbb{R}^n$,

where we used that (Figs. 1.1 and 1.2)

$$\begin{aligned}
&|e^{-\alpha\sigma z} + e^{-\beta\sigma z}|^2 = (e^{-\alpha\sigma z^*} + e^{-\beta\sigma z^*})(e^{-\alpha\sigma z} + e^{-\beta\sigma z})\\
&= e^{-2\alpha\sigma x} + e^{-2\beta\sigma x} + e^{-\sigma[\alpha(x-iy)+\beta(x+iy)]} + e^{-\sigma[\alpha(x+iy)+\beta(x-iy)]}\\
&= e^{-2\alpha\sigma x} + e^{-2\beta\sigma x} + e^{-\sigma(\alpha x - i\alpha y + \beta x + i\beta y)} + e^{-\sigma(\alpha x + i\alpha y + \beta x - i\beta y)}\\
&= e^{-2\alpha\sigma x} + e^{-2\beta\sigma x} + e^{-\sigma(\alpha+\beta)x}[e^{i\sigma(\alpha-\beta)y} + e^{-i\sigma(\alpha-\beta)y}]\\
&= e^{-2\alpha\sigma x} + e^{-2\beta\sigma x} + 2e^{-\sigma(\alpha+\beta)x}\cos[\sigma(\alpha-\beta)y]\\
&= e^{-\sigma(\alpha+\beta)x}\left\{e^{-\sigma(\alpha-\beta)x} + e^{\sigma(\alpha-\beta)x} + 2\cos[\sigma(\alpha-\beta)y]\right\}\\
&= 2e^{-\sigma(\alpha+\beta)x}\,\{\cosh[\sigma(\alpha-\beta)x] + \cos[\sigma(\alpha-\beta)y]\}\ ,
\end{aligned}$$

for every $z = x + iy \in \mathbb{C} \setminus (-\infty, 0]$, $x, y, \sigma, \alpha, \beta \in \mathbb{R}$.

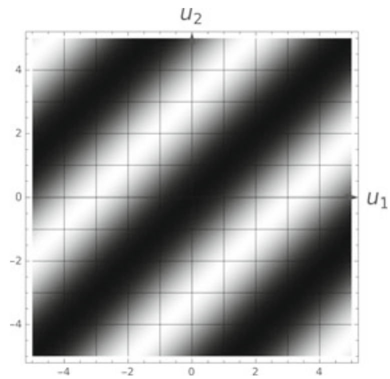


Fig. 1.2 Density plot of the oscillating factor for $t = m/(2\hbar\kappa^2)$, in the probability distribution (1.26) for the position of the particle in the u_1, u_2-plane, of the superposed Gaussians, displaying interference, for $n = 3$, $\sigma = 1$, $u_0 = (1, 0, 0)$, $v_0 = (0, 1, 0)$. Relatively darker colors indicate relatively higher probabilities

Superposition of Gaussians: Asymptotic for Large Times

We note that

$$\left| e^{-i\,\frac{t}{\hbar}\hat{H}}\, \frac{\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)}{\|\exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - u_0|^2) + \exp(-\sigma|\mathrm{id}_{\mathbb{R}^n} - v_0|^2)\|_2} \right|^2 \tag{1.27}$$
$$\underset{t\to\pm\infty}{\sim} \frac{e^{\frac{\sigma\,|u_0 - v_0|^2}{4}}}{(2\pi\sigma)^{\frac{n}{2}}\cosh\left(\frac{\sigma\,|u_0-v_0|^2}{4}\right)} \left(\frac{\hbar}{2\varepsilon_0|t|}\right)^n ,$$

for every $\sigma > 0$, $u_0 \in \mathbb{R}^n$ and $v_0 \in \mathbb{R}^n$.

1.6 Perturbations of the Free Hamilton Operator in $\leqslant 3$ Space Dimensions

A Point-Particle of Mass $m > 0$ Subject to an External Potential V

In the following, we are going to show for $n \leqslant 3$ that the densely-defined, linear and symmetric operator

$$\hat{H}_{V0} : C_0^2(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n)$$

in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, defined by

$$\hat{H}_{V0} f := -\frac{\hbar^2 \kappa^2}{2m} \triangle f + V f = \frac{\hbar^2 \kappa^2}{2m} \left(-\triangle f + \frac{2m}{\hbar^2 \kappa^2} V f \right) ,$$

for every $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$, where $V \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$.[a] Then $\hat{H}_{V0}$ is essentially self-adjoint. In addition,

$$\overline{\hat{H}_{V0}} = \hat{H} + T_V ,$$

where $\hat{H}$ is the free Hamiltonian from Sect. 1.4, and T_V denotes the maximal multiplication operator with V in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, and[b]

$$D\left(\overline{\hat{H}_{V0}}\right) = D(\hat{H}) \subset C_\infty(\mathbb{R}^n, \mathbb{C}) .$$

We note that the potential corresponding to the case of an electron in the Coulomb field of an nucleus containing Z protons,

$$V = -\frac{Ze^2\kappa}{|\;|} ,$$

where e denotes the charge of an electron, is an element of $L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$.

[a] We note that V coincides with the classical potential function only up to a scale factor. The value of the classical potential function at the point $x \in \mathbb{R}^n$ is given by $V(\kappa x)$.

[b] We note that is not difficult to show that $D(\hat{H})$ is equal to the Sobolev space $W^2_{\mathbb{C}}(\mathbb{R}^n)$, i.e., the subspace of $L^2_{\mathbb{C}}(\mathbb{R}^n)$, consisting of those elements that are weakly differentiable to every order $\alpha \in \mathbb{N}^n$ with $|\alpha| \leqslant 2$ and such that these weak derivatives are square integrable. It is interesting to note that there is a connection between the concept of domains of self-adjoint operators and Sobolev spaces, at least for simple potentials.

For this purpose, we are going to use the Rellich-Kato theorem, whose proof is given in the Appendix, see Theorem 12.4.11 in the Appendix.

Theorem 1.6.1 (Relatively bounded perturbations of self-adjoint operators, Rellich-Kato theorem) *Let* $(X, \langle\,|\,\rangle)$ *be a complex Hilbert space, A, B be densely-defined, linear, symmetric operators in X and* $0 \leqslant a < 1$, $b \geqslant 0$ *such that* $D(B) \supset D(A)$ *and*

$$\|Bf\|^2 \leqslant a^2 \|Af\|^2 + b^2 \|f\|^2 \tag{1.28}$$

for every $f \in D(A)$. *If A is in addition essentially self-adjoint, then* $A + B$ *is densely-defined, linear and essentially self-adjoint such that*

$$\overline{A + B} = \bar{A} + \bar{B} .$$

For the proof that $\hat{H}_0$ is essentially self-adjoint, we recall that

$$A : C_0^2(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n) \ , \tag{1.29}$$

defined for every $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$ by

$$Af := -\triangle f \ ,$$

is a densely-defined, linear, positive symmetric and essentially self-adjoint operator in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, whose closure $\bar{A}$ has the spectrum

$$\sigma(\bar{A}\,) = [0, \infty) \ .$$

Further, for every bounded and universally measurable function $f : [0, \infty) \to \mathbb{C}$:

$$f(\bar{A}\,) = F_2^{-1} \circ T_{f \circ |\ |^2} \circ F_2 \ ,$$

where $T_{f \circ |\ |^2}$ is the maximal multiplication operator with the function $f \circ |\ |^2$, defined by

$$T_{f \circ |\ |^2} g := (f \circ |\ |^2) \cdot g \ ,$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. In particular,

$$(\bar{A} + 1)^{-1} = F_2^{-1} \circ T_{\frac{1}{1+|\ |^2}} \circ F_2 \ ,$$

and

$$(\bar{A} + 1)^{-1} f = F_2^{-1} (1 + |\ |^2)^{-1} F_2 f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. We note that

$$\frac{1}{1 + |\ |^2} \in L^2_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

for $n \leqslant 3$, but not for $n \geqslant 4$. From the theory of the Fourier transformation, it follows that

$$f * g = F_1[(F_2^{-1} f) \cdot (F_2^{-1} g)] \ ,$$

for all $f, g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $*$ denotes the convolution product. Hence for $n \leqslant 3$, it follows further that

$$\begin{aligned}
(\bar{A} + 1)^{-1} f &= F_2^{-1} (1 + |\ |^2)^{-1} F_2 f = F_2\, (1 + |\ |^2)^{-1} F_2^{-1} f \\
&= \frac{1}{(2\pi)^{n/2}}\, F_1\, (1 + |\ |^2)^{-1} F_2^{-1} f \\
\Bigg(&= \frac{1}{(2\pi)^{n/2}}\, [F_2\, (1 + |\ |^2)^{-1}] * f \Bigg) \ ,
\end{aligned}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. In particular,

$$(\bar{A}+1)^{-1} f \in C_\infty(\mathbb{R}^n, \mathbb{C})$$

and

$$\begin{aligned}\|(\bar{A}+1)^{-1} f\|_\infty &= \left\| \frac{1}{(2\pi)^{n/2}} \, F_1 \, (1+|\ |^2)^{-1} F_2^{-1} f \right\|_\infty \\ &\leqslant \frac{1}{(2\pi)^{n/2}} \, \left\| (1+|\ |^2)^{-1} F_2^{-1} f \right\|_1 \\ &\leqslant c_n \, \|f\|_2 \ ,\end{aligned}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where

$$c_n := \frac{1}{(2\pi)^{n/2}} \, \left\| (1+|\ |^2)^{-1} \right\|_2$$

and Hoelder's inequality was used. As a consequence, for $n \leqslant 3$, we arrive at the following Sobolev inequality

$$\|f\|_\infty \leqslant c_n \, \|(\bar{A}+1)f\|_2 \leqslant c_n \left(\|\bar{A}f\|_2 + \|f\|_2 \right) \ , \tag{1.30}$$

for every $f \in D(\bar{A})$. In a further step, with the help of Hoelder's inequality, it follows for $U \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ that

$$\begin{aligned}\|Uf\|_2^2 &\leqslant \|U\|_2^2 \cdot \|f\|_\infty^2 \leqslant c_n^2 \, \|U\|_2^2 \left(\|\bar{A}f\|_2 + \|f\|_2 \right)^2 \\ &\leqslant 2c_n^2 \, \|U\|_2^2 \left(\|\bar{A}f\|_2^2 + \|f\|_2^2 \right)\end{aligned}$$

and hence that

$$\|Uf\|_2^2 \leqslant 2c_n^2 \, \|U\|_2^2 \left(\|\bar{A}f\|_2^2 + \|f\|_2^2 \right) \ , \tag{1.31}$$

for every $f \in D(\bar{A})$. Hence if $U = U_1 + U_2$, where $U_1 \in L^2(\mathbb{R}^n)$, $U_2 \in L^\infty(\mathbb{R}^n)$, we define for every $\nu \in \mathbb{N}^*$ a corresponding $U_{1\nu} \in L^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ by

$$U_{1\nu} := \chi_{U_1^{-1}([-\nu,\nu])} \cdot U_1 \ .$$

Then, it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \|U_{1\nu} - U\|_2 = 0$$

and hence the existence of a $\nu_0 \in \mathbb{N}^*$ such that

$$2c_n^2 \|U_{1\nu_0} - U\|_2^2 < 1 \ .$$

As consequence,

$$U = U_1 - U_{1\nu_0} + U_{1\nu_0} + U_2 \ ,$$

where

$$U_1 - U_{1\nu_0} \in L^2(\mathbb{R}^n) \text{ and } U_{1\nu_0} + U_2 \in L^\infty(\mathbb{R}^n) \ .$$

In a first step, it follows from (1.30) and the Rellich-Kato theorem that

$$A + T_{U_1 - U_{1\nu_0}}$$

is essentially self-adjoint, where

$$T_{U_1 - U_{1\nu_0}}$$

denotes the maximal multiplication operator with $U_1 - U_{1\nu_0}$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$. In addition, it follows that

$$\overline{A + T_{U_1 - U_{1\nu_0}}} = \bar{A} + T_{U_1 - U_{1\nu_0}}$$

and that

$$D\left(\overline{A + T_{U_1 - U_{1\nu_0}}}\right) = D(\bar{A}) \ ,$$

the latter since $D(\bar{A}) \subset C_\infty(\mathbb{R}^n, \mathbb{C})$. Further, since

$$U_{1\nu_0} + U_2 \in L^\infty(\mathbb{R}^n) \ ,$$

it follows that the maximal multiplication operator

$$T_{U_{1\nu_0} + U_2}$$

with

$$U_{1\nu_0} + U_2$$

in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ is a bounded linear operator on $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Hence, it follows from the Rellich-Kato theorem that

$$A + T_{U_1 - U_{1\nu_0}} + T_{U_{1\nu_0} + U_2} = A + T_U$$

is essentially self-adjoint, where T_U denotes the maximal multiplication operator with U in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ and therefore also that $\hat{H}_0$ is essentially self-adjoint. In addition, it follows that

$$\begin{aligned} \overline{A + T_U} &= \overline{A + T_{U_1 - U_{1\nu_0}}} + T_{U_{1\nu_0} + U_2} \\ &= \bar{A} + T_{U_1 - U_{1\nu_0}} + T_{U_{1\nu_0} + U_2} = \bar{A} + T_U \end{aligned}$$

and that

$$D\left(\overline{A + T_U}\right) = D(\bar{A}) \ ,$$

the latter since $D(\bar{A}) \subset C_\infty(\mathbb{R}^n, \mathbb{C})$.

Equality of the Essential Spectrum of the Free Hamiltonian and the Essential Spectra of a Class of Perturbed Hamiltonians

In the following, we are going to show that the essential spectrum $\sigma_e(\hat{H})$ of the free Hamiltonian $\hat{H}$ and the essential spectrum, $\sigma_e(\overline{\hat{H}_{V0}})$, of $\overline{\hat{H}_{V0}}$ coincide and are given by the interval $[0, \infty)$:

$$\sigma_e(\overline{\hat{H}_{V0}}) = \sigma_e(\hat{H}) = [0, \infty) \ ,$$

where V is such that there is a sequence $V_1, V_2, \ldots$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ satisfying

$$\lim_{\nu \to \infty} \|V_\nu - V\|_\infty = 0 \ .$$

We note that the potential corresponding to the case of an electron in the Coulomb field of an nucleus containing Z protons,

$$V = -\frac{Ze^2\kappa}{|\ |} \ ,$$

where e denotes the charge of an electron, is satisfying this condition.

For the proof, in a first step, we are going to show for $U \in L^2(\mathbb{R}^n)$ that $T_U\,(\bar{A}+1)^{-1}$ is a Hilbert-Schmidt operator and hence compact. We note that for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$

$$\begin{aligned} T_U\,(\bar{A}+1)^{-1} f &= \frac{1}{(2\pi)^{n/2}}\, U \cdot [F_2\,(1+|\ |^2)^{-1}] * f \\ &= U \cdot (h * f) = \mathrm{Int}(K) f \ , \end{aligned}$$

where $h \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ is defined by

$$h := \frac{1}{(2\pi)^{n/2}}\, F_2\,(1+|\ |^2)^{-1} \ ,$$

for almost all u and $\bar{u} \in \mathbb{R}^n$

$$K(u, \bar{u}) := U(u)\, h(u-\bar{u}) = U(u)\, h(\bar{u}-u)$$

and $\mathrm{Int}(K)$ denotes the integral operator on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ that is associated with K. In addition, it follows that K is measurable, a fact that is shown in the derivation of the elementary properties of the convolution product. Also, for every u in the domain $D(U)$ of U,

$$|U(u)|^2 \cdot |h|^2(\cdot - u) \in L^1(\mathbb{R}^n) \ ,$$

and

$$\begin{pmatrix} D(U) \to \mathbb{R} \\ u \mapsto \int_{\mathbb{R}^n} |U(u)|^2 \cdot |h|^2(\cdot - u)\, dv^n \end{pmatrix} = \begin{pmatrix} D(U) \to \mathbb{R} \\ u \mapsto \| |h|^2 \|_1 \cdot |U(u)|^2 \end{pmatrix}$$

is integrable since $U \in L^2(\mathbb{R}^n)$. Hence it follows from Tonelli's theorem as well as Fubini's theorem that $K \in L^2_{\mathbb{C}}((\mathbb{R}^n)^2)$ and that

$$\|K\|_2^2 = \| |U|^2 \|_1 \cdot \| |h|^2 \|_1 = \|U\|_2^2 \cdot \|h\|_2^2 \ .$$

Hence $T_U\,(\bar{A}+1)^{-1}$ is a Hilbert-Schmidt operator and therefore compact. Further, if U is such that there is a sequence $U_1, U_2, \dots$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ satisfying

$$\lim_{\nu \to \infty} \|U_\nu - U\|_\infty = 0 \ ,$$

then

$$T_U\,(\bar{A}+1)^{-1} = T_{U_\nu}\,(\bar{A}+1)^{-1} + T_{U-U_\nu}\,(\bar{A}+1)^{-1} \ ,$$

for every $\nu \in \mathbb{N}^*$. Hence, it follows that

$$\begin{aligned} &\|T_{U_\nu}\,(\bar{A}+1)^{-1} - T_U\,(\bar{A}+1)^{-1}\| = \|T_{U_\nu - U}\,(\bar{A}+1)^{-1}\| \\ &\leqslant \|U_\nu - U\|_\infty \cdot \|(\bar{A}+1)^{-1}\| \ . \end{aligned}$$

As a consequence,

$$\lim_{\nu \to \infty} \|T_{U_\nu}\,(\bar{A}+1)^{-1} - T_U\,(\bar{A}+1)^{-1}\| = 0 \ ,$$

and therefore $T_U\,(\bar{A}+1)^{-1}$ is compact as a limit, with respect to the operator norm $\|\ \|$, of compact operators. Hence, according to Corollary 12.5.21 in the Appendix, T_U is compact relative to $\bar{A}$. Therefore, according to Theorem 12.5.23 in the Appendix, the essential spectra of $\bar{A}$ and $\bar{A} + T_U$ coincide. As noted before, the spectrum of $\bar{A}$ is given by the closed interval $[0, \infty)$. In particular, $\bar{A}$ has no discrete spectral values and hence, see Theorem 12.5.18 in the Appendix, the essential spectrum of $\bar{A}$ is given by $[0, \infty)$.

For later use, we are going to calculate

$$e^{-\sigma \bar{A}} \ ,$$

for $\sigma \in (0, \infty) \times \mathbb{R}$.

A Representation of $e^{-\sigma\bar{A}}$

For every $\sigma \in (0, \infty) \times \mathbb{R}$

$$e^{-\sigma\bar{A}} f = \frac{1}{(4\pi\sigma)^{n/2}} \, e^{-|\ |^2/(4\sigma)} * f \in C_\infty(\mathbb{R}^n, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

and

$$\|e^{-\sigma\bar{A}} f\|_\infty \leqslant \left(\frac{|\sigma|}{8\pi^2 \mathrm{Re}(\sigma)}\right)^{n/2} \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$.

For the proof, we note that

$$e^{-\sigma\bar{A}} = F_2^{-1} \circ T_{e^{-\sigma|\ |^2}} \circ F_2 \ ,$$

and

$$e^{-\sigma\bar{A}} f = F_2^{-1} e^{-\sigma|\ |^2} F_2 f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. Since according to the theory of the Fourier transformation

$$f * g = F_1[(F_2^{-1} f) \cdot (F_2^{-1} g)] \ ,$$

for all $f, g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $*$ denotes the convolution product, it follows further that

$$\begin{aligned} e^{-\sigma\bar{A}} f &= F_2^{-1} e^{-\sigma|\ |^2} F_2 f = F_2 e^{-\sigma|\ |^2} F_2^{-1} f \\ &= \frac{1}{(2\pi)^{n/2}} \, F_1 \, e^{-\sigma|\ |^2} F_2^{-1} f = \frac{1}{(2\pi)^{n/2}} \, (F_2 \, e^{-\sigma|\ |^2}) * f \\ &= \frac{1}{(4\pi\sigma)^{n/2}} \, e^{-|\ |^2/(4\sigma)} * f \ , \end{aligned}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where we used Corollary 12.9.24 from the Appendix. We note that it follows in particular that

$$e^{-\sigma\bar{A}} f \in C_\infty(\mathbb{R}^n, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

and

$$\begin{aligned} &\|e^{-\sigma\bar{A}} f\|_\infty \leqslant \frac{1}{(8\pi^2|\sigma|)^{n/2}} \left\| e^{-|\ |^2/(4\sigma)} \right\|_2 \cdot \|f\|_2 \\ &= \frac{1}{(8\pi^2|\sigma|)^{n/2}} \left(\int_{\mathbb{R}^n} e^{-\mathrm{Re}(\sigma)\cdot|\ |^2/(2|\sigma|^2)} \right)^{1/2} \cdot \|f\|_2 = \left(\frac{|\sigma|}{8\pi^2 \mathrm{Re}(\sigma)}\right)^{n/2} \ , \end{aligned}$$

where we used Lemma 12.9.26 and Corollary 12.9.24 from the Appendix.

2 Commutators, Symmetries and Invariances

2.1 Commuting Operators

In the discussion of the canonical commutation rule for the position and the momentum operator for the harmonic oscillator in [7], the commutator bracket $[\ ,\ ]$ was used. In the following, we are going to use this bracket more systematically, but only for bounded linear operators. For bounded linear operators A, B on a Hilbert space, we define the commutator of A and B as the bounded linear operator given by

$$[A, B] := A \circ B - B \circ A \ .$$

For unbounded operators, the analogous definition turned out inconclusive, and we are not going to use the notation $[A, B]$ in the following, if at least one of the involved operators is unbounded.

On the other hand, the notion of that two, possibly unbounded, observables A and B commute allows a clear cut mathematical definition, with important implications, namely that the commutator of each member of the spectral family E^A of A commutes with each member of the spectral family E^B of B,

$$[E^A_{\lambda_1}, E^B_{\lambda_2}] = 0 \ ,$$

for all $\lambda_1, \lambda_2 \in \mathbb{R}$. The following theorem, whose proof is given in the Appendix, see Theorem 12.9.1, gives equivalent criteria for the commuting of observables.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_2.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_2

Theorem 2.1.1 (Commuting Observables) *Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ and $B : D(B) \to X$ densely-defined, linear and self-adjoint operators in X, with corresponding spectra $\sigma(A)$ and $\sigma(B)$, respectively, and E^A and E^B the spectral families that are associated with A and B, respectively. We say that B and A commute, if*

$$\left[E^B_s, E^A_t\right] = 0 \ ,$$

for all $s, t \in \mathbb{R}$. Finally, let $U_A := (A - i)(A + i)^{-1}$ and $U_B := (B - i)(B + i)^{-1}$ be the Cayley transforms of A and B, respectively, which are unitary linear operators on X.

(i) If in addition $B \in L(X, X)$, then the following statements are equivalent.

(a)

$$[g(B), f(A)] = 0 \ ,$$

for all $g \in \overline{U^s_{\mathbb{C}}(\sigma(B))}$ and $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

(b) B and A commute.

(c) $[B, U_A] = 0$.

(d) $[B, e^{itA}] = 0$, for all $t \in \mathbb{R}$.

(e) $A \circ B \supset B \circ A$.

(ii) The following statements are equivalent.

(a)

$$[g(B), f(A)] = 0 \ ,$$

for all $g \in \overline{U^s_{\mathbb{C}}(\sigma(B))}$ and $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

(b) B and A commute.

(c) $[e^{isB}, e^{itA}] = 0$, for all $s, t \in \mathbb{R}$.

(d) $[U_B, U_A] = 0$.

Physically relevant examples of commuting operators are the operators corresponding to the measurement of the kth and lth, $k, l \in \{1, \dots, n\}$, component of the position and the operators corresponding to the measurement of the kth and lth component of momentum. Also, the kth, $k \in \{1, \dots, n\}$, component of momentum commutes with the Hamiltonian describing free motion in $\mathbb{R}^n$. These facts are simple consequences of Theorem 2.1.1, (1.1), (1.12) and (1.16). Also the operators corresponding to the 3rd component of angular momentum $\hat{L}_3$ and the square of angular momentum $\hat{L}^2$ commute, see Sect. 2.4.5. In Sect. 2.7.3, we are going to show that the free Hamiltonian commutes with space translations and orthogonal transformations and that the members of a class of perturbations of the free Hamiltonian by central potentials commute with orthogonal transformations.

According to the previous theorem, Theorem 2.1.1, observables A and B commute if and only if the commutators of each pair of operators from the functional calculi corresponding to A and B, respectively, vanish. This includes the spectral projections corresponding to A and B which are relevant for the measurement process. All these operators are bounded linear operators.[1]

For example, if the physical system is in a state $\mathbb{C}.f$, where $f \in X \setminus \{0\}$, and a measurement of the observable A determined that the values of the observable belong to an interval $I \subset \sigma(A)$, where $\sigma(A)$ denotes the spectrum of A, then, if A and B commute, a subsequent measurement of the values of the observable B does not affect this result of the measurement of the values of observable A, i.e., in this case a subsequent measurement of the values of observable A will still find the values of A to belong to the interval I. On the other hand, this is true only if there is no time delay between these measurements, which is not very realistic, but refers to a limit where the time delay between the measurement processes approaches 0. Even in a theory that uses Newtonian ideas of space and time,[2] like quantum mechanics, such processes take time, and after the measurement of the values of the observable A the resulting state is subject to time evolution until the measurement of the values of the observable B. Generically, if A does not commute with the Hamiltonian operator H, a subsequent measurement of the values of the observable A will not lead on the same values as in a previous measurement. On the other hand, it needs to be remembered that this process of time evolution between the measurements is deterministic. There is no loss of information during this time.

The previous indicates that what is really physically relevant is the commuting of the spectral projections of two observables, A and B. This leads on the concept of closed invariant subspaces, leading to the reduction of observables and a decomposition of their spectras and the concept of symmetries.

For motivation of closed invariant subspaces, say, we know, due to a previous measurement of an observable A, that a system is in state belonging to a projection space of a spectral projection of A, a closed subspace Y of the state space X, and perform a further measurement of an observable B that commutes with A. The measurement process corresponds to the application of a spectral projection P of B, which commute with those of A. Hence, *the measurement leaves Y invariant*, i.e., after the measurement the state is still an element of Y. More precisely, the state is an element of the intersection, $(\text{Ran } P) \cap Y$, of Y with the range of the spectral projection P, $\text{Ran } P$, a closed subspace of X. The space $(\text{Ran } P) \cap Y$

---

[1] Observables can be viewed a labels of the associated functional calculi of bounded linear operators, and it is the latter that is of primary importance. So, one might ask for the reason why observables in quantum theory are generically unbounded DSLO's. The answer is given by the so called Hellinger-Toeplitz theorem, Theorem 12.4.4 (xi). As a consequence, an observable is unbounded if and only if its spectrum is unbounded. Now if the range of values of a classical observable is unbounded, there is no reason why quantization should lead to a bounded spectrum for the corresponding observable in quantum theory.

[2] In particular, like in classical Newtonian physics, quantum mechanics assumes instantaneous propagation of any action.

is a closed subspace of the state space and generically a proper restriction of Y, and in this way the measurement of the observable can be considered to "refine" the measurement of the observable A.

2.2 Closed Invariant Subspaces of Observables

For explanation, we consider a observable A.

Definition of Closed Invariant Subspaces

A subspace Y of the state space X is called an closed invariant subspace of A, if Y is closed and the orthogonal projection $P \in L(X, X)$ onto Y commutes with A, i.e.,

$$A \circ P \supset P \circ A \ , \tag{2.1}$$

i.e., $A \circ P$ is an extension of $P \circ A$. We note that, according to Theorem 2.1.1, the latter implies that

$$[f(A), P] = 0 \ ,$$

i.e., $f(A)$ maps leaves Y invariant,[a] for every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

[a] Equivalently, every element of Y is mapped into an element of Y.

We remind that we always assume compositions to be maximally defined. So the domain $D(A \circ P)$ of $A \circ P$ is defined by

$$D(A \circ P) := \{f \in X : Pf \in D(A)\} \ .$$

Hence, an equivalent way of formulating (2.1) is that for every $f \in D(A)$, we have

$$Pf \in D(A) \text{ and } APf = PAf \ .$$

We note that this implies for every $f \in D(A)$ that $(1 - P)f \in D(A)$,

$$A\,(1 - P)f = Af - APf = Af - PAf = (1 - P)Af$$

and hence that

$$A \circ (1 - P) \supset (1 - P) \circ A \ , \tag{2.2}$$

i.e., the orthogonal complement X_2 of X_1 is also a closed invariant subspace of A. Hence, we arrive at the decomposition of A into reduced operators A_1 and A_2,

$$A = A_1 \oplus A_2 \ ,$$

where

$$A_1 := (D(A) \cap X_1 \to X_1, f \mapsto Af) \ ; \ A_2 := (D(A) \cap X_2 \to X_2, f \mapsto Af) \ .$$

We are no going to continue this particular analysis, but give in the following more in depth results of the reduction of observables, using invariant subspaces.

The following lemma is proved in the Appendix, see Lemma 12.9.2. It shows that a closed invariant subspace of an DLSO leads to a reduced DLSO in the invariant subspace, that the spectrum of the reduced operator is part of the spectrum of the original operator and that restriction of the functional calculus of the original operator to the invariant subspace coincides with functional calculus of the reduced operator.

Lemma 2.2.1 (Reduction of Observables I) *Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $(\phi \neq)$ $\sigma(A)$ $(\subset \mathbb{R})$ the spectrum of A, $P \in L(X, X)$ a non-trivial orthogonal projection such that $A \circ P \supset P \circ A$ and $Y :=$ Ran P the non-trivial and closed projection space corresponding to P (which is a closed invariant subspace of A). Then the following is true.*

(i) By $A_P := (D(A) \cap Y \to Y, f \mapsto Af)$, there is defined a densely-defined, linear and self-adjoint Operator in Y. The spectrum $\sigma(A_P)$ of A_P is part of $\sigma(A)$.
(ii) For every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$,

$$f\big|_{\sigma(A_P)} \in \overline{U^s_{\mathbb{C}}(\sigma(A_P))} \text{ and } \big(f\big|_{\sigma(A_P)}\big)(A_P) = (Y \to Y, g \mapsto f(A)g) \ .$$

The starting point in applications is usually a symmetric DLO, not a DSLO. The latter are created through appropriate extension of a symmetric DLO. In particular, a priori closed invariant subspaces are not known. The following lemma, proved in the Appendix, see Lemma 12.9.3, starts from a decomposition of the underlying Hilbert space into a sequence of orthogonal closed subspaces and a symetric DLO that induces symmetric DLO's in these subspaces that are in addition essentially self-adjoint and gives that the original symmetric DLO is essentially self-adjoint, too, and that the original closed subspaces are closed invariant subspaces of its closure. This Lemma and the subsequent Corollary are crucial in the discussion below of the angular momentum operators in Sect. 2.4 as well as for the quantization of a particle subject to a central potential in Chap. 4.

Lemma 2.2.2 (Reduction of Observables II) *Let $(X, \langle | \rangle)$ be a non-trivial complex Hilbert space and $A : D(A) \to X$ a densely defined, linear and symmetric operator in X. Moreover, let $P_0, P_1, \dots$ be a sequence of orthogonal projections on X with pairwise orthogonal projection spaces and such that*

$$\lim_{n\to\infty} \sum_{j=0}^{n} P_j f = f \ ,$$

for every $f \in X$. Finally, for each $j \in \mathbb{N}$, let D_j be a dense subspace of $Ran(P_j)$ with

$$D_j \subset D(A) \ , \ A(D_j) \subset Ran(P_j) \ , \tag{2.3}$$

and such that densely-defined, linear and symmetric operator $A_j := (D_j \to \mathrm{Ran}\, P_j, f \mapsto Af)$ in $\mathrm{Ran}\, P_j$ is essentially self-adjoint. Then A is essentially self-adjoint and the therefore self-adjoint closure $\bar{A}$ of A commutes strongly with every P_j, $j \in \mathbb{N}$, i.e.,

$$\bar{A} \circ P_j \supset P_j \circ \bar{A} \tag{2.4}$$

holds for each $j \in \mathbb{N}$.

Corollary 2.2.3 *Under the assumptions of Lemma 2.2.2, it follows that*

$$\bar{A}|_{D(\bar{A}) \cap \mathrm{Ran}(P_j)} = \bar{A}_j \ , \tag{2.5}$$

for every $j \in \mathbb{N}$, where $\bar{A}_j$ denotes the closure of A_j in $\mathrm{Ran}(P_j)$.

Note that, since $D_j \subset \mathrm{Ran}(P_j)$ for every $j \in \mathbb{N}$, (2.3) are "invariance conditions" and that $\mathrm{Ran}(P_0), \mathrm{Ran}(P_1), \dots$ is a sequence of invariant subspaces of $\bar{A}$ such that the span of the union of these spaces is dense in X. Further, we note that the assumptions of Lemma 2.2.2 do not exclude that only finitely many of the projection spaces of $P_0, P_1, \dots$ are non-trivial.

A decomposition of an operator as in Lemma 2.2.2 induces a decomposition of the spectrum of that operator. Also the proof of the following theorem is given in the Appendix, see Theorem 12.9.5.

Theorem 2.2.4 (Induced Decomposition of Spectra) *Let $(X, \langle | \rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $(\phi \neq) \, \sigma(A) \, (\subset \mathbb{R})$ the spectrum of A. In addition, let $(P_n)_{n\in\mathbb{N}}$ be a sequence of orthogonal projections with pairwise orthogonal projection spaces that commute with A. According to Lemma 2.2.2, for every $n \in \mathbb{N}$ by $A_n := (D(A) \cap \mathrm{Ran}\, P_n \to \mathrm{Ran}\, P_n, \ f \mapsto Af)$, there is defined a densely-defined, linear and self-adjoint operator in $\mathrm{Ran}\, P_n$. Finally, let $\sigma(A_n), \sigma_p(A_n)$ be the spectrum of A_n and the point spectrum, i.e., the set of all eigenvalues, of A_n, respectively. We note that $\sigma(A_n) = \phi$, if $\mathrm{Ran}\, P_n = \{0\}$. Then*

$$\sigma_p(A) = \bigcup_{n\in\mathbb{N}} \sigma_p(A_n) \ , \ \ \sigma(A) = \overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)} \ .$$

Often, the reduction of operators proceeds by use of representation changes induced by coordinate transformations. This usually leads to the introduction of coordinate singularities into the transformed operators which in turn affects the choice of the domain of the operator A. As a result, it can very well happen that some of the induced operators in Theorem 2.2.2 are not essentially self-adjoint. For instance, such a case occurs in the quantization of a particle subject to a central potential. As a consequence, in these cases, the induced operators that fail to be essentially self-adjoint need to be extended to essentially self-adjoint operators, which in turn affects the domain of the original operator A. Fortunately, it is easy to combine a sequence of symmetric DLO that are essentially self-adjoint to a symmetric DLO that is essentially self-adjoint. Also, the following Lemma is proved in the Appendix, see Lemma 12.9.6.

Lemma 2.2.5 (Reduction of Observables III) *Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $P_0, P_1, \dots$ be a sequence of orthogonal projections on X with pairwise orthogonal projection spaces and such that*

$$\lim_{n\to\infty} \sum_{j=0}^{n} P_j f = f \ ,$$

for every $f \in X$. Further, for each $j \in \mathbb{N}$, let $A_j : D_j \to Ran(P_j)$ be a densely-defined, linear, symmetric and essentially self-adjoint operator in $Ran(P_j)$. We define the subspace $D \leqslant X$ by

$$D := \left\{ \sum_{j=0}^{n} f_j \ : \ n \in \mathbb{N} \textit{ and } f_j \in D_j, \textit{ for every } j \in \{1, \dots, n\} \right\} \ ,$$

and $A : D \to X$ by

$$A \sum_{j=0}^{n} f_j := \sum_{j=0}^{n} A_j f_j \ ,$$

where $n \in \mathbb{N}$ and $f_j \in D_j$, for every $j \in \{0, \dots, n\}$. Then A is a densely-defined, linear, symmetric and essentially self-adjoint operator in X, whose closure $\bar{A}$ commutes strongly with every P_j, $j \in \mathbb{N}$, i.e.,

$$\bar{A} \circ P_j \supset P_j \circ \bar{A}$$

holds for each $j \in \mathbb{N}$.

2.3 Insert: Decomposition of Spectra of DSLO's

There are 2 main decompositions of the spectrum of a DSLO A.
The first is rarely used in the text, but becomes important in the formal scattering theory, which is not treated in this text. Also, the results given below in this connection are not proved here. For this, we refer to [60], Volume I. The decomposition in question is the result of a decomposition of the underlying Hilbert space X into a direct orthogonal sum of closed invariant subspaces, due to particular properties of the spectral measures that are associated to the operator and every element of X.

For this purpose, we define the so called "discontinuous subspace" X_p of X to consist of all $f \in X$ for which there is a countable subset $N \subset \mathbb{R}$ such that $\mathbb{R} \backslash N$ is a set of measure 0 of the spectral measure ψ_f that corresponds to A and f, and the so called "continuous subspace" X_c of X to consist of all $f \in X$ for which every $\lambda \in \mathbb{R}$ is a set of measure 0 of ψ_f.

Then X_p and X_c are closed invariant subspaces of X, X_p coincides with the closure of the span of the eigenvectors of A and

$$\boxed{X_p^{\perp} = X_c \ .}$$

As a consequence, we arrive at a representation of X as a direct orthogonal sum of the closed invariant subspaces X_p and X_c

$$\boxed{X = X_p \otimes X_c \ ,}$$

which according to Theorem 2.2.4 leads to reduced DSLO's, the so called "discontinuous part of A," A_p, and the so called "continuous part of A," A_c, and the associated decomposition of the spectrum $\sigma(A)$ of A into the spectrum $\sigma(A_p)$ of A_p and the spectrum $\sigma_c(A)$ of A_c

$$\sigma(A) = \sigma(A_p) \cup \sigma_c(A) \ .$$

Since, $\sigma(A_p)$ coincides with closure of the point spectrum $\sigma_p(A)$ of A, i.e., the set of eigenvalues of A, we have that

$$\boxed{\sigma(A) = \overline{\sigma_p(A)} \cup \sigma_c(A) \ .}$$

The continuous subspace X_c of X allows a further useful decomposition.

> For this purpose, we define the so called "singular subspace" X_s of X to consist of all $f \in X$ for which there is a set $N \subset \mathbb{R}$ of Lebesgue measure 0 such that $\mathbb{R}\backslash N$ is a set of ψ_f-measure 0, and the so called "absolutely continuous subspace" X_{ac} of X to consist of all $f \in X$ such that the Lebesgue measure is absolutely continuous with respect to ψ_f, i.e., every set of ψ_f-measure 0 is a set of Lebesgue measure 0.

Also X_s and X_{ac} are closed invariant subspaces of X and, in particular,

$$\boxed{X_s^{\perp} = X_{ac}\ .}$$

We note that

$$X_p \subset X_s\ ,$$

since if $f \in X_p$, then there is a countable subset $N \subset \mathbb{R}$, i.e., a set of Lebesgue measure 0, such that $\mathbb{R}\backslash N$ is a set of ψ_f-measure 0. As a consequence,

$$X_c = X_p^{\perp} \supset X_s^{\perp} = X_{ac}\ ,$$

i.e.,

$$X_{ac} \subset X_c\ .$$

Further, we have that

$$X_{ac}^{\perp} \cap X_c = X_s^{\perp\perp} \cap X_c = X_s \cap X_c$$

Also $X_s \cap X_c$ is a closed invariant subspace X, and we arrive at a representation of X as a direct orthogonal sum of the closed invariant subspaces X_p, X_{ac} and $X_s \cap X_c$

$$\boxed{X = X_p \otimes X_{ac} \otimes (X_s \cap X_c)\ ,}$$

which according to Theorem 2.2.4 leads to reduced DSLO's, the discontinuous part A_p of A, the so called "absolutely continuous part of A," A_{ac}, and the "singular continuous part of A," A_{sc}, of A. This decomposition induces a decomposition of the spectrum $\sigma(A)$ of A into the spectrum $\sigma(A_p)$ of A_p, the spectrum $\sigma_{ac}(A)$ of A_{ac} and the spectrum $\sigma_{sc}(A)$ of A_{sc}

$$\boxed{\sigma(A) = \overline{\sigma_p(A)} \cup \sigma_{ac}(A) \cup \sigma_{sc}(A)\ .}$$

If A is the Hamiltonian of a quantum system, then the set $\overline{\sigma_p(A)}$ is the closure of the set of eigenvalues of A, usually corresponding to the bound states, i.e., energies smaller than 0, of the system, the absolutely continuous part $\sigma_{ac}(A)$ of $\sigma(A)$ is interpreted as the scattering spectrum, usually corresponding to states of energies greater than 0 and the singular continuous spectrum $\sigma_{sc}(A)$ is usually empty. On the other hand, the latter is not always easy to show.

Occasionally, we mention that a spectrum of an DLSO is purely absolutely continuous. For instance, this is true for the position operators, momentum operators and the free Hamiltonian. Per definitionem, this means that $\sigma(A) = \sigma_{ac}(A)$, i.e., that the Lebesgue measure is absolutely continuous with respect to ψ_f, for every $f \in X$, which is relatively easy to decide, once the functional calculus of the operator in question is known.

The second main decomposition of the spectrum of a DSLO A comes from perturbation theory and is used in various places in the text. Corresponding proofs are given in Sects. 12.5.2 and 12.5.4 in the Appendix.

A Disjoint Decomposition of the Spectrum of a DSLO

We have the following decomposition of the spectrum $\sigma(A)$ of A

$$\sigma(A) = \sigma_e(A) \,\dot{\cup}\, \sigma_d(A) \ ,$$

where the discrete spectrum $\sigma_d(A)$ of A is defined by

$$\sigma_d(A) := \{\lambda \in \sigma(A) : \lambda \text{ is an isolated point of } \sigma(A) \\ \text{as well as an eigenvalue of } A \text{ of finite multiplicity}\}$$

and the essential spectrum $\sigma_e(A)$ contains all real λ for which there is a sequence $f_1, f_2, \ldots$ in $D(A)$ such that $\|f_\nu\| = 1$ for every $\nu \in \mathbb{N}^*$, $f_1, f_2, \ldots$ has no convergent subsequence, and $\lim_{\nu\to\infty}(A - \lambda)f_\nu = 0$.

Further, the essential spectrum of A is stable under certain small perturbations.

Stability of the Essential Spectrum

If $B : D(B) \to X$ a linear, symmetric, such that $D(B) \supset D(A)$ and such that $B \circ (A - \lambda)^{-1}$ is a compact linear operator on X, for some λ in the resolvent set of A, then $A + B$ is self-adjoint, and $\sigma_e(A + B) = \sigma_e(A)$.

2.4 Quantization of Angular Momentum

In the following, we are going to analyze the angular momentum operators in 3-space dimensions, using closed invariant subspaces. In classical mechanics, the angular momentum $\vec{L} = {}^t(L_1, L_2, L_3)$ of a particle is given by the cross product of its position $\vec{q} = {}^t(q_1, q_2, q_3)$ and its momentum $\vec{p} = {}^t(p_1, p_2, p_3)$,

$$\vec{L} = \begin{pmatrix} L_1 \\ L_2 \\ L_3 \end{pmatrix} = \vec{q} \times \vec{p} = \begin{pmatrix} q_2\, p_3 - q_3\, p_2 \\ q_3\, p_1 - q_1\, p_3 \\ q_1\, p_2 - q_2\, p_1 \end{pmatrix} .$$

Hence, corresponding minimal operators in quantum mechanics are $\hat{L}_{k0} : C^1_0(\mathbb{R}^3, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^3)$, $k \in \{1, 2, 3\}$, defined by

$$\hat{L}_{10} f := \frac{\hbar}{i} \left(u_2 \, \frac{\partial f}{\partial u_3} - u_3 \, \frac{\partial f}{\partial u_2} \right) \ , \ \hat{L}_{20} f := \frac{\hbar}{i} \left(u_3 \, \frac{\partial f}{\partial u_1} - u_1 \, \frac{\partial f}{\partial u_3} \right) \ ,$$
$$\hat{L}_{30} f := \frac{\hbar}{i} \left(u_1 \, \frac{\partial f}{\partial u_2} - u_2 \, \frac{\partial f}{\partial u_1} \right) \ ,$$

for every $f \in C^1_0(\mathbb{R}^3, \mathbb{C})$, where $u_k : \mathbb{R}^3 \to \mathbb{R}$ denotes the kth coordinate projection, $k \in \{1, 2, 3\}$, defined by $u_k(\bar{u}) := \bar{u}_k$ for all $\bar{u} = (\bar{u}_1, \bar{u}_2, \bar{u}_3) \in \mathbb{R}^3$.
These operators are pairwise unitarily equivalent, where the corresponding unitary transformation is induced by a cyclic permutation of the coordinate projections. The proof is left to the reader.

Exercise 1

Prove that the operators $\hat{L}_{10}$, $\hat{L}_{20}$ and $\hat{L}_{30}$ are unitarily equivalent.

Hence, we need to analyze only the operator $\hat{L}_{30}$. Since $C^1_0(\mathbb{R}^3, \mathbb{C})$ is a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R}^3)$, $\hat{L}_{30}$ is densely-defined. Further, $\hat{L}_{30}$ is obviously linear. As a consequence of "partial integration," $\hat{L}_{30}$ is symmetric:

$$
\begin{aligned}
\left\langle f|\hat{L}_{30}g\right\rangle &= \frac{\hbar}{i}\int_{\mathbb{R}^3} f^* \cdot \left(u_1\frac{\partial g}{\partial u_2} - u_2\frac{\partial g}{\partial u_1}\right) du_1 du_2\, du_3 \\
&= -\frac{\hbar}{i}\int_{\mathbb{R}^3} \left(u_1\frac{\partial f^*}{\partial u_2} - u_2\frac{\partial f^*}{\partial u_1}\right) \cdot g\, du_1 du_2\, du_3 \\
&= -\frac{\hbar}{i}\int_{\mathbb{R}^3} \left(u_1\frac{\partial f}{\partial u_2} - u_2\frac{\partial f}{\partial u_1}\right)^* \cdot g\, du_1 du_2\, du_3 \\
&= \int_{\mathbb{R}^3} \left[\frac{\hbar}{i}\left(u_1\frac{\partial f}{\partial u_2} - u_2\frac{\partial f}{\partial u_1}\right)\right]^* \cdot g\, du_1 du_2\, du_3 \\
&= \left\langle \hat{L}_{30} f|g\right\rangle \ ,
\end{aligned}
$$

for all $f, g \in C_0^1(\mathbb{R}^3, \mathbb{C})$, where Lemma 1.2.1 has been used.
In the next step, we change the representation, using a unitary transformation U induced by spherical coordinates.

2.4.1 A Change of Representation Induced by Introduction of Spherical Coordinates

First, we note the following Lemma.

Lemma 2.4.1 (Transformation of $\hat{L}_{30}$ into Spherical Coordinates) *For this, let $\Omega \subset \mathbb{R}^3$ be non-empty and open. In addition, let $\Omega_{sph} \subset \mathbb{R}^3$ be a non-empty open subset such*

$$g(\Omega_{sph}) = \Omega \ ,$$

where $g \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ is defined by

$$g(u, \theta, \varphi) := (u \sin(\theta)\cos(\varphi), u \sin(\theta)\sin(\varphi), u\cos(\theta)) \ ,$$

for all $(u, \theta, \varphi) \in \Omega_{sph}$. Finally, let $f \in C^1(\Omega, \mathbb{R})$. Then

$$\left(u_1\frac{\partial f}{\partial u_2} - u_2\frac{\partial f}{\partial u_1}\right)(g(u, \theta, \varphi)) = \frac{\partial \bar{f}}{\partial \varphi}(u, \theta, \varphi) \ , \tag{2.6}$$

for all $(u, \theta, \varphi) \in \Omega_{sph}$, where $\bar{f} \in C^1(\Omega_{sph}, \mathbb{R})$ is defined by

$$\bar{f}(u, \theta, \varphi) := (f \circ g)(u, \theta, \varphi) = f(u \sin(\theta)\cos(\varphi), u \sin(\theta)\sin(\varphi), u\cos(\theta)) \ ,$$

for all $(u, \theta, \varphi) \in \Omega_{sph}$.

Exercise 2

Prove Lemma 2.4.1.

The map g induces the unitary transformation

$$U : L^2_{\mathbb{C}}(\mathbb{R}^3) \to L^2_{\mathbb{C}}(\Omega, u^2 \sin(\theta)) \ ,$$

where $\Omega := (0, \infty) \times (0, \pi) \times (-\pi, \pi)$, defined by

$$Uf := f \circ g|_{\Omega} \ , \tag{2.7}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^3)$. The inverse U^{-1} of U is given by

$$U^{-1} f := f \circ (g|_{\Omega})^{-1} \ ,$$

for every $f \in L^2_{\mathbb{C}}(\Omega, u^2 \sin(\theta))$, where $(g|_{\Omega})^{-1} : \mathbb{R}^3 \backslash \mathcal{Z} \to \Omega$ is given by

$$(g|_{\Omega})^{-1}(u) = \begin{cases} (\,|u|\,, \arccos(u_3/|u|\,)\,, \arccos(u_1/\sqrt{u_1^2 + u_2^2}\,)) & \text{if } u_2 \geqslant 0 \\ (\,|u|\,, \arccos(u_3/|u|\,)\,, -\arccos(u_1/\sqrt{u_1^2 + u_2^2}\,)) & \text{if } u_2 < 0 \end{cases} ,$$

for all $u = (u_1, u_2, u_3) \in \mathbb{R}^3 \backslash \mathcal{Z}$, where $\mathcal{Z} := (-\infty, 0] \times \{0\} \times \mathbb{R}$ is a closed set of Lebesgue measure zero. The proof that U is indeed an unitary linear transformation is mainly an application of Lebesgue's change of variable formula and is left to the reader.

Exercise 3

Show that U is an unitary linear transformation.

As a consequence of Lemma 2.4.1,

$$U \hat{L}_{30}\, f = \frac{\hbar}{i} \frac{\partial}{\partial \varphi} Uf \ ,$$

for every $f \in C^1_0(\mathbb{R}^3, \mathbb{C})$.[3] Hence, $U \hat{L}_{30}\, U^{-1}$ is given by

[3] To simplify notation here and in the following, the same symbol can denote a coordinate projection or a coordinate of a point. For instance, interchangeably u, θ and φ will denote real numbers from the intervals $(0, \infty)$, $(0, \pi)$ and $(-\pi, \pi)$ or the coordinate projections of $\mathbb{R}^3 \backslash (\{0\} \times \{0\} \times \mathbb{R})$ onto the open intervals $(0, \infty)$, $(0, \pi)$ and $(-\pi, \pi)$, respectively. The definition used will be clear from the context. In addition we assume composition of maps (which includes addition, multiplication etc.) always to be maximally defined. For instance, the addition of two maps (if at all possible to define) is defined on the intersection of the corresponding domains.

$$U\hat{L}_{30}\,U^{-1}f = \frac{\hbar}{i}\,\frac{\partial f}{\partial\varphi}\ ,$$

for every $f \in C_0^1(\Omega, \mathbb{C})$.

In the next step, we are going to use the spherical symmetry of the system to decompose into a countable number of densely-defined, linear, symmetric and essentially self-adjoint operators. The basis for the reduction is Lemma 2.2.2.

2.4.2 Spherical Harmonics

A widely known decomposition of m

$$X := L^2_{\mathbb{C}}(\Omega, u^2\sin(\theta)) \tag{2.8}$$

in physics, into pairwise orthogonal closed subspaces suitable for an application of Lemma 2.2.2 to spherically symmetric operators, is induced by spherical harmonics.

Lemma 2.4.2 (Spherical Harmonics) *Let $I = (-1, 1)$ and $J := (-\pi, \pi)$. For $m \in \mathbb{N}$, $v \in \mathbb{R}$, we define Ferrers function of the first kind, $P_v^{-m} \in C^\infty(I, \mathbb{R})$ according to [56] 14.3.1 by*

$$P_v^{-m}(x) := \frac{1}{m!}\cdot(1+x)^{-m/2}\cdot(1-x)^{m/2}\cdot F\left(-v, v+1, m+1, \frac{1}{2}\cdot(1-x)\right)\ ,$$

where the Gauss hypergeometric function F is defined according to [1], for all $x \in I$. Further, according to [56] 14.3.5, we define for all $m \in \mathbb{N}$, $\ell \in \{m, m+1, \ldots\}$ Ferrers function of the first kind, $P_\ell^m \in C^\infty(I, \mathbb{R})$, by

$$P_\ell^m := (-1)^m\cdot\frac{(\ell+m)!}{(\ell-m)!}\cdot P_\ell^{-m}\ .$$

Finally, for $\ell \in \mathbb{N}$, $m \in \{-\ell, -\ell+1, \ldots, \ell\}$, we define $\bar{Y}_{\ell m} \in C^\infty(I \times J, \mathbb{C})$ by

$$\bar{Y}_{\ell m} := \sqrt{\frac{1}{2\pi}\cdot\left(\ell+\frac{1}{2}\right)\cdot\frac{(\ell-m)!}{(\ell+m)!}}\cdot P_\ell^m \otimes e^{im\cdot id_J}.$$

Then, the following is true.

(i) $\left\{\frac{1}{\sqrt{2\pi}}\cdot e^{im.id_J} : m \in \mathbb{Z}\right\}$ *is a Hilbert basis for $L^2_{\mathbb{C}}(J)$.*

(ii) For each $m \in \mathbb{Z}$ is

Table 2.1 Table of associated Legendre polynomials, where $x \in (-1, 1)$. For fixed $m \in \mathbb{Z}$, ℓ runs through the natural numbers from $|m|$ to ∞. As a consequence of (2.9), associated Legendre polynomials corresponding to negative m are multiples of those with positive m

$P_\ell^m(x)$	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$
$m = 0$	1	x	$\frac{1}{2}\left(3x^2 - 1\right)$	$\frac{x}{2}\left(5x^2 - 3\right)$
$m = 1$	N/A	$-\sqrt{1-x^2}$	$-3x\sqrt{1-x^2}$	$-\frac{3}{2}\left(5x^2 - 1\right)\sqrt{1-x^2}$
$m = 2$	N/A	N/A	$3\left(1 - x^2\right)$	$15x\left(1 - x^2\right)$
$m = 3$	N/A	N/A	N/A	$-15\left(1 - x^2\right)^{3/2}$

$$\left\{\sqrt{\left(l + \frac{1}{2}\right) \cdot \frac{(\ell - m)!}{(\ell + m)!}} \cdot P_\ell^m : \ell \in \{|m|, |m| + 1, \ldots\}\right\}$$

a Hilbert basis for $L^2_{\mathbb{C}}(I)$ (Table 2.1).

(iii)

$$\left\{\bar{Y}_{\ell m} : (\ell, m) \in \bigcup_{k \in \mathbb{N}} (\{k\} \times \{-k, -k+1, \ldots, k\})\right\}$$

is a Hilbertbasis for $L^2_{\mathbb{C}}(I \times J)$.

The corresponding proof is not given here, but left as an exercise. We note that for every $m \in \mathbb{N}$ and $\ell \in \{m, m+1, \ldots\}$, it follows that

$$P_\ell^{-m} = (-1)^m \cdot \frac{(\ell - m)!}{(\ell + m)!} \cdot P_\ell^m \,, \tag{2.9}$$

and hence that

$$\begin{aligned}
&\sqrt{\left(l + \frac{1}{2}\right) \cdot \frac{(\ell + m)!}{(\ell - m)!}} \cdot P_\ell^{-m} \\
&= (-1)^m \cdot \sqrt{\left(l + \frac{1}{2}\right) \cdot \frac{(\ell + m)!}{(\ell - m)!}} \cdot \frac{(\ell - m)!}{(\ell + m)!} \cdot P_\ell^m \\
&= (-1)^m \cdot \sqrt{\left(l + \frac{1}{2}\right) \cdot \frac{(\ell - m)!}{(\ell + m)!}} \cdot P_\ell^m \,,
\end{aligned}$$

resulting

$$\bar{Y}_{\ell(-m)} = (-1)^m \cdot \bar{Y}^*_{\ell m} \,. \tag{2.10}$$

Table 2.2 Table of spherical harmonics, where $(\theta, \varphi) \in (0, \pi) \times (-\pi, \pi)$. For fixed $m \in \mathbb{Z}$, ℓ runs through the natural numbers from $|m|$ to ∞. As a consequence of (2.10), it follows for every $m \in \mathbb{N}$ and $\ell \in \{m, m+1, \ldots\}$ that $Y_{\ell\,(-m)} = (-1)^m \cdot Y_{\ell m}^*$

$Y_{\ell m}(\theta, \varphi)$	$\ell = 0$	$\ell = 1$	$\ell = 2$
$m = 0$	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta)$	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\,[\,3\cos^2(\theta) - 1\,]$
$m = 1$	N/A	$-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta)\,e^{i\varphi}$	$-\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin(\theta)\cos(\theta)\,e^{i\varphi}$
$m = 2$	N/A	N/A	$\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2(\theta)\,e^{2i\varphi}$

We decompose X into subspaces $X_{\ell m}$,

$$(\ell, m) \in \mathcal{I} := \bigcup_{\bar{\ell} \in \mathbb{N}} \{(\bar{\ell}, \bar{m}) : \bar{m} \in \{-\bar{\ell}, -\bar{\ell} + 1, \ldots, \bar{\ell} - 1, \bar{\ell}\,\}\} \ ,$$

using spherical harmonics. For this purpose, we use the following notation:

$$I := (0, \infty) \ , \ \ J := (0, \pi) \ , \ \ K := (-\pi, \pi)$$

and for each $f \in L^2_{\mathbb{C}}(I, u^2)$, $g \in L^2_{\mathbb{C}}(J \times K, \sin(\theta))$, where u denotes the identity map on I and θ denotes the projection of $J \times K$ onto the first component, $f \otimes g \in X$ is defined by

$$(f \otimes g)(u, \theta, \varphi) := f(u) \cdot g(\theta, \varphi),$$

for all u from the domain of f and all (θ, φ) from the domain of g.

For every $(\ell, m) \in \mathcal{I}$, the space $X_{\ell m}$ is then given by the range of the linear isometry $U_{\ell m} : L^2_{\mathbb{C}}(I, u^2) \to X$, defined by

$$U_{lm} f := f \otimes Y_{lm} \ , \tag{2.11}$$

for all $f \in L^2_{\mathbb{C}}(I, u^2)$, where

$$Y_{lm}(\theta, \varphi) := \bar{Y}_{lm}(\cos(\theta), \varphi) \ ,$$

for all $\theta \in J$ and $\varphi \in K$ (Table 2.2).

The fact that $U_{\ell m}$ is isometric is not difficult to prove by using Fubini's theorem, partial integration and the orthonormality relations for the spherical harmonics. The pairwise orthogonality of the subspaces $X_{\ell m}$ of X for all $(\ell, m) \in \mathcal{I}$ follows by the same methods. Finally, the fact that the span of the union of these spaces is dense in X is a consequence of the completeness of the spherical harmonics.

The corresponding sequence of dense subspaces $\mathcal{D}_{\ell m}$ of $X_{\ell m}$, needed for an application of Lemma 2.2.2 is chosen as follows:

$$\mathcal{D}_{\ell m} := U_{\ell m} C_0^1(I, \mathbb{C}) \ ,$$

for all $(\ell, m) \in \mathcal{I}$. That these spaces are also subspaces of

$$D(U \hat{L}_{30} \, U^{-1}) = U(C_0^1(\mathbb{R}^3, \mathbb{C}))$$

follows from the fact that there is unique harmonic homogeneous polynomial of degree ℓ, $p_\ell^m : \mathbb{R}^3 \to \mathbb{C}$ such that

$$u^\ell \, Y_{\ell m}(\theta, \varphi) = p_\ell^m(g(u, \theta, \varphi)) \ ,$$

for every $(u, \theta, \varphi) \in \Omega$, e.g., see [67]. Therefore, it follows for every $f \in C_0^1(I, \mathbb{C})$ that

$$\begin{aligned}
&(U_{\ell m} f)(u, \theta, \varphi) = f(u) \cdot Y_{\ell m}(\theta, \varphi) = f(u) \cdot u^{-\ell} \, p_\ell^m(g(u, \theta, \varphi)) \\
&= (\mathrm{id}_I^{-\ell} f)(|g(u, \theta, \varphi)|) \cdot p_\ell^m(g(u, \theta, \varphi)) = \left\{[(\mathrm{id}_I^{-\ell} f) \circ |\ |] \cdot p_\ell^m\right\}(g(u, \theta, \varphi)) \\
&= \{U[(\mathrm{id}_I^{-\ell} f) \circ |\ |] \cdot p_\ell^m\}(u, \theta, \varphi) \ ,
\end{aligned}$$

for all $(u, \theta, \varphi) \in \Omega$ and hence that

$$U_{\ell m} f = U \, [(\mathrm{id}_I^{-\ell} f) \circ |\ |] \cdot p_\ell^m \ ,$$

where

$$[(\mathrm{id}_I^{-\ell} f) \circ |\ |] \cdot p_\ell^m \in C_0^1(\mathbb{R}^3, \mathbb{C}) \ .$$

Further, for every $(\ell, m) \in \mathcal{I}$ and $f \in C_0^1(I, \mathbb{C})$, it follows that

$$\boxed{U \hat{L}_{30} \, U^{-1} f \otimes Y_{\ell m} = \frac{\hbar}{i} \frac{\partial}{\partial \varphi} f \otimes Y_{\ell m} = m\hbar f \otimes Y_{\ell m} \ .}$$

2.4.3 Analysis of the Reduced Operators

The final step in the application of Lemma 2.2.2 consists in the analysis of the reduced operators that are unitarily equivalent to the, densely-defined, linear and symmetric, operators $\hat{L}_{30\ell m} : C_0^1(I, \mathbb{C}) \to L^2_{\mathbb{C}}(I, u^2)$, $(\ell, m) \in \mathcal{I}$, defined by

Reduced Operators

$$\hat{L}_{30\ell m} f = m\hbar f \ , \ \text{ for every } f \in C_0^1(I, \mathbb{C}).$$

These reduced operators are restrictions of real multiples of the identical operator to the dense subspace $C_0^1(I, \mathbb{C})$ of $L^2_{\mathbb{C}}(I, u^2)$ and therefore essentially self-adjoint. Hence, it follows from Lemma 2.2.2 that $\hat{L}_{30}$ is essentially self-adjoint. Further, it follows from Theorem 2.2.4 that the spectrum $\sigma(\hat{L}_3)$ of the closure $\hat{L}_3$ of $\hat{L}_{30}$ is given by

$$\sigma(\hat{L}_3) = \hbar.\mathbb{Z} \ ,$$

and consists of eigenvalues of infinite multiplicity, and there is a complete set eigenvectors of $\hat{L}_3$. Such a spectrum is called a pure point spectrum. The spectrum of $\hat{L}_3$ is not purely discrete, since the eigenvalues are of infinite multiplicity. Finally, we arrive at the following result (Fig. 2.1).

Angular Momentum Operators

The angular momentum operators $\hat{L}_{10}$, $\hat{L}_{20}$ and $\hat{L}_{30}$ are densely-defined, linear, symmetric and essentially self-adjoint operators in $L^2_{\mathbb{C}}(\mathbb{R}^3)$ with a pure point spectrum given by $\hbar.\mathbb{Z}$, consisting of eigenvalues of infinite multiplicity. Hence the spectrum is not purely discrete. We note that this result differs significantly from classical mechanics, since the values of components of the angular momentum operator in classical mechanics are not quantized, but can assume any real value.

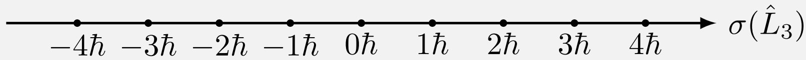


Fig. 2.1 The spectral values of $\hat{L}_3$, i.e., all integer multiples of $\hbar$, are indicated by points.

2.4.4 The Operator Corresponding to the Square of Angular Momentum

We define the minimal operator $\hat{L}_0^2 : C_0^2(\mathbb{R}^3, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^3)$ corresponding to the square of angular momentum by

$$\hat{L}_0^2 f := (\hat{L}_{10}^2 + \hat{L}_{20}^2 + \hat{L}_{30}^2) f \ ,$$

for every $f \in C_0^2(\mathbb{R}^3, \mathbb{C})$. We repeat the steps from Sect. 2.4. First, we note the following Lemma.

Lemma 2.4.3 (Transformation of $\hat{L}_0^2$ into Spherical Coordinates) *For this, let* $\Omega \subset \mathbb{R}^3 \setminus (\{0\} \times \{0\} \times \mathbb{R})$ *be non-empty and open. In addition, let* $\Omega_{sph} \subset \mathbb{R}^3$ *be a non-empty open subset such*

$$g(\Omega_{sph}) = \Omega \ ,$$

where $g \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ is defined as in Lemma 2.4.1. Finally, let $f \in C^2(\Omega, \mathbb{R})$. Then

$$\left\{\left[\left(u_2\,\frac{\partial}{\partial u_3} - u_3\,\frac{\partial}{\partial u_2}\right)^2 + \left(u_3\,\frac{\partial}{\partial u_1} - u_1\,\frac{\partial}{\partial u_3}\right)^2 \right.\right. \tag{2.12}$$
$$\left.\left. + \left(u_1\,\frac{\partial}{\partial u_2} - u_2\,\frac{\partial}{\partial u_1}\right)^2\right] f\right\}(g(u,\theta,\varphi))$$
$$= \frac{1}{\sin^2(\theta)}\left[\frac{\partial^2 \bar{f}}{\partial \varphi^2}(u,\theta,\varphi) + \sin^2(\theta)\,\frac{\partial^2 \bar{f}}{\partial \theta^2}(u,\theta,\varphi) + \sin(\theta)\cos(\theta)\,\frac{\partial \bar{f}}{\partial \theta}(u,\theta,\varphi)\right] ,$$

for all $(u,\theta,\varphi) \in \Omega_{sph}$, where $\bar{f} \in C^2(\Omega_{sph}, \mathbb{R})$ is defined by

$$\bar{f}(u,\theta,\varphi) := (f \circ g)(u,\theta,\varphi) = f(u\sin(\theta)\cos(\varphi), u\sin(\theta)\sin(\varphi), u\cos(\theta))$$

for all $(u,\theta,\varphi) \in \Omega_{sph}$.

The proof of this Lemma is left to the reader.

Exercise 4

Prove Lemma 2.4.3.

Further, we define $U : L^2_{\mathbb{C}}(\mathbb{R}^3) \to L^2_{\mathbb{C}}(\Omega, u^2\sin(\theta))$ by (2.7), where $\Omega := (0,\infty) \times (0,\pi) \times (-\pi,\pi)$. As a consequence of Lemma 2.4.3, $U\hat{L}_0^2 U^{-1}$ is given by

$$U\hat{L}_0^2 U^{-1} f = -\frac{\hbar^2}{\sin^2(\theta)}\left[\frac{\partial^2}{\partial\varphi^2} + \sin^2(\theta)\,\frac{\partial^2}{\partial\theta^2} + \sin(\theta)\cos(\theta)\,\frac{\partial}{\partial\theta}\right] f ,$$

for every $f \in C^2_0(\Omega, \mathbb{C})$.

In the next step, we are going to use the spherical symmetry of the system to decompose into a countable number of densely-defined, linear, symmetric and essentially self-adjoint operators. The basis for the reduction is Lemma 2.2.2. We define, $X := L^2_{\mathbb{C}}(\Omega, u^2\sin(\theta))$, for every $(\ell, m) \in \mathcal{I}$ a corresponding linear isometry $U_{\ell m} : L^2_{\mathbb{C}}(I, u^2) \to X$, where $I := (0,\infty)$, by (2.11) and the corresponding closed subspace $X_{\ell m}$ of X as the range of $U_{\ell m}$. Further, we define the dense subspaces $\mathcal{D}_{\ell m}$ of $X_{\ell m}$ by

$$\mathcal{D}_{\ell m} := U_{\ell m} C^2_0(I, \mathbb{C}) ,$$

for all $(\ell, m) \in \mathcal{I}$. Then, it follows for every $(\ell, m) \in \mathcal{I}$ and $f \in C^2_0(I, \mathbb{C})$

$$
\begin{aligned}
&U\hat{L}_0^2 U^{-1} f \otimes Y_{\ell m} \\
&= -\frac{\hbar^2}{\sin^2(\theta)}\left[\frac{\partial^2}{\partial\varphi^2} + \sin^2(\theta)\,\frac{\partial^2}{\partial\theta^2} + \sin(\theta)\cos(\theta)\,\frac{\partial}{\partial\theta}\right] f \otimes Y_{\ell m} \\
&= \hbar^2 \ell(\ell+1) f \otimes Y_{\ell m} m \ ,
\end{aligned}
$$

where we used that

$$
-\frac{1}{\sin^2(\theta)}\left\{\frac{\partial^2}{\partial\varphi^2} + \left[\sin(\theta)\,\frac{\partial}{\partial\theta}\right]^2\right\} Y_{\ell m} = \ell(\ell+1)\cdot Y_{\ell m} \ .
$$

The final step in the application of Lemma 2.2.2 consists in the analysis of the reduced operators that are unitarily equivalent to the, densely-defined, linear and symmetric operators $\hat{L}_{0\ell m}^2 : C_0^2(I,\mathbb{C}) \to L_{\mathbb{C}}^2(I,u^2)$, defined by

Reduced Operators

$$
\hat{L}_{0\ell m}^2 f = \hbar^2 \ell(\ell+1) f \ , \ \text{ for every } f \in C_0^2(I,\mathbb{C}).
$$

These reduced operators are restrictions of real multiples of the identical operator to the dense subspace $C_0^2(I,\mathbb{C})$ of $L_{\mathbb{C}}^2(I,u^2)$ and therefore essentially self-adjoint. Hence, it follows from Lemma 2.2.2 that $\hat{L}_0^2$ is essentially self-adjoint and from Theorem 2.2.4 that the spectrum $\sigma(\hat{L}^2)$ of the closure $\hat{L}^2$ of $\hat{L}_0^2$ is given by

$$
\sigma(\hat{L}^2) = \hbar^2.\{\ell(\ell+1) : \ell \in \mathbb{N}\} \ ,
$$

consists of eigenvalues of infinite multiplicity, and that there is a complete set eigenvectors of $\hat{L}^2$, i.e., the spectrum is a pure point spectrum. The spectrum of $\hat{L}^2$ is not purely discrete, since the eigenvalues are of infinite multiplicity. Finally, we arrive at the following result (Fig. 2.2).

Angular Momentum Operators

The square of the angular momentum $\hat{L}_0^2$ is a densely-defined, linear, symmetric and essentially self-adjoint operator in $L_{\mathbb{C}}^2(\mathbb{R}^3)$ with a pure point spectrum given by

$$
\hbar^2.\{\ell(\ell+1) : \ell \in \mathbb{N}\} \ ,
$$

consisting of eigenvalues of infinite multiplicity. Hence the spectrum is not purely discrete. Again, we note that this result differs significantly from classical mechanics, since the values of the square of the angular momentum in classical mechanics are not quantized, but can assume any positive real value.

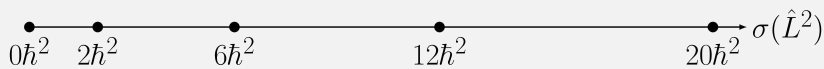


Fig. 2.2 The spectral values of $\hat{L}^2$, i.e., all positive integer multiples of $\hbar^2$ of the form $\ell(\ell+1)\hbar^2$, where $l \in \mathbb{N}$, are indicated by points.

2.4.5 The Commuting of the Operators $\hat{L}_3$ and $\hat{L}^2$

For the proof, we note that according to the analysis inside the Sects. 2.4.4, 2.4.3 and Corollary 2.2.3, the operators $U\hbar^{-1}\hat{L}_3\,U^{-1}$ and $U\hbar^{-2}\hat{L}^2\,U^{-1}$, where the unitary transformation $U : L^2_{\mathbb{C}}(\mathbb{R}^3) \to X := L^2_{\mathbb{C}}(\Omega, u^2\sin(\theta))$ is defined by (2.7), coincide with the operator

$$m.\mathrm{id}_{X_{\ell m}}$$

and the operator

$$\ell(\ell+1).\mathrm{id}_{X_{\ell m}}\ ,$$

respectively, on the pairwise orthogonal subspaces $X_{\ell m} \leqslant X$, $(\ell, m) \in \mathcal{I}$, defined by (2.11). Hence, it follows from Lemma 2.2.1 and for $\sigma, \tau \in \mathbb{R}$ that

$$e^{i\sigma U\hbar^{-1}\hat{L}_3\,U^{-1}}|_{X_{\ell m}} = e^{i\sigma m}.\mathrm{id}_{X_{\ell m}}\ ,\quad e^{i\tau U\hbar^{-2}\hat{L}^2\,U^{-1}}|_{X_{\ell m}} = e^{i\tau\ell(\ell+1)}.\mathrm{id}_{X_{\ell m}}\ .$$

As a consequence,

$$\left[e^{i\sigma U\hbar^{-1}\hat{L}_3\,U^{-1}}, e^{i\tau U\hbar^{-2}\hat{L}^2\,U^{-1}}\right]\Big|_{X_{\ell m}} = 0\ .$$

Since the span of the union of all $X_{\ell m}$, $(\ell, m) \in \mathcal{I}$, is dense in X, this implies that

$$\left[e^{i\sigma U\hbar^{-1}\hat{L}_3\,U^{-1}}, e^{i\tau U\hbar^{-2}\hat{L}^2\,U^{-1}}\right] = 0\ .$$

Taking into account that this is true for all $\sigma, \tau \in \mathbb{R}$, it follows from Theorem 2.1.1 that $U\hbar^{-1}\hat{L}_3\,U^{-1}$ and $U\hbar^{-2}\hat{L}^2\,U^{-1}$ commute and hence also that $\hat{L}_3$ and $\hat{L}^2$ commute.

2.5 Symmetry and Invariance

Symmetry transformations are of fundamental importance in the whole of physics. For instance, Euclidean space is homogeneous and isotropic, i.e., there is no preferred location

or direction in space. Therefore, a free particle in space cannot "know" its location nor orientation in space, and hence the physical system is in some sense "invariant" under rigid transformations, the symmetry transformations of Euclidean space. On the other hand, in general, interactions need not be compatible with rigid transformations.
In quantum mechanics, to every rigid transformation, there corresponds a unitary linear operator $U : X \to X$ on the state space X. The physical system is invariant under U if U leaves the time evolution operators invariant.

Definition of a Symmetry of a Quantum Mechanical System

In the following, we are going to adopt the definition that a symmetry of quantum mechanical system is given by a unitary linear operator $\mathcal{U}$ on the state space X that leaves invariant every member of the family $(U(t))_{t\in\mathbb{R}}$ of time evolution operators, see (3.2), i.e., $\mathcal{U}$ is an unitary linear operator such that $[\mathcal{U}, U(t)] = 0$, for every $t \in \mathbb{R}$.

Hence if $\mathcal{U}$ is a symmetry of the system and

$$(\mathbb{R} \to X, t \mapsto U(t - t_0)f)$$

is the path in the state space, of the system corresponding to the initial data $f \in X\setminus\{0\}$ at time $t_0 \in \mathbb{R}$, then

$$(\mathbb{R} \to X, t \mapsto \mathcal{U}\, U(t - t_0)f)$$

is the path of the system corresponding to the initial data $\mathcal{U}f \in X\setminus\{0\}$ at time t_0. We note that for this to be true, it is essential that $\mathcal{U}$ is unitary.
In the context of time evolution, we remind the reader the method of the book, to deal with physical dimensions in operator theory. In this text, physical operators are always of a particular form, namely multiples of dimensionless operators. The only place, where the physical dimension appears in observables is in the constant multiplying the dimensionless operator, in this way giving the operator as well as its spectrum the right physical dimension. In particular, in the case of time evolution, the situation is as follows. The Hamilton operator $\hat{H}$ is of the form $\hat{H} = \varepsilon_0 A$, where A is a dimensionless operator and $\varepsilon_0 > 0$ is a constant with the dimension of an energy. Hence

$$U(t) = e^{-i\frac{t}{\hbar}\hat{H}} = e^{-i\frac{\varepsilon t}{\hbar}A} \ ,$$

where $\frac{\varepsilon t}{\hbar}$, for every $t \in \mathbb{R}$, and A are dimensionless, in this way, allowing a clean application of the spectral theorem for the operator A. Having this in mind, we are going to prove a sufficient condition for a symmetry of a physical system.

A Sufficient Condition for a Symmetry

If $\hat{H}$ is the Hamilton operator of the system, and $\mathcal{U}$ is an unitary linear operator such that

$$\hat{H}\mathcal{U} \supset \mathcal{U}\hat{H} \ , \tag{2.13}$$

i.e., if for every $f \in D(\hat{H})$, it follows that $Uf \in D(\hat{H})$ as well as that $\hat{H}Uf = U\hat{H}f$, then $\mathcal{U}$ is a symmetry of the system.

For the proof, we note that if $\mathcal{U}$ is an unitary linear operator that satisfies (2.13), then $\mathcal{U}$ leaves the domain $D(\hat{H})$ of $\hat{H}$ invariant, i.e.,

$$\mathcal{U}D(\hat{H}) \subset D(\hat{H}) \ .$$

Further, for $f \in D(\hat{H})$, the unique solution $u : \mathbb{R} \to D(\hat{H})$ of the Schrödinger equation

$$i\hbar.u'(t) = \hat{H}u(t)$$

such that $u(0) = f$, where $'$ denotes the ordinary derivative of a X-valued path, is given by

$$u(t) := U(t)f$$

for all $t \in \mathbb{R}$. Hence $\mathcal{U} \circ u : \mathbb{R} \to D(\hat{H})$ is differentiable such that

$$\begin{aligned} i\hbar.(\mathcal{U} \circ u)'(t) &= \mathcal{U}i\hbar.u'(t) = \mathcal{U}\hat{H}u(t) = \hat{H}\mathcal{U}u(t) = \hat{H}(\mathcal{U} \circ u)(t) \ , \\ (\mathcal{U} \circ u)(0) &= \mathcal{U}f \ . \end{aligned}$$

for every $t \in \mathbb{R}$. Hence, it follows from Stone's theorem that

$$\mathcal{U}U(t)f = (\mathcal{U} \circ u)(t) = U(t)\mathcal{U}f \ ,$$

for every $t \in \mathbb{R}$. Hence, it follows for every $t \in \mathbb{R}$ that the bounded linear operators $\mathcal{U}U(t)$ and $U(t)\mathcal{U}$ coincide on $D(\hat{H})$. Since $D(\hat{H})$ is dense in the representation space X, this implies that

$$[\mathcal{U}, U(t)] = 0 \ ,$$

for every $t \in \mathbb{R}$ and hence that $\mathcal{U}$ is a symmetry.

Generically, the exact domain of Hamilton operator is unknown, so that (2.13) can rarely be checked explicitly. What is usually known, is a core for $\hat{H}$ that is invariant under U. Indeed, it is sufficient to check (2.13) for the restriction of $\hat{H}$ to such a core.

A Sufficient Condition for a Symmetry II

If $\hat{H}$ is the Hamilton operator of the system, $D \subset D(\hat{H})$ a core for $\hat{H}$, and $\mathcal{U}$ an unitary linear operator that leaves D invariant and such that for every $f \in D$, it follows that $\hat{H}Uf = U\hat{H}f$, then $\mathcal{U}$ is a symmetry of the system.

For the proof, let $f \in D(\hat{H})$. Since $D \subset D(\hat{H})$ is a core for $\hat{H}$, there is a sequence $f_1, \ldots, f_n$ in D such that

$$\lim_{\nu\to\infty} f_\nu = f \text{ and } \lim_{\nu\to\infty} \hat{H}f_\nu = \hat{H}f \ .$$

Hence,

$$\lim_{\nu\to\infty} Uf_\nu = Uf \text{ and } U\hat{H}f = \lim_{\nu\to\infty} U\hat{H}f_\nu = \lim_{\nu\to\infty} \hat{H}Uf_\nu \ .$$

Since $\hat{H}$ is closed, if follows that $Uf \in D(\hat{H})$ and $\hat{H}Uf = U\hat{H}f$.

We note that if $\mathcal{U}$ is an unitary linear operator on the state space satisfying (2.13), then it follows from the spectral theorem, Theorem 12.6.4, that U commutes with every function $f(\hat{H})$ of $\hat{H}$,

$$[\mathcal{U}, f(\hat{H})] = 0 \ ,$$

for every $f \in \overline{U^s_{\mathbb{C}}(\sigma(\hat{H}))}$. In particular, $\mathcal{U}$ commutes with the spectral projections corresponding to $\hat{H}$ *and, in particular, leaves its eigenspaces invariant.*.

In the following, as an example of the treatment of rigid transformations in quantum mechanics, we consider unitary representations of the translation group, $(\mathbb{R}^n, +)$ and the orthogonal group, $O(n)$, in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, $n \in \mathbb{N}^*$. Only later, we switch to the case that $n = 3$, which is of primary interest.

2.6 An Unitary Representation of Translations in Euclidean Space

For every $v \in \mathbb{R}^n$, we define a corresponding translation $T_v \in L(\mathbb{R}^n, \mathbb{R}^n)$ on $(\mathbb{R}^n, +)$ by

$$T_v(u) := u - v \ ,$$

for every $u \in \mathbb{R}^n$. Further, for every $v \in \mathbb{R}^n$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, we define

$$U_{T_v} f := f \circ T_v^{-1} \ .$$

Since is $T_v^{-1} = T_{-v}$ is in particular a C^1-diffeomorphism, it follows that $f \circ T_v^{-1} \in L^2_{\mathbb{C}}(\mathbb{R}^n)$,

$$\|U_{T_v} f\|_2^2 = \int_{\mathbb{R}^n} |U_{T_v} f|^2 \, dv^n = \int_{\mathbb{R}^n} |f \circ T_v^{-1}|^2 \cdot |\det(T_v^{-1\prime})| \, dv^n$$
$$= \int_{T_v^{-1}(\mathbb{R}^n)} |f|^2 \, dv^n = \int_{\mathbb{R}^n} |f|^2 \, dv^n = \|f\|_2^2 \ ,$$

and hence that

$$\|U_{T_v} f\|_2 = \|f\|_2 \ .$$

Further, U_{T_v} is obviously linear. In addition,

$$U_{T_0} = \mathrm{id}_{L^2_{\mathbb{C}}(\mathbb{R}^n)} \ , \ U_{T_{v_1} \circ T_{v_2}} = U_{T_{v_1}} \circ U_{T_{v_2}} \ ,$$

for all $v_1, v_2 \in \mathbb{R}^n$. As a consequence, for every $v \in \mathbb{R}^n$, the corresponding U_{T_v} is a linear isometry, with a linear isometric inverse and hence unitary linear, where we use the polarization identities for $\mathbb{C}$-Sesquilinear forms on complex vector spaces, see Theorem 12.3.3 (ii) in the Appendix. Hence, we arrive at a unitary representation of $(\mathbb{R}^n, +)$ on $L^2_{\mathbb{C}}(\mathbb{R}^n)$,

$$U : (\mathbb{R}^n, +) \to L(L^2_{\mathbb{C}}(\mathbb{R}^n), L^2_{\mathbb{C}}(\mathbb{R}^n)) \ ,$$

defined by

$$U(v) := U_{T_v} \ ,$$

for every $v \in \mathbb{R}^n$, i.e., U has its images in the set of unitary linear operators on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ and satisfies

$$U(0) = \mathrm{id}_{L^2_{\mathbb{C}}(\mathbb{R}^n)} \ , \ U(v_1 + v_2) = U(v_1) \circ U(v_2) \ .$$

for all $v_1, v_2 \in \mathbb{R}^n$.

In addition, U is strongly continuous. i.e., if $v_1, v_2, \dots$ is a sequence in $\mathbb{R}^n$ that converges componentwise to $v \in \mathbb{R}^n$, then

$$\lim_{\nu \to \infty} \|[U(v_\nu) - U(v)]f\|_2 = 0 \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. For the proof, we note that for every $v \in \mathbb{R}^n$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$,

$$U(v)f = f \circ T_v^{-1} = f \circ T_{-v} \ .$$

Hence if $v_1, v_2, \dots$ is a sequence in $\mathbb{R}^n$ that converges componentwise to $v \in \mathbb{R}^n$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, then it follows that the corresponding sequence $U(v_1)f, U(v_2)f, \dots$ convergences a.e. pointwise to $U(v)f$. This implies that the sequence

$$|[U(v_1) - U(v)]f|^2, |[U(v_2) - U(v)]f|^2, \dots$$

convergences a.e. pointwise to 0. For the next step, we assume temporarily that f is in particular continuous, with a compact support contained in $U_R(0)$, for some $R > 0$. Then, it follows for very $\nu \in \mathbb{N}^*$ that $U(v_\nu)f$ is continuous such that

$$\operatorname{supp}(U(v_\nu)f) \subset -v_\nu + U_R(0) \ ,$$

since T_{v_ν} is in particular continuous, implying in particular that $U(v_\nu)f$ is continuous with a compact support and that

$$|U(v_\nu)f| \leqslant \|f\|_\infty \, \chi_{-v_\nu + U_R(0)} \ .$$

Since $v_1, v_2, \ldots$ converges componentwise to $v \in \mathbb{R}^n$, it follows that the sequence $|v_1|, |v_2|, \ldots$ is in particular bounded by some $\rho > 0$. This implies that

$$|U(v_\nu)f| \leqslant \|f\|_\infty \, \chi_{U_{\rho+R}(0)} \ ,$$

for every $\nu \in \mathbb{N}^*$, and hence that the members of the sequence of integrable functions

$$|[U(v_1) - U(v)]f|^2, |[U(v_2) - U(v)]f|^2, \ldots$$

are dominated by an integrable function. Hence it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \|U(v_\nu)f - U(v)f\|_2 = 0 \ .$$

In the next step, we go back to the general case. Since $C_0(\mathbb{R}^n, \mathbb{C})$ is a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R}^n)$, for every $\mu \in \mathbb{N}^*$, there is $f_\mu \in C_0(\mathbb{R}^n, \mathbb{C})$ such that

$$\|f_\mu - f\|_2 \leqslant \frac{1}{\mu} \ .$$

Hence it follows for every $\nu \in \mathbb{N}^*$ and every $\mu \in \mathbb{N}^*$ that

$$\begin{aligned}
&\|U(v_\nu)f - U(v)f\|_2 \\
&= \|U(v_\nu)f - U(v_\nu)f_\mu + U(v_\nu)f_\mu - U(v)f_\mu + U(v)f_\mu - U(v)f\|_2 \\
&\leqslant \|U(v_\nu)(f - f_\mu)\|_2 + \|U(v_\nu)f_\mu - U(v)f_\mu\|_2 + \|U(v)(f_\mu - f)\|_2 \\
&\leqslant \frac{2}{\mu} + \|U(v_\nu)f_\mu - U(v)f_\mu\|_2 \ .
\end{aligned}$$

If $\varepsilon > 0$ and $\mu \in \mathbb{N}^*$ is such that $\mu \geqslant 4/\varepsilon$, then

$$\|U(v_\nu)f - U(v)f\|_2 \leqslant \frac{\varepsilon}{2} + \|U(v_\nu)f_\mu - U(v)f_\mu\|_2 \ .$$

Further, since

$$\lim_{\nu\to\infty} \|U(v_\nu)f_\mu - U(v)f_\mu\|_2 = 0 \ ,$$

there is $\nu_0 \in \mathbb{N}^*$, such that

$$\|U(v_\nu)f_\mu - U(v)f_\mu\|_2 \leqslant \frac{\varepsilon}{2} \ ,$$

for every $\nu \in \mathbb{N}^*$ such that $\nu \geqslant \nu_0$. Hence, it follows that

$$\|U(v_\nu)f - U(v)f\|_2 \leqslant \varepsilon \ ,$$

for every $\nu \in \mathbb{N}^*$ such that $\nu \geqslant \nu_0$. Since this is true for every $\varepsilon > 0$, we conclude that

$$\lim_{\nu\to\infty} \|U(v_\nu)f - U(v)f\|_2 = 0 \ .$$

2.6.1 Generators Corresponding to Continuous One-Parameter Subgroups

In the following, let $v \in \mathbb{R}^n$. Then $V : \mathbb{R} \to \mathbb{R}^n$, defined by

$$V(s) := s\,v \ ,$$

for $s \in \mathbb{R}$, is a continuous group homomorphism, i.e., such that

$$V(s_1 + s_2) = V(s_1) + V(s_2) \ ,$$

for all $s_1, s_2 \in \mathbb{R}$ and such that, for every sequence $s_1, s_2, \dots$ in $\mathbb{R}$ that is convergent to $s \in \mathbb{R}$, the corresponding sequence $V(s_1), V(s_2), \dots$ converges componentwise to $V(s)$, then $U \circ V$ is a strongly continuous one-parameter unitary group. According to Stone's theorem, there is a unique densely-defined, linear and self-adjoint operator A_V in $X := L^2_{\mathbb{C}}(\mathbb{R}^n)$ such that

$$\exp(isA_V) = (U \circ V)(s) \ ,$$

for every $s \in \mathbb{R}$ and, in particular, that $A_V : D(A_V) \to X$ is given by

$$D(A_V) = \left\{ f \in X : \lim_{s\to 0, s\neq 0} \frac{1}{s}\,[(U \circ V)(s) - \mathrm{id}_X]\,f \ \text{exists} \right\}$$

and for every $f \in D(A_V)$

$$A_V f = \frac{1}{i} \lim_{s\to 0, s\neq 0} \frac{1}{s}\,[(U \circ V)(s) - \mathrm{id}_X]\,f \ .$$

If $f \in C_0^1(\mathbb{R}^n, \mathbb{C})$, then it follows from the mean value theorem in several variables the existence of $C \geqslant 0$ such that

$$|f(v) - f(u)| \leqslant C\,|v - u| \ ,$$

for all $u, v \in \mathbb{R}^n$. Further, if $R > 0$ is such that $\text{supp}(f) \subset U_R(0)$, we conclude for every $s \in \mathbb{R}$, $u \in \mathbb{R}^n$ that

$$\left|[(U \circ V)(s)f](u) - f(u)\right|^2 = \left|f(u + sv) - f(u)\right|^2 \leqslant C^2|v|^2\,s|^2$$

and hence that

$$\left|\frac{1}{s}\,[(U \circ V)(s)f - f]\right|^2 \leqslant C^2|v|^2\,\chi_{U_{R+|v|\cdot|s|}(0)} \ ,$$

for every $s \in \mathbb{R}^*$. Further,

$$\lim_{s \to 0, s \neq 0} \frac{1}{s}\,\{[(U \circ V)(s) - \text{id}_X]\,f\}\,(u) = (v \cdot \nabla f)(u) \ ,$$

for every $u \in \mathbb{R}^n$. As a consequence, if $s_1, s_2, \ldots$ is a sequence in $\mathbb{R}^*$ that is convergent to 0, then

$$\left(\left|\frac{1}{s_\nu}\,[(U \circ V)(s_\nu)f - f] - v \cdot \nabla f\right|^2\right)_{\nu \in \mathbb{N}^*}$$

is a sequence of integrable functions that is everywhere on $\mathbb{R}^n$ convergent to the 0-function on $\mathbb{R}^3$ and whose members are dominated by the integrable function

$$2\,C^2|v|^2\,\chi_{U_{R+S|v|}(0)} + 2\,|v \cdot \nabla f|^2 \ ,$$

where $S \geqslant 0$ is a upper bound for the sequence $|s_1|, |s_2|, \ldots$. Hence, it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \int_{\mathbb{R}^n} \left|\frac{1}{s_\nu}\,[(U \circ V)(s_\nu)f - f] - v \cdot \nabla f\right|^2 dv^n = 0 \ ,$$

i.e., that

$$\lim_{\nu \to \infty} \left\|\frac{1}{s_\nu}\,[(U \circ V)(s_\nu)f - f] - v \cdot \nabla f\right\|_2 = 0 \ .$$

We conclude that $C_0^1(\mathbb{R}^n, \mathbb{C}) \subset D(A_V)$ a well as that

$$A_V f = \frac{1}{i}\,v \cdot \nabla f \ ,$$

for every $f \in C_0^1(\mathbb{R}^n, \mathbb{C})$. Hence, for every $k \in \{1, \dots, n\}$, A_{e_k} is a self-adjoint extension of $(\hbar\kappa)^{-1}\hat{p}_{k0}$. Since $\hat{p}_{k0}$ is essentially self-adjoint, with self-adjoint extension $\hat{p}_k$, this implies that

$$\hat{p}_k = \hbar\kappa \, A_{e_k} \ .$$

Hence, we arrive at the following.

Connection Between Space Translations and the Components of Momentum

For every $k \in \{1, \dots, n\}$, the following representation is true

$$\exp\Big(i \, \frac{s}{\hbar\kappa} \, \hat{p}_k\Big) \, f = f \circ (\mathrm{id}_{\mathbb{R}^n} + s e_k) \ , \tag{2.14}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $s \in \mathbb{R}$.

Using (2.14) and (1.1), for $k, l \in \{1, \dots, n\}$, it follows that

$$\begin{aligned}
&\exp\Big(i \, \frac{\tau}{\hbar\kappa} \, \hat{p}_k\Big) \exp(i\sigma\kappa \, \hat{q}_l) f = \exp\Big(i \, \frac{\tau}{\hbar\kappa} \, \hat{p}_k\Big) \exp(i\sigma u_l) f \\
&= \exp[i\sigma \, (u_l + \tau \, \delta_{kl})] \cdot [f \circ (\mathrm{id}_{\mathbb{R}^n} + \tau \, e_k)] \\
&= \exp(i\sigma\tau \, \delta_{kl}) \exp(i\sigma u_l) \cdot [f \circ (\mathrm{id}_{\mathbb{R}^n} + \tau \, e_k)] \\
&= \exp(i\tau\sigma \, \delta_{kl}) \exp(i\sigma u_l) \exp\Big(i \, \frac{\tau}{\hbar\kappa} \, \hat{p}_k\Big) \, f \\
&= \exp(i\tau\sigma \, \delta_{kl}) \exp(i\sigma\kappa \, \hat{q}_l) \exp\Big(i \, \frac{\tau}{\hbar\kappa} \, \hat{p}_k\Big) \, f \ ,
\end{aligned}$$

where $\tau, \sigma \in \mathbb{R}$, $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and δ_{kl} is defined as 1 if $k = l$ and 0, otherwise.

Hence we arrive at Weyl's form of the canonical commutation relations. These relations are required to be satisfied by the quantizations of the canonically conjugate observables of the classical system, momentum and position.

Weyl's form of the Canonical Commutation Relations for the Components of Momentum and Position

For every $k \in \{1, \dots, n\}$,

$$e^{i\tau\,(\hbar\kappa)^{-1}\hat{p}_k} e^{i\sigma\kappa\,\hat{q}_l} \, f = e^{i\tau\sigma\delta_{kl}} e^{i\sigma\kappa\,\hat{q}_l} e^{i\tau\,(\hbar\kappa)^{-1}\hat{p}_k} \ , \tag{2.15}$$

where $\tau, \sigma \in \mathbb{R}$, $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and δ_{kl} is defined as 1 if $k = l$ and 0, otherwise.

The reader might wonder, whether there is a connection of the components of the position operator $\hat{q}_1, \ldots, \hat{q}_n$ to an one-parameter unitary group of translations. Indeed, this is the case. For the proof, we assume that $k \in \{1, \ldots, n\}$. Then

$$\begin{aligned} F_2^{-1} \exp(isA_{e_k})\, F_2 f &= F_2^{-1}[(F_2 f) \circ (\mathrm{id}_{\mathbb{R}^n} + se_k)] = F_2^{-1} F_2\, e^{-isu_k} f \\ &= e^{-is\kappa\,(u_k/\kappa)} f = \exp(-is\kappa\, \hat{q}_k) f \ , \end{aligned}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $s \in \mathbb{R}$, where we used (1.1). Hence, it follows that

$$\exp(is\kappa\, \hat{q}_k) f = F_2^{-1}[(F_2 f) \circ (\mathrm{id}_{\mathbb{R}^n} - se_k)] = F_2^{-1} \exp(-isA_{e_k})\, F_2 f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $s \in \mathbb{R}$. As a consequence, $\exp(is\kappa\, \hat{q}_k)$ corresponds to a translation in momentum space, for every $s \in \mathbb{R}$. Further,

$$\hat{q}_k = F_2^{-1}\left(-\frac{1}{\kappa}\, A_{e_k}\right) F_2 \ .$$

and hence $\hat{q}_k$ coincides with the closure of

$$F_2^{-1}\left(C_0^\infty(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n),\ f \mapsto \frac{i}{\kappa}\, \frac{\partial f}{\partial v_k}\right) F_2 \ .$$

Hence, we arrive at the following.

Connection Between Translations in Momentum Space and the Components of Position

Using in addition (1.1), we arrive for every $k \in \{1, \ldots, n\}$ at the following representations,

$$\exp(is\kappa\, \hat{q}_k) f = \exp(isu_k) f = F_2^{-1}[(F_2 f) \circ (\mathrm{id}_{\mathbb{R}^n} - se_k)] \ , \tag{2.16}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $s \in \mathbb{R}$, where $u_k : \mathbb{R}^n \to \mathbb{R}$ denotes the kth coordinate projection, defined by $u_k(\bar{u}) := \bar{u}_k$ for all $\bar{u} = (\bar{u}_1, \ldots, \bar{u}_n) \in \mathbb{R}^n$. In addition, $\hat{q}_k$ coincides with the closure of

$$F_2^{-1}\left(C_0^\infty(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n),\ f \mapsto \frac{i}{\kappa}\, \frac{\partial f}{\partial v_k}\right) F_2 \ .$$

2.7 An Unitary Representation of Orthogonal Transformations in Euclidean Space

For every $n \in \mathbb{N}^*$, we define $O(n)$ to consist of all real $n \times n$ matrices M satisfying

$$M^* \cdot M = E \ , \tag{2.17}$$

where $\cdot$ denotes matrix multiplication, E the $n \times n$ unit matrix and M^* the transpose of M. We note that the latter implies that

$$1 = \det(E) = \det(M^* \cdot M) = \det(M^*) \cdot \det(M) = [\det(M)]^2$$

and hence that

$$\det(M) \in \{-1, 1\} \ .$$

Therefore M is invertible and $M^{-1} = M^*$, i.e., M is an orthogonal matrix. Also, according to definition, every orthogonal matrix M is invertible such that $M^{-1} = M^*$ and hence is satisfying (2.17). As a consequence, $O(n)$ coincides with the set of orthogonal $n \times n$-matrices. Also, since

$$(M_1 M_2)^* M_1 M_2 = M_2^* M_1^* M_1 M_2 = E \ , \ \ E^* E = EE = E \ ,$$
$$\left(M^{-1}\right)^* M^{-1} = \left(M^*\right)^* M^{-1} = M M^{-1} = E \ ,$$

for all $M_1, M_2 \in O(n)$, $O(n)$ is a subgroup of the general linear group, the so called orthogonal group in dimension n.

For every real $n \times n$ matrix M, we define the corresponding transformation $T_M \in L(\mathbb{R}^n, \mathbb{R}^n)$ by

$$T_M u := M \cdot u := \left(\sum_{k=1}^{n} M_{1k} u_k \, , \ldots , \sum_{k=1}^{n} M_{nk} u_k \right) \ ,$$

for every $u = {}^t(u_1, \ldots, u_n) \in \mathbb{R}^n$, where $u_1, \ldots, u_n \in \mathbb{R}$ are the components of the vector u. For every $M \in O(n)$, we note that

$$\begin{aligned}
\langle T_M u | T_M u \rangle_c &= \sum_{j=1}^{n} (T_M u)_j \cdot (T_M u)_j = \sum_{j=1}^{n} \left(\sum_{k=1}^{n} M_{jk} u_k \right) \cdot \left(\sum_{l=1}^{n} M_{jl} u_l \right) \\
&= \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} M_{jk} M_{jl} u_k u_l = \sum_{k=1}^{n} \sum_{l=1}^{n} \left(\sum_{j=1}^{n} M_{kj}^* M_{jl} \right) u_k u_l \\
&= \sum_{k=1}^{n} \sum_{l=1}^{n} E_{kl} u_k u_l = \sum_{k=1}^{n} u_k^2 = \langle u | u \rangle_c \ ,
\end{aligned}$$

for every $\langle \, | \, \rangle_c : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ denotes the canonical scalar product for $\mathbb{R}^n$, defined by

$$\langle v|w\rangle_c := v_1 w_1 + \ldots v_n w_n \ ,$$

for all vectors $v = {}^{\mathrm{t}}(v_1, \ldots, v_n), w = {}^{\mathrm{t}}(w_1, \ldots, w_n) \in \mathbb{R}^n$, where $v_1, \ldots, v_n \in \mathbb{R}$ and $w_1, \ldots, w_n \in \mathbb{R}$ are the components of the vector v and w, respectively. Hence, T_M preserves the scalar product, i.e., is a orthogonal linear transformation. As consequence, T_M is injective and hence also bijective.

On the other hand, if $T \in L(\mathbb{R}^n, \mathbb{R}^n)$ preserves the canonical scalar product and M is the representation matrix of T with respect to the canonical basis of $\mathbb{R}^n$,

$$\begin{aligned} \langle T_M e_m | T_M e_{m'} \rangle_c &= \sum_{k=1}^{n} \sum_{l=1}^{n} \left(\sum_{j=1}^{n} M^*_{kj} M_{jl} \right) (e_m)_k \, (e_{m'})_l \\ &= \sum_{j=1}^{n} M^*_{mj} M_{jm'} = \langle e_m | e_{m'} \rangle_c = E_{mm'} \end{aligned}$$

and hence that (2.17) is true. Here, $e_1, \ldots, e_n \in \mathbb{R}^n$ is the canonical basis of $\mathbb{R}^n$.

As a consequence, if $T \in L(\mathbb{R}^n, \mathbb{R}^n)$ and M is the representation matrix of T with respect to the canonical basis of $\mathbb{R}^n$, then T is orthogonal if and only if (2.17) is true.

Further, we note that

$$T_E = \mathrm{id}_{\mathbb{R}^n} \ , \ T_{\alpha M_1 + \beta M_2} = \alpha \, T_{M_1} + \beta \, T_{M_2} \ , \ T_{M_1 \cdot M_2} = T_{M_1} \circ T_{M_2} \ ,$$

for all $\alpha, \beta \in \mathbb{R}$ and real $n \times n$ matrices M_1, M_2. In particular, it follows for $M \in O(n)$ that

$$\mathrm{id}_{\mathbb{R}^n} = T_E = T_{M^{-1} \cdot M} = T_{M^{-1}} \circ T_M \ ,$$

implying that

$$T_M^{-1} = T_{M^{-1}} = T_{M^*} \ .$$

For later use, we note that for every real $n \times n$ matrix M and $v = {}^{\mathrm{t}}(v_1, \ldots, v_n) \in \mathbb{R}^n$, where $v_1, \ldots, v_n \in \mathbb{R}$ are the components of the v, it follows that

$$\begin{aligned} |T_M v|^2 &= \sum_{j=1}^{n} \left(\sum_{k=1}^{n} M_{jk} v_k \right)^2 \leqslant \sum_{j=1}^{n} \left[\left(\sum_{k=1}^{n} M_{jk}^2 \right) \left(\sum_{k=1}^{n} v_k^2 \right) \right] \\ &= \left(\sum_{j=1}^{n} \sum_{k=1}^{n} M_{jk}^2 \right) \cdot |v|^2 \ , \end{aligned}$$

where we define

$$|w| := \langle w|w \rangle_c^{1/2} = \left(\sum_{j=1}^{n} w_j^2 \right)^{1/2} \ ,$$

for every $w = {}^{t}(w_1, \dots, w_n) \in \mathbb{R}^n$, where $w_1, \dots, w_n \in \mathbb{R}$ are the components of the vector w. Hence

$$|T_M v| \leqslant \left(\sum_{j=1}^{n} \sum_{k=1}^{n} M_{jk}^2 \right)^{1/2} \cdot |v| \tag{2.18}$$

as well as for all real $n \times n$ matrices M_1, M_2

$$|(T_{M_2} - T_{M_1})v| \leqslant \left(\sum_{j=1}^{n} \sum_{k=1}^{n} |M_{2jk} - M_{1jk}|^2 \right)^{1/2} \cdot |v|$$

for every $v \in \mathbb{R}^n$. Hence, if $M_1, M_2, \dots$ is a sequence of real $n \times n$ matrices that converges componentwise to a real $n \times n$ matrix M, then

$$\lim_{\nu \to \infty} |T_{M_\nu} v - T_M v| = 0 \ , \tag{2.19}$$

for every $v \in \mathbb{R}^n$.

2.7.1 An Unitary Representation of $O(n)$ on $L^2_{\mathbb{C}}(\mathbb{R}^n)$

For every orthogonal $T \in L(\mathbb{R}^n, \mathbb{R}^n)$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, we define

$$U_T f := f \circ T^{-1} \ .$$

Since is T^{-1} is in particular a C^1-diffeomorphism, it follows that $f \circ T^{-1} \in L^2_{\mathbb{C}}(\mathbb{R}^n)$,

$$\begin{aligned} \|U_T f\|_2^2 &= \int_{\mathbb{R}^n} |U_T f|^2 \, dv^n = \int_{\mathbb{R}^n} |f \circ T^{-1}|^2 \cdot |\det(T^{-1\prime})| \, dv^n \\ &= \int_{T^{-1}(\mathbb{R}^n)} |f|^2 \, dv^n = \int_{\mathbb{R}^n} |f|^2 \, dv^n = \|f\|_2^2 \ , \end{aligned}$$

and hence that

$$\|U_T f\|_2 = \|f\|_2 \ .$$

Further, U_T is obviously linear. In addition,

$$U_{\mathrm{id}_{\mathbb{R}^n}} = \mathrm{id}_{L^2_{\mathbb{C}}(\mathbb{R}^n)} \ , \ U_{T_1 \circ T_2} = U_{T_1} \circ U_{T_2} \ ,$$

for all orthogonal $T_1, T_2 \in L(\mathbb{R}^n, \mathbb{R}^n)$. Hence, we arrive at a map

$$U : O(n) \to L(L^2_{\mathbb{C}}(\mathbb{R}^n), L^2_{\mathbb{C}}(\mathbb{R}^n)) \ ,$$

defined by

$$U(M) := U_{T_M} \ ,$$

for every $M \in O(n)$, satisfying

$$U(E) = \mathrm{id}_{L^2_{\mathbb{C}}(\mathbb{R}^n)} \ , \ U(M_1 \cdot M_2) = U(M_1) \circ U(M_2) \ , \tag{2.20}$$

for all $M_1, M_2 \in O(n)$. As a consequence, for every $M \in O(n)$, the corresponding $U(M)$ is a linear isometry, with a linear isometric inverse and hence unitary linear, where we use the polarization identities for $\mathbb{C}$-Sesquilinear forms on complex vector spaces, see Theorem 12.3.3 (ii) in the Appendix. Hence, U is a unitary representation of $O(n)$ on $L^2_{\mathbb{C}}(\mathbb{R}^n)$, since it images are in the set of unitary linear operators on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ and since it is satisying (2.20), for all $M_1, M_2 \in O(n)$.

In addition, U is strongly continuous, i.e., if $M_1, M_2, \dots$ is a sequence in $O(n)$ that converges componentwise to $M \in O(n)$, then

$$\lim_{\nu \to \infty} \| [U(M_\nu) - U(M)] f \|_2 = 0 \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. For the proof, we note that for every $M \in O(n)$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$,

$$U(M) f = U_{T_M} f = f \circ T_M^{-1} = f \circ T_{M^*} \ .$$

Hence if $M_1, M_2, \dots$ is a sequence in $O(n)$ that converges componentwise to $M \in O(n)$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, then it follows from (2.19) that the corresponding sequence $U(M_1)f, U(M_2)f, \dots$ convergences a.e. pointwise to $U(M)f$. This implies that the sequence

$$|[U(M_1) - U(M)]f|^2, |[U(M_2) - U(M)]f|^2, \dots$$

convergences a.e. pointwise to 0. For the next step, we assume temporarily that f is in particular continuous, with a compact support. Then, it follows for very $\nu \in \mathbb{N}^*$ that $U(M_\nu)f$ is continuous such that

$$\mathrm{supp}(U(M_\nu)f) \subset T_{M_\nu}(\mathrm{supp}(f)) \ ,$$

since T_{M_ν} is in particular continuous, implying in particular that $U(M_\nu)f$ is continuous with a compact support and that

$$|U(M_\nu)f| \leqslant \|f\|_\infty \, \chi_{T_{M_\nu}(\mathrm{supp}(f))} \ .$$

Since $M_1, M_2, \dots$ converges componentwise to $M \in O(n)$, it follows from (2.18) the existence of $C \geqslant 0$ such that for every $\nu \in \mathbb{N}^*$

$$|T_{M_\nu} v| \leqslant C \cdot |v| \ ,$$

for every $v \in \mathbb{R}^n$ and at the same time such that

$$|T_M v| \leqslant C \cdot |v| \ ,$$

for every $v \in \mathbb{R}^n$. In particular, this implies that

$$|U(M_\nu)f| \leqslant \|f\|_\infty \, \chi_{C.(\text{supp}(f))} \ .$$

and hence that the members of the sequence of integrable functions

$$|[U(M_1) - U(M)]f|^2, |[U(M_2) - U(M)]f|^2, \ldots$$

are dominated by an integrable function. Hence it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \|U(M_\nu)f - U(M)f\|_2 = 0 \ .$$

In the next step, we go back to the general case. Since $C_0(\mathbb{R}^n, \mathbb{C})$ is a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R}^n)$, for every $\mu \in \mathbb{N}^*$, there is $f_\mu \in C_0(\mathbb{R}^n, \mathbb{C})$ such that

$$\|f_\mu - f\|_2 \leqslant \frac{1}{\mu} \ .$$

Hence it follows for every $\nu \in \mathbb{N}^*$ and every $\mu \in \mathbb{N}^*$ that

$$\begin{aligned}
&\|U(M_\nu)f - U(M)f\|_2 \\
&= \|U(M_\nu)f - U(M_\nu)f_\mu + U(M_\nu)f_\mu - U(M)f_\mu + U(M)f_\mu - U(M)f\|_2 \\
&\leqslant \|U(M_\nu)(f - f_\mu)\|_2 + \|U(M_\nu)f_\mu - U(M)f_\mu\|_2 + \|U(M)(f_\mu - f)\|_2 \\
&\leqslant \frac{2}{\mu} + \|U(M_\nu)f_\mu - U(M)f_\mu\|_2 \ .
\end{aligned}$$

If $\varepsilon > 0$ and $\mu \in \mathbb{N}^*$ is such that $\mu \geqslant 4/\varepsilon$, then

$$\|U(M_\nu)f - U(M)f\|_2 \leqslant \frac{\varepsilon}{2} + \|U(M_\nu)f_\mu - U(M)f_\mu\|_2 \ .$$

Further, since

$$\lim_{\nu \to \infty} \|U(M_\nu)f_\mu - U(M)f_\mu\|_2 = 0 \ ,$$

there is $\nu_0 \in \mathbb{N}^*$, such that

$$\|U(M_\nu)f_\mu - U(M)f_\mu\|_2 \leqslant \frac{\varepsilon}{2} \ ,$$

for every $\nu \in \mathbb{N}^*$ such that $\nu \geqslant \nu_0$. Hence, it follows that

$$\|U(M_\nu)f - U(M)f\|_2 \leqslant \varepsilon \ ,$$

for every $\nu \in \mathbb{N}^*$ such that $\nu \geqslant \nu_0$. Since this is true for every $\varepsilon > 0$, we conclude that

$$\lim_{\nu \to \infty} \|U(M_\nu)f - U(M)f\|_2 = 0 \ .$$

2.7.2 Generators Corresponding to Rotations About the Coordinate Axes in 3 Space Dimensions

If

$$M : (\mathbb{R}, +) \to O(n)$$

is a continuous group homomorphism, i.e., such that

$$M(s_1 + s_2) = M(s_1) \cdot M(s_2) \ ,$$

for all $s_1, s_2 \in \mathbb{R}$ and such that, for every sequence $s_1, s_2, \dots$ in $\mathbb{R}$ that is convergent to $s \in \mathbb{R}$, the corresponding sequence $M(s_1), M(s_2), \dots$ converges componentwise to $M(s)$, then $U \circ M$ is a strongly continuous one-parameter unitary group. According to Stone's theorem, there is a unique densely-defined, linear and self-adjoint operator A_M in $X := L^2_{\mathbb{C}}(\mathbb{R}^n)$ such that

$$\exp(isA_M) = (U \circ M)(s) \ ,$$

for every $s \in \mathbb{R}$ and, in particular, that $A_M : D(A_M) \to X$ is given by

$$D(A_M) = \{ f \in X : \lim_{s \to 0, s \neq 0} \frac{1}{s} \, [(U \circ M)(s) - \mathrm{id}_X] \, f \ \text{exists} \}$$

and for every $f \in D(A_M)$

$$A_M f = \frac{1}{i} \lim_{s \to 0, s \neq 0} \frac{1}{s} \, [(U \circ M)(s) - \mathrm{id}_X] \, f \ .$$

In the following, our main cases of interest is $n = 3$ and rotations about the coordinate axes,

$$M_j : \mathbb{R} \to O(3) \ ,$$

$j \in \{1, 2, 3\}$, where

$$M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(s) & \sin(s) \\ 0 & -\sin(s) & \cos(s) \end{pmatrix} \ , \ M_2 = \begin{pmatrix} \cos(s) & 0 & -\sin(s) \\ 0 & 1 & 0 \\ \sin(s) & 0 & \cos(s) \end{pmatrix} \ ,$$

$$M_3 = \begin{pmatrix} \cos(s) & \sin(s) & 0 \\ -\sin(s) & \cos(s) & 0 \\ 0 & 0 & 1 \end{pmatrix} \ .$$

In the following, we analyze $U \circ M_3$. If $f \in C^1_0(\mathbb{R}^3, \mathbb{C})$, then it follows from the mean value theorem in several variables the existence of $C \geqslant 0$ such that

$$|f(v) - f(u)| \leqslant C \, |v - u| \ ,$$

for all $u, v \in \mathbb{R}^3$. Further, if $R > 0$ is such that $\text{supp}(f) \subset U_R(0)$, we conclude for every $s \in \mathbb{R}$, $u = (u_1, u_2, u_3) \in U_R(0)$ that

$$\begin{aligned}
&\left|[(U \circ M_3)(s) f](u) - f(u)\right|^2 \\
&= \left|f(\cos(s)u_1 - \sin(s)u_2, \sin(s)u_1 + \cos(s)u_2, u_3) - f(u_1, u_2, u_3)\right|^2 \\
&\leqslant C^2 \cdot \left|((\cos(s) - 1)u_1 - \sin(s)u_2, \sin(s)u_1 + (\cos(s) - 1)u_2, 0)\right|^2 \\
&= C^2\,[(\cos(s) - 1)^2 + \sin^2(s)](u_1^2 + u_2^2) = 2\,C^2\,[1 - \cos(s)](u_1^2 + u_2^2) \\
&= 4\,C^2 \sin^2\!\left(\frac{s}{2}\right)(u_1^2 + u_2^2) \leqslant C^2 R^2 s^2
\end{aligned}$$

and hence that

$$\left|\frac{1}{s}\,[(U \circ M_3)(s) f - f]\right|^2 \leqslant C^2\,R^2\,\chi_{U_R(0)}\ ,$$

for every $s \in \mathbb{R}^*$. Further,

$$\lim_{s \to 0, s \neq 0} \frac{1}{s}\,\{[(U \circ M_3)(s) - \text{id}_X]\,f\}\,(u) = \left(u_1\,\frac{\partial f}{\partial u_2} - u_2\,\frac{\partial f}{\partial u_1}\right)(u)$$

for every $u \in \mathbb{R}^3$. As a consequence, if $s_1, s_2, \ldots$ is a sequence in $\mathbb{R}^*$ that is convergent to 0, then

$$\left(\left|\frac{1}{s_\nu}\,[(U \circ M_3)(s_\nu) f - f] - \left(u_1\,\frac{\partial f}{\partial u_2} - u_2\,\frac{\partial f}{\partial u_1}\right)\right|^2\right)_{\nu \in \mathbb{N}^*}$$

is a sequence of integrable functions that is everywhere on $\mathbb{R}^3$ convergent to the 0-function on $\mathbb{R}^3$ and whose member are dominated by the integrable function

$$2\,C^2\,R^2\,\chi_{U_R(0)} + 2\left|u_1\,\frac{\partial f}{\partial u_2} - u_2\,\frac{\partial f}{\partial u_1}\right|^2\ .$$

Hence, it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu \to \infty} \int_{\mathbb{R}^3} \left|\frac{1}{s_\nu}\,[(U \circ M_3)(s_\nu) f - f] - \left(u_1\,\frac{\partial f}{\partial u_2} - u_2\,\frac{\partial f}{\partial u_1}\right)\right|^2 dv^3 = 0\ ,$$

i.e., that

$$\lim_{\nu \to \infty} \left\|\frac{1}{s_\nu}\,[(U \circ M_3)(s_\nu) f - f] - \left(u_1\,\frac{\partial f}{\partial u_2} - u_2\,\frac{\partial f}{\partial u_1}\right)\right\|_2 = 0\ .$$

We conclude that $C_0^1(\mathbb{R}^3, \mathbb{C}) \subset D(A_{M_3})$ a well as that

$$A_{M_3} f = \frac{1}{i}\left(u_1\,\frac{\partial f}{\partial u_2} - u_2\,\frac{\partial f}{\partial u_1}\right)\ ,$$

for every $f \in C_0^1(\mathbb{R}^3, \mathbb{C})$. Hence, A_{M_3} is a self-adjoint extension of $\hbar^{-1}\hat{L}_{30}$. Since $\hat{L}_{30}$ is essentially self-adjoint, with self-adjoint extension $\hat{L}_3$, this implies that

$$\hat{L}_3 = \hbar \, A_{M_3} \ .$$

Analogously, it follows that

$$\hat{L}_1 = \hbar \, A_{M_1} \ , \ \hat{L}_2 = \hbar \, A_{M_2} \ .$$

Hence, we arrive at the following

Connection Between Rotations About the Coordinate Axes and the Components of the Angular Momentum

For every $k \in \{1, 2, 3\}$, the following representation is true

$$\exp\Big(i \, \frac{s}{\hbar} \, \hat{L}_k\Big) \, f = f \circ (M_k(s) \cdot \mathrm{id}_{\mathbb{R}^3}) \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^3)$ and $s \in \mathbb{R}$, where $M_k : (\mathbb{R}, +) \to O(n)$ is given by

$$M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(s) & -\sin(s) \\ 0 & \sin(s) & \cos(s) \end{pmatrix} \ , \ M_2 = \begin{pmatrix} \cos(s) & 0 & \sin(s) \\ 0 & 1 & 0 \\ -\sin(s) & 0 & \cos(s) \end{pmatrix} \ ,$$

$$M_3 = \begin{pmatrix} \cos(s) & -\sin(s) & 0 \\ \sin(s) & \cos(s) & 0 \\ 0 & 0 & 1 \end{pmatrix} \ .$$

2.7.3 Symmetries of Perturbations of the Free Hamilton Operator

In the first step, we study the transformation of $\triangle f$, where $f \in C^2(\mathbb{R}^n, \mathbb{C})$, under coordinate transformations $h \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$. For this purpose, we define

$$\bar{f} := f \circ h^{-1}$$

such that

$$f = \bar{f} \circ h \ .$$

Then it follows by the chain rule

$$\frac{\partial f}{\partial u_j}(u) = \sum_{l=1}^{n} \frac{\partial h_l}{\partial u_j}(u)\, \frac{\partial \bar{f}}{\partial u_l}(h(u)) \ ,$$

$$\begin{aligned} &\frac{\partial^2 f}{\partial u_i \partial u_j}(u) \\ &= \sum_{l=1}^{n} \frac{\partial^2 h_l}{\partial u_i \partial u_j}(u)\, \frac{\partial \bar{f}}{\partial u_l}(h(u)) + \sum_{k,l=1}^{n} \frac{\partial h_l}{\partial u_j}(u)\, \frac{\partial h_k}{\partial u_i}(u)\, \frac{\partial^2 \bar{f}}{\partial u_k \partial u_l}(h(u)) \\ &= \sum_{k,l=1}^{n} \frac{\partial h_k}{\partial u_i}(u)\, \frac{\partial h_l}{\partial u_j}(u)\, \frac{\partial^2 \bar{f}}{\partial u_k \partial u_l}(h(u)) + \sum_{k=1}^{n} \frac{\partial^2 h_k}{\partial u_i \partial u_j}(u)\, \frac{\partial \bar{f}}{\partial u_k}(h(u)) \ , \end{aligned}$$

for every $u \in \mathbb{R}^n$ and $i, j \in \{1, \ldots, n\}$.

Next, we consider the case that h coincides with a space translation, $h = T_v$, for some $v \in \mathbb{R}^n$. Then

$$\frac{\partial f}{\partial u_i}(u) = \frac{\partial \bar{f}}{\partial u_i}(h(u)) \ , \quad \frac{\partial^2 f}{\partial u_i \partial u_j}(u) = \frac{\partial^2 \bar{f}}{\partial u_i \partial u_j}(h(u)) \ ,$$

for every $u \in \mathbb{R}^n$ and $i, j \in \{1, \ldots, n\}$. Hence if $v \in \mathbb{R}^n$, then

$$\triangle f = (\triangle \bar{f}\,) \circ h \ ,$$

or equivalently,

$$(\triangle f) \circ h^{-1} = \triangle (f \circ h^{-1}) \ .$$

We note that

$$U(v) f = U_{T_v} f = f \circ T_v^{-1} \ ,$$

for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. Hence it follows for $f \in C^2_0(\mathbb{R}^n, \mathbb{C})$ that

$$U(v) \triangle f = \triangle\, U(v) f \ ,$$

where we use that $U(v) f = f \circ T_v^{-1} \in C^2_0(\mathbb{R}^n, \mathbb{C})$. Since $C^2_0(\mathbb{R}^n, \mathbb{C})$ is a core for the free Hamiltonian $\hat{H}$ that is left invariant by $U(v)$, it follows that

> For every $v \in \mathbb{R}^n$, the corresponding unitary linear operator $U(v)$ on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ is a symmetry of the free Hamiltonian $\hat{H}$ from Sect. 1.4.

Further, going back to beginning of this section, we assume that h is linear. Then all partial derivatives of the first order are constant, and it follows that

$$\frac{\partial f}{\partial u_i}(u) = \sum_{k=1}^{n} M_{ki} \, \frac{\partial \bar{f}}{\partial u_k}(h(u)) \ ,$$
$$\frac{\partial^2 f}{\partial u_i \partial u_j}(u) = \sum_{k,l=1}^{n} M_{ki} \, M_{lj} \, \frac{\partial^2 \bar{f}}{\partial u_k \partial u_l}(h(u)) \ ,$$

for every $u \in \mathbb{R}^n$ and $i, j \in \{1, \dots, n\}$, where the real $n \times n$-matrix M is defined by

$$M_{ij} := \frac{\partial h_i}{\partial u_j} \ ,$$

for all $i, j \in \{1, \dots, n\}$. As a consequence,

$$\begin{aligned}(\triangle f)(u) &= \sum_{k,l=1}^{n} \left(\sum_{i=1}^{n} M_{ki} \, M_{li} \right) \frac{\partial^2 \bar{f}}{\partial u_k \partial u_l}(h(u)) \\ &= \sum_{k,l=1}^{n} \left(\sum_{i=1}^{n} M_{ki} \, M^*_{il} \right) \frac{\partial^2 \bar{f}}{\partial u_k \partial u_l}(h(u)) \\ &= \sum_{k,l=1}^{n} (M \cdot M^*)_{kl} \, \frac{\partial^2 \bar{f}}{\partial u_k \partial u_l}(h(u)) \ ,\end{aligned}$$

for every $u \in \mathbb{R}^n$. Hence, if $M \in O(n)$, then

$$\triangle f = (\triangle \bar{f}\,) \circ h \ ,$$

or equivalently,

$$(\triangle f) \circ h^{-1} = \triangle (f \circ h^{-1}) \ .$$

We note that

$$U(M) f = U_{T_M} f = f \circ T_M^{-1} \ ,$$

for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, and

$$T_M u := M \cdot u := \left(\sum_{k=1}^{n} M_{1k} u_k \, , \dots , \sum_{k=1}^{n} M_{nk} u_k \right) \ ,$$

for every $u = {}^{\mathrm{t}}(u_1, \dots, u_n) \in \mathbb{R}^n$. Hence

$$\frac{\partial (T_M)_i}{\partial u_j} = M_{ij} \ ,$$

for all $i, j \in \{1, \dots, n\}$, and it follows for $M \in O(n)$ and $f \in C^2_0(\mathbb{R}^n, \mathbb{C})$ that

$$U(M) \triangle f = \triangle \, U(M) f \ ,$$

where we use that $U(M)f = f \circ T_M^{-1} \in C_0^2(\mathbb{R}^n, \mathbb{C})$.[4] Since $C_0^2(\mathbb{R}^n, \mathbb{C})$ is a core for the free Hamiltonian $\hat{H}$ that is left invariant by $U(M)$, it follows that

> For every $M \in O(n)$, the corresponding unitary linear operator $U(M)$ on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ is a symmetry of the free Hamiltonian $\hat{H}$ from Sect. 1.4.

In Sect. 1.6, we showed for $n \leqslant 3$ and $V \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$ that the densely-defined, linear and symmetric operator

$$\hat{H}_{V0} : C_0^2(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n)$$

in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, defined by

$$\hat{H}_{V0} f := -\frac{\hbar^2\kappa^2}{2m} \triangle f + Vf = \frac{\hbar^2\kappa^2}{2m}\left(-\triangle f + \frac{2m}{\hbar^2\kappa^2}\, Vf\right) ,$$

for every $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$, is essentially self-adjoint. In addition,

$$\overline{\hat{H}_{V0}} = \hat{H} + T_V \ ,$$

where $\hat{H}$ is the free Hamiltonian from Sect. 1.4 and T_V denotes the maximal multiplication operator with V in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, and

$$D\left(\overline{\hat{H}_{V0}}\right) = D(\hat{H}) \subset C_\infty(\mathbb{R}^n, \mathbb{C}) \ .$$

If V is in addition a central potential, possibly singular at the origin, of the form $V \circ |\ |$, where $V : (0, \infty) \to \mathbb{R}$, then it follows for $M \in O(n)$ and $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$ that

$$U(M)\hat{H}_{V0} f = \hat{H}_{V0}\, U(M) f \ ,$$

where we use that $U(M)f = f \circ T_M^{-1} \in C_0^2(\mathbb{R}^n, \mathbb{C})$. Since $C_0^2(\mathbb{R}^n, \mathbb{C})$ is a core for $\hat{H} + T_V$ that is left invariant by $U(M)$, it follows that

[4] The latter can be seen as follows. Since $T_M^{-1} \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$, we have $U(M)f \in C^2(\mathbb{R}^n, \mathbb{C})$. Further, if $u \notin T_M(\text{supp}(f))$, then $T_M^{-1} u \notin \text{supp}(f)$ and hence $(U(M)f)(u) = 0$. As consequence, $(U(M)f)^{-1}(\mathbb{C}^*) \subset T_M(\text{supp}(f))$ as well as $\text{supp}(U(M)f) \subset T_M(\text{supp}(f))$, since $T_M(\text{supp}(f))$ is compact, as image of a compact subset of $\mathbb{R}^n$ under a continuous map. Hence $\text{supp}(U(M)f)$ is a compact subset of $\mathbb{R}^n$ and $U(M)f \in C_0^2(\mathbb{R}^n, \mathbb{C})$.

If $n \leqslant 3$ and $V \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$ is in addition a central potential, of the form $V \circ |\ |$, for some a.e. on $\mathbb{R}$ defined function, then for every $M \in O(n)$, the corresponding unitary linear operator $U(M)$ on $L^2_{\mathbb{C}}(\mathbb{R}^n)$ is a symmetry of $\hat{H} + T_V$, where $\hat{H}$ is the free Hamiltonian from Sect. 1.4, and T_V denotes the maximal multiplication operator with V in $L^2_{\mathbb{C}}(\mathbb{R}^n)$.

We note that the potential corresponding to the case of an electron in the Coulomb field of a nucleus containing Z protons,

$$V = -\frac{Ze^2\kappa}{|\ |} \ ,$$

where e denotes the charge of an electron, is a central potential satisfying $V \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$.

2.8 An One-Parameter Group of Symmetries

The potential functions of classical physics are not unique. The addition of a constant to a potential function leads to another physically equivalent potential function, since the force fields, given by the negative of the gradients, corresponding to both functions coincide. In short, potential functions of classical physics are unique only up to constant. This fact has its reflection in quantum mechanics. The easiest way to see this is as follows.

If $\hat{H}$ is the Hamiltonian of a quantum mechanical system and $f \in D(\hat{H})$, the unique solution $u : \mathbb{R} \to D(\hat{H})$ of the Schrödinger equation,

$$i\hbar.u'(t) = \hat{H}u(t) \ ,$$

such that $u(0) = f$, where $'$ denotes the ordinary derivative of a X-valued path and $(X, \langle\,|\,\rangle)$ is the representation space, is given by

$$u(t) = e^{-i\,(t/\hbar)\hat{H}} f$$

for every $t \in \mathbb{R}$. For the next step, let $\omega \in \mathbb{R}$, have the dimension $1/\text{Time}$. Then, we define $v : \mathbb{R} \to D(\hat{H})$ by

$$v(t) := e^{i\omega t} u(t) \ ,$$

for every $t \in \mathbb{R}$. In this, it is important that according to our definition of physical states, for every $t \in \mathbb{R}$ the corresponding $u(t)$ *and* $v(t)$ *describe the same physical state*, if $f \neq 0$. Further, we note for $t \in \mathbb{R}$ that

$$\begin{aligned}\frac{1}{\tau}\,[v(t+\tau)-v(\tau)] &= \frac{1}{\tau}\,[e^{i\omega(t+\tau)}u(t+\tau)-e^{i\omega t}u(t)] \\ &= \frac{e^{i\omega t}}{\tau}\left[e^{i\omega\tau}u(t+\tau)-u(t)\right] \\ &= e^{i\omega t}\left\{e^{i\omega\tau}\frac{1}{\tau}\,[u(t+\tau)-u(t)]+\frac{e^{i\omega\tau}-1}{\tau}\,u(t)\right\}\ ,\end{aligned}$$

for every $\tau \neq 0$ and hence that v is differentiable in t, with the derivative

$$v'(t) = e^{i\omega t}[u'(t) + i\omega u(t)]$$

and hence that

$$\begin{aligned}&i\hbar.v'(t) = e^{i\omega t}[i\hbar.u'(t) - \hbar\omega u(t)] = e^{i\omega t}(\hat{H} - \hbar\omega)u(t) = (\hat{H} - \hbar\omega)v(t)\ , \\ &\quad v(0) = u(0) = f\ .\end{aligned}$$

Since $D(H)$ is dense in X, we conclude that

$$e^{-(it/\hbar)(\hat{H}-\hbar\omega)} = e^{i\omega t}e^{-i\,(t/\hbar)\hat{H}}\ .$$

Hence, for every $f \in X\backslash\{0\}$

$$\mathbb{C}^* e^{-(it/\hbar)(\hat{H}-\hbar\omega)} f = \mathbb{C}^* e^{-i\,(t/\hbar)\hat{H}} f\ ,$$

for every $t \in \mathbb{R}$.

> Hence physically, the Hamiltonians $\hat{H} - E$ and $\hat{H}$ generate the same time evolution, where $E \in \mathbb{R}$ has the dimension of an energy. As a consequence, only energy differences are measurable, or the measuring of the value of the energy of Hamiltonian system is possible only through comparison with a reference energy.

2.9 Galilean Invariance

We consider two observers O and O' who move relative to each other, with translational uniform motion. Therefore, observer O sees observer O' moving with velocity $\vec{v} = {}^t(v_1, v_2, v_3) \in \mathbb{R}^3$, while O' sees O moving with velocity $-\vec{v}$. We choose, for simplicity, that at $t = 0$, O and O' are coincident and that the Cartesian coordinate axes of both coordinate systems coincide. Hence the coordinate axes remain parallel to each other during the motion. Then, the coordinates (t, x_1, x_2, x_3) and (t', x_1', x_2', x_3') of events in space and time, corresponding to the observer O and O', respectively, are related by a Galilean transformation

$$x_1' = x_1 - v_1 t \ , \ \ x_2' = x_2 - v_2 t \ , \ \ x_3' = x_3 - v_3 t \ ,$$

and

$$t' = t \ ,$$

where we assume the existence of an absolute time t, as is assumed in Newtonian physics. As a consequence, the momenta $\vec{p}$ and $\vec{p}\,'$ of a particle, as observed from O and O', respectively, are related by

$$\vec{p}\,' = \vec{p} - \vec{v} \ .$$

The latter indicates also how time evolution of a quantum mechanical system is perceived from both coordinate systems. In this context, we need to remember that translations in "momentum space" are governed by the position operator, see (2.16).

In the following, we consider more generally free motion in $n \in \mathbb{N}^*$ space dimensions and define

$$\sigma_k := \frac{m v_k}{\hbar \kappa} \ ,$$

for every $k \in \{1, \ldots, n\}$, where $\vec{v} = (v_1, \ldots, v_n) \in \mathbb{R}^n$ is the relative velocity of the system O' with respect to O.

According to Weyl's commutation rules for the operators corresponding to the components of position and momentum, (2.15), we have for $\tau \in \mathbb{R}$

$$e^{i\sigma_k \kappa\, \hat{q}_k} e^{i\tau\, (\hbar\kappa)^{-1} \hat{p}_k} e^{-i\sigma_k \kappa\, \hat{q}_k} f = e^{-i\tau\sigma_k} e^{i\tau\, (\hbar\kappa)^{-1} \hat{p}_k}$$

and hence

$$e^{i\sigma_k \kappa\, \hat{q}_k} (\hbar\kappa)^{-1} \hat{p}_k e^{-i\sigma_k \kappa\, \hat{q}_k} = (\hbar\kappa)^{-1} \hat{p}_k - \sigma_k = (\hbar\kappa)^{-1} (\, \hat{p}_k - m v_k) \ .$$

We note that if $k, l \in \{1, \ldots, n\}$ such that $l \neq k$, then

$$\begin{aligned} e^{i\sigma_l \kappa\, \hat{q}_l} e^{i\sigma_k \kappa\, \hat{q}_k} (\hbar\kappa)^{-1} \hat{p}_k e^{-i\sigma_k \kappa\, \hat{q}_k} e^{-i\sigma_l \kappa\, \hat{q}_l} &= (\hbar\kappa)^{-1} \hat{p}_k - \sigma_k \\ &= (\hbar\kappa)^{-1} (\, \hat{p}_k - m v_k) \ , \end{aligned}$$

since $\hat{q}_l$ and $\hat{p}_k$ commute. Hence

$$U_v\, \hat{p}_k U_v^{-1} = \hat{p}_k - m v_k \ ,$$

for every $k \in \{1, \ldots, n\}$, where the unitary linear operator U is defined by

$$U_v := e^{i\sigma_1 \kappa\, \hat{q}_1} \ldots e^{i\sigma_n \kappa\, \hat{q}_n} \ .$$

We note that

$$U_v \hat{q}_k U_v^{-1} = \hat{q}_k \ ,$$

for every $k \in \{1, \ldots, n\}$.

Further, according to Sect. 1.4, the Hamilton operator corresponding to the free motion in $n \in \mathbb{N}^*$ space dimensions is given by

$$\hat{H} = \varepsilon_0 . F_2^{-1} T_{|\ |^2} F_2 \ ,$$

where $T_{|\ |^2}$ denotes the maximal multiplication in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ with $|\ |^2$ and

$$\varepsilon_0 := \frac{\hbar^2 \kappa^2}{2m} \ .$$

Also, the spectrum of $\hat{H}$ consists of the interval $[0, \infty)$ and is purely absolutely continuous. Further, for every bounded universally measurable function $f : [0, \infty) \to \mathbb{C}$:

$$f(\hat{H}) = F_2^{-1} \circ T_{f \circ (\varepsilon_0 . |\ |^2)} \circ F_2 \ ,$$

where $T_{f \circ (\varepsilon_0 . |\ |^2)}$ is the maximal multiplication operator with the function $f \circ (\varepsilon_0 . |\ |^2)$, defined by

$$T_{f \circ (\varepsilon_0 . |\ |^2)} g := [f \circ (\varepsilon_0 . |\ |^2)] \cdot g \ ,$$

for every $g \in X := L^2_{\mathbb{C}}(\mathbb{R}^n)$. In particular, for $\tau \in \mathbb{R}$

$$e^{i\,(\tau/\varepsilon_0)\,\hat{H}} = e^{i\,\tau\,(\varepsilon_0^{-1} \hat{H}\,)} = F_2^{-1} \circ T_{e^{i\tau |\ |^2}} \circ F_2 \ .$$

Also, according to (2.16), it follows for $k \in \{1, \ldots, n\}$ that

$$e^{i\sigma\kappa\,\hat{q}_k} f = e^{i\sigma(\kappa\,\hat{q}_k)} f = e^{i\sigma u_k} f = F_2^{-1}[(F_2 f) \circ (\mathrm{id}_{\mathbb{R}^n} - \sigma e_k)] \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $\sigma \in \mathbb{R}$, where $u_k : \mathbb{R}^n \to \mathbb{R}$ denotes the kth coordinate projection, defined by $u_k(\bar{u}) := \bar{u}_k$ for all $\bar{u} = (\bar{u}_1, \ldots, \bar{u}_n) \in \mathbb{R}^n$.

Hence, it follows for $k \in \{1, \ldots, n\}$ further that

$$\begin{aligned}
e^{i\,(\tau/\varepsilon_0)\,\hat{H}} e^{-i\sigma_k\kappa\,\hat{q}_k} f &= F_2^{-1} e^{i\tau |\ |^2} [(F_2 f) \circ (\mathrm{id}_{\mathbb{R}^n} + \sigma_k e_k)] \\
&= F_2^{-1} \left\{ [e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k|^2} F_2 f] \circ (\mathrm{id}_{\mathbb{R}^n} + \sigma_k e_k) \right\} \\
&= e^{-i\sigma_k u_k} F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k|^2} F_2 f \\
&= e^{-i\sigma_k\kappa\,\hat{q}_k} F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k|^2} F_2 f \ ,
\end{aligned}$$

and hence that

$$e^{i\sigma_k\kappa\,\hat{q}_k} e^{i\,(\tau/\varepsilon_0)\,\hat{H}} e^{-i\sigma_k\kappa\,\hat{q}_k} f = F_2^{-1} T_{e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k|^2}} F_2 f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. We note that if $k, l \in \{1, \dots, n\}$, then

$$\begin{aligned}
& e^{i\sigma_l \kappa \, \hat{q}_l} e^{i\sigma_k \kappa \, \hat{q}_k} e^{i\,(\tau/\varepsilon_0)\,\hat{H}} e^{-i\sigma_k \kappa \, \hat{q}_k} f \\
&= e^{i\sigma_l \kappa \, \hat{q}_l} F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k|^2} F_2 f \\
&= F_2^{-1} \{ [e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k|^2} F_2 f] \circ (\mathrm{id}_{\mathbb{R}^n} - \sigma_l e_l) \} \\
&= F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k - \sigma_l e_l|^2} [(F_2 f) \circ (\mathrm{id}_{\mathbb{R}^n} - \sigma_l e_l)] \\
&= F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k - \sigma_l e_l|^2} F_2 (e^{i\sigma_l u_l} f) \\
&= F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k - \sigma_l e_l|^2} F_2 \, e^{i\sigma_l \kappa \, \hat{q}_l} f
\end{aligned}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and hence that

$$e^{i\sigma_l \kappa \, \hat{q}_l} e^{i\sigma_k \kappa \, \hat{q}_k} e^{i\,(\tau/\varepsilon_0)\,\hat{H}} e^{-i\sigma_k \kappa \, \hat{q}_k} e^{-i\sigma_l \kappa \, \hat{q}_l} f = F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \sigma_k e_k - \sigma_l e_l|^2} F_2 f \ \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. As a consequence, it follows also that

$$U_v e^{i\,(\tau/\varepsilon_0)\,\hat{H}} U_v^{-1} f = F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}|^2} F_2 f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where

$$\sigma := \sum_{k=1}^{n} \sigma_k e_k \in \mathbb{R}^n \ .$$

Now,

$$(\mathbb{R} \to L(X, X), \tau \mapsto U_v e^{i\,(\tau/\varepsilon_0)\,\hat{H}} U_v^{-1})$$

is a strongly continuous one-parameter unitary group, with generator

$$\varepsilon_0^{-1} U_v \hat{H} U_v^{-1} \ ,$$

and

$$(\mathbb{R} \to L(X, X), \tau \mapsto F_2^{-1} e^{i\tau |\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}|^2} F_2)$$

is a strongly continuous one-parameter unitary group, with generator

$$F_2^{-1} T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}|^2} F_2 \ ,$$

where

$$T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}|^2}$$

denotes the maximal multiplication operator in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ with the function $|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}|^2$. Hence,

$$U_v \hat{H} U_v^{-1} = \varepsilon_0 F_2^{-1} T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}|^2} F_2 \ . \tag{2.21}$$

In the following, we are going to investigate the connection of the right hand side of of the previous equation with the components of momentum. For this purpose, we consider the linear operator $(\,\hat{\vec{p}} - m\vec{v}\,)^2$, defined by

$$(\,\hat{\vec{p}} - m\vec{v}\,)^2 f := \sum_{k=1}^{n} \left(\,\hat{p}_k - m v_k\right)^2 f \ ,$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$. We conclude from known properties of F_2 that

$$\begin{aligned} F_2\,(\,\hat{\vec{p}} - m\vec{v}\,)^2 F_2^{-1} f &= \sum_{k=1}^{n} \left(\hbar\kappa\, T_{w_k} - m v_k\right)^2 f \\ &= (\hbar\kappa)^2 T_{\sum_{k=1}^{n}(w_k - \sigma_k)^2} f = (\hbar\kappa)^2 T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}\,|^2} \ , \end{aligned}$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$, where for every $k \in \{1, \dots, n\}$, $w_k : \mathbb{R}^n \to \mathbb{R}$ denotes the kth coordinate projection, defined by $w_k(\bar{w}) := \bar{w}_k$ for all $\bar{w} = {}^t(\bar{w}_1, \dots, \bar{w}_n) \in \mathbb{R}^n$. According to the characterization of essential self-adjointness from Theorem 12.4.9, the restriction of $T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}\,|^2}$ to $\mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ is essentially self-adjoint since

$$T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}\,|^2 \pm i}\, \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

contain $C_0^\infty(\mathbb{R}^n, \mathbb{C})$ and are therefore dense in $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Since F_2 is unitary, this implies also the essential self-adjointness of $(\,\hat{\vec{p}} - m\vec{v}\,)^2$ and that

$$\overline{(\,\hat{\vec{p}} - m\vec{v}\,)^2} = (\hbar\kappa)^2 F_2^{-1} T_{|\mathrm{id}_{\mathbb{R}^n} - \vec{\sigma}\,|^2} F_2 \ .$$

Hence, it follows from (2.21) that

$$U_v \hat{H} U_v^{-1} = \frac{1}{2m}\, \overline{(\,\hat{\vec{p}} - m\vec{v}\,)^2} \ .$$

Position, Momentum and Hamilton Operators Corresponding to the Observer O'

Summarizing the previous, the operators corresponding to the components of position, the components of momentum and the Hamilton operator in the system corresponding to the observer O', that is moving relative to the observer O with speed $\vec{v} = {}^t(v_1, \dots, v_k) \in \mathbb{R}^n$, are given by

$$\begin{aligned} &U_v \hat{q}_k U_v^{-1} = \hat{q}_k \ , \ U_v \hat{p}_k U_v^{-1} = \hat{p}_k - m v_k \ , \\ &U_v \hat{H} U_v^{-1} = \frac{1}{2m}\, \overline{(\,\hat{\vec{p}} - m\vec{v}\,)^2} \ , \end{aligned} \tag{2.22}$$

for $k \in \{1, \dots, n\}$, were $\overline{(\,\hat{\vec{p}} - m\vec{v}\,)^2}$ is the closure of the densely-defined, linear, symmetric and essentially self-adjoint operator in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, defined by

$$(\,\hat{\vec{p}} - m\vec{v}\,)^2 f := \sum_{k=1}^{n} \left(\,\hat{p}_k - m v_k\right)^2 f \ , \tag{2.23}$$

for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$, and the unitary linear transformation U_v to the relatively moving system is given by

$$U_v = e^{i\,\frac{m v_1}{\hbar}\,\hat{q}_1} \dots e^{i\,\frac{m v_n}{\hbar}\,\hat{q}_n} \ . \tag{2.24}$$

2.10 Gauge Invariance

We remind the reader of Maxwell's equations[5] in Minkowski space, for the electromagnetic field $\vec{E}, \vec{B} \in C^1(\Omega, \mathbb{R}^3)$ in Gaussian units

$$\begin{aligned} &\frac{\partial \vec{E}}{\partial t} = c\,\vec{\nabla} \times \vec{B} - 4\pi\,\vec{j}\ ,\ \ \frac{\partial \vec{B}}{\partial t} = -c\,\vec{\nabla} \times \vec{E}\ , \\ &\vec{\nabla} \cdot \vec{E} = 4\pi\rho\ ,\ \ \vec{\nabla} \cdot \vec{B} = 0\ , \end{aligned} \tag{2.25}$$

where $\Omega \subset \mathbb{R}^4$ is non-empty and open, $t, x_1, x_2, x_3 : \mathbb{R}^4 \to \mathbb{R}$ are inertial coordinates, c denotes the speed of light, $\rho \in C(\Omega, \mathbb{R})$ the charge density and $\vec{j} \in C(\Omega, \mathbb{R}^3)$ the current density. The conservation of charge is described by the conservation law

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0\ ,$$

and the Lorentz force on a particle with charge q is given by

$$\vec{F} = q\left(\vec{E} + \frac{1}{c}\,\vec{v} \times \vec{B}\right)\ .$$

[5] The source free Maxwell's equations are invariant under the Poincaré group, i.e., consistent with the theory of special relativity, where the speed of light sets a limit for the speed of propagation of any action. On the other hand, as we already know, quantum mechanics uses Newtonian ideas of space and time, where there is instantaneous propagation of any action, and hence inconsistent with the special theory of relativity. Therefore, the following incorporation of the effects of the electromagnetic field into quantum mechanics can be expected to be valid only if the expectation values of the speeds of the involved particles are small compared to the speed of light.

The classical Hamiltonian function H is given by

$$H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\,\vec{A}\right)^2 + q\,\phi = \frac{1}{2mc^2}\left(c\,\vec{p} - q\vec{A}\right)^2 + q\,\phi\ ,$$

where $\vec{A} \in C^2(\Omega, \mathbb{R}^3)$ and $\phi \in C^2(\Omega, \mathbb{R})$ are the vector and scalar potential, respectively, that are connected to the physical field $\vec{E}$, $\vec{B}$ by

$$\vec{E} = -\frac{1}{c}\,\frac{\partial \vec{A}}{\partial t} - \vec{\nabla}\phi\ ,\ \ \vec{B} = \vec{\nabla} \times \vec{A}\ . \tag{2.26}$$

If the Lorenz gauge condition

$$\frac{1}{c}\,\frac{\partial \phi}{\partial t} + \vec{\nabla}\cdot\vec{A} = 0\ , \tag{2.27}$$

and the inhomogeneous wave equations

$$\frac{1}{c^2}\,\frac{\partial^2 \phi}{\partial t} - \triangle\phi = 4\pi\rho\ ,\ \ \frac{1}{c^2}\,\frac{\partial^2 \vec{A}}{\partial t^2} - \triangle\vec{A} = \frac{4\pi}{c}\,\vec{j} \tag{2.28}$$

are satisfied, then the physical field $\vec{E}$, $\vec{B}$ defined by (2.26) satisfies Maxwell's equations (2.25). The physical field is left invariant by a (joint) gauge transformation of the potentials

$$\vec{A} \to \vec{A} + \vec{\nabla}\Lambda\ ,\ \ \phi \to \phi - \frac{1}{c}\,\frac{\partial\Lambda}{\partial t}\ ,$$

where $\Lambda \in C^3(\Omega, \mathbb{R})$. Under such a gauge transformation, H is mapped into

$$H_\Lambda = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\,\vec{\nabla}\Lambda - \frac{q}{c}\,\vec{A}\right)^2 + q\cdot\left(\phi - \frac{1}{c}\,\frac{\partial\Lambda}{\partial t}\right)\ .$$

In the following, we restrict attention to time-independent physical fields, i.e., $\Omega \subset \mathbb{R}^3$ is non-empty and open. Then,

$$H_\Lambda = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\,\vec{\nabla}\Lambda - \frac{q}{c}\,\vec{A}\right)^2 + q\phi\ .$$

Under quantization, the operators corresponding to H and H_Λ need to be unitarily equivalent. In the following, we assume that $q \neq 0$. A candidate for the Hamiltonian operator corresponding to H_Λ is given by the closure of

$$\hat{H}_{\Lambda 0} : C_0^2(\kappa\Omega, \mathbb{C}) \to L^2_{\mathbb{C}}(\kappa\Omega)\ ,$$

defined by[6]

[6] In the following, we are going to use the conventions that $(\vec{a}\cdot\nabla + b)g := \vec{a}\cdot\nabla g + b\cdot g$, $(\vec{a}\cdot\nabla + b)^0 g := g$, $(\vec{a}\cdot\nabla + b)^{m+1} g := (\vec{a}\cdot\nabla + b)(\vec{a}\cdot\nabla + b)^m g$ for every $m \in \mathbb{N}$, where $\vec{a} \in (C(U, \mathbb{C}))^n$, $b \in C(U, \mathbb{C})$, $g \in C^1(U, \mathbb{C})$ and U is a non-empty open subset of $\mathbb{R}^n$, $n \in \mathbb{N}^*$.

$$\begin{aligned}
\hat{H}_{\Lambda 0} f &:= \left\{ \frac{1}{2m} \sum_{k=1}^{3} \left[\frac{\hbar\kappa}{i} \frac{\partial}{\partial u_k} - \frac{q}{c} \Lambda_{,k}\left(\frac{1}{\kappa}\cdot\right) - \frac{q}{c} \vec{A}_k\left(\frac{1}{\kappa}\cdot\right) \right]^2 + q\,\phi\left(\frac{1}{\kappa}\cdot\right) \right\} f \\
&= \frac{(\hbar\kappa)^2}{2m} \left[\sum_{k=1}^{3} \left(\frac{1}{i} \frac{\partial}{\partial u_k} - \alpha \bar{\Lambda}_{,k} - \alpha \bar{\vec{A}}_k \right)^2 + \bar{\phi} \right] f \\
&= \frac{(\hbar\kappa)^2}{2m} \left\{ -\triangle f - \frac{\alpha}{i} \left[(\bar{\vec{A}} + \vec{\nabla}\bar{\Lambda}) \cdot \vec{\nabla} f + \vec{\nabla} \cdot [f\,(\bar{\vec{A}} + \vec{\nabla}\bar{\Lambda})] \right] \right. \\
&\qquad \left. + \left(\alpha^2 |\bar{\vec{A}} + \vec{\nabla}\bar{\Lambda}|^2 + \bar{\phi} \right) f \right\} , \\
&= \frac{(\hbar\kappa)^2}{2m} \left[-\triangle f - \frac{2\alpha}{i} (\bar{\vec{A}} + \vec{\nabla}\bar{\Lambda}) \cdot \vec{\nabla} f \right. \\
&\qquad \left. + \left(\alpha^2 |\bar{\vec{A}} + \vec{\nabla}\bar{\Lambda}\,|^2 - \frac{\alpha}{i} \vec{\nabla} \cdot (\bar{\vec{A}} + \vec{\nabla}\bar{\Lambda}) + \bar{\phi} \right) f \right] ,
\end{aligned}$$

for every $f \in C_0^2(\kappa\Omega, \mathbb{C})$, where $\Lambda_{,k} := (e_k \cdot \vec{\nabla})\Lambda$, $\bar{\Lambda}_{,k} := \frac{\partial \bar{\Lambda}}{\partial u_k}$, for every $k \in \{1, 2, 3\}$, and

$$\begin{aligned}
&\bar{\Lambda}(u) := \frac{1}{q} \Lambda\left(\frac{1}{\kappa} u\right) , \ \bar{\vec{A}}(u) := \frac{1}{\kappa q} \vec{A}\left(\frac{1}{\kappa} u\right) , \\
&\bar{\phi}(u) := \frac{2\,mq}{(\hbar\kappa)^2} \phi\left(\frac{1}{\kappa} u\right) , \ \alpha := \frac{q^2}{\hbar c} > 0 ,
\end{aligned}$$

for every $u \in \kappa\Omega$. Here $\bar{\vec{A}} \in C^2(\kappa\Omega, \mathbb{R})$, $\bar{\Lambda} \in C^3(\kappa\Omega, \mathbb{R})$, $\bar{\phi} \in C^2(\kappa\Omega, \mathbb{R})$ are dimensionless functions and α is dimensionless. In particular,

$$\hat{H}_{00} : C_0^2(\kappa\Omega, \mathbb{C}) \to L^2_{\mathbb{C}}(\kappa\Omega) ,$$

defined by

$$\begin{aligned}
\hat{H}_{00} f &:= \left\{ \frac{1}{2m} \sum_{k=1}^{3} \left[\frac{\hbar\kappa}{i} \frac{\partial}{\partial u_k} - \frac{q}{c} \vec{A}_k\left(\frac{1}{\kappa}\cdot\right) \right]^2 + q\,\phi\left(\frac{1}{\kappa}\cdot\right) \right\} f \\
&= \frac{(\hbar\kappa)^2}{2m} \left\{ \sum_{k=1}^{3} \left(\frac{1}{i} \frac{\partial}{\partial u_k} - \alpha \bar{\vec{A}}_k \right)^2 + \bar{\phi} \right] f \\
&= \frac{(\hbar\kappa)^2}{2m} \left\{ -\triangle f - \frac{\alpha}{i} \left[\bar{\vec{A}} \cdot \vec{\nabla} f + \vec{\nabla} \cdot (f \bar{\vec{A}}\,) \right] + \left(\alpha^2 |\bar{\vec{A}}\,|^2 + \bar{\phi} \right) f \right\} , \\
&= \frac{(\hbar\kappa)^2}{2m} \left[-\triangle f - \frac{2\alpha}{i} \bar{\vec{A}} \cdot \vec{\nabla} f + \left(\alpha^2 |\bar{\vec{A}}\,|^2 - \frac{\alpha}{i} \vec{\nabla} \cdot \bar{\vec{A}} + \bar{\phi} \right) f \right] ,
\end{aligned}$$

for every $f \in C_0^2(\kappa\Omega, \mathbb{C})$, is the candidate whose closure corresponds to H. Hence, $\hat{H}_{00}$ and $\hat{H}_{0\Lambda}$ are densely-defined, linear operators in $L^2_{\mathbb{C}}(\kappa\Omega)$. Further, it follows by partial integration that $\hat{H}_{00}$ and $\hat{H}_{0\Lambda}$ are symmetric as well as that

$$
\begin{aligned}
\left\langle f|\hat{H}_{0\Lambda} f\right\rangle &= \frac{(\hbar\kappa)^2}{2m}\left\{\left\langle f|\sum_{k=1}^{3}\left[\frac{1}{i}\frac{\partial}{\partial u_k} - \alpha\,(\bar{\vec{A}} + \vec{\nabla}\Lambda_k)\right]^2 f\right\rangle + \langle f|\bar{\phi} f\rangle\right\} \\
&= \frac{(\hbar\kappa)^2}{2m}\left\{\sum_{k=1}^{3}\left\langle f|\left[\frac{1}{i}\frac{\partial}{\partial u_k} - \alpha\,(\bar{\vec{A}} + \vec{\nabla}\Lambda_k)\right]^2 f\right\rangle + \langle f|\bar{\phi} f\rangle\right\} \\
&= \frac{(\hbar\kappa)^2}{2m}\left\{\sum_{k=1}^{3}\left\|\left[\frac{1}{i}\frac{\partial}{\partial u_k} - \alpha\,(\bar{\vec{A}} + \vec{\nabla}\Lambda_k)\right] f\right\|^2 + \langle f|\bar{\phi} f\rangle\right\} \geqslant \frac{(\hbar\kappa)^2}{2m}\,\langle f|\bar{\phi} f\rangle\ , \\
\left\langle f|\hat{H}_{00} f\right\rangle &\geqslant \frac{(\hbar\kappa)^2}{2m}\,\langle f|\bar{\phi} f\rangle\ ,
\end{aligned}
\tag{2.29}
$$

for every $f \in C_0^2(\kappa\Omega, \mathbb{C})$. The latter inequalities give lower bounds of the spectrum of $\hat{H}_{00}$ and $\hat{H}_{0\Lambda}$, see Corollary 12.5.5 in the Appendix. In addition, we arrive at the following result.

The operators $\hat{H}_{0\Lambda}$ and $\hat{H}_{00}$ are unitarily equivalent, i.e.,

$$
\hat{H}_{\Lambda 0} = T_{\exp(i\alpha\bar{\Lambda})}\,\hat{H}_{00}\,(T_{\exp(i\alpha\bar{\Lambda})})^{-1}\ .
$$

There is a one-to-one correspondence of self-adjoint extensions of the operators $\hat{H}_{00}$ and $\hat{H}_{\Lambda 0}$. Every self-adjoint extension of $\hat{H}_{\Lambda 0}$ is of the form

$$
T_{\exp(i\alpha\bar{\Lambda})}\,\hat{H}\,(T_{\exp(i\alpha\bar{\Lambda})})^{-1}\ ,
$$

where $\hat{H}$ is a self-adjoint extension of $\hat{H}_{00}$. Every self-adjoint extension of $\hat{H}_{00}$ is of the form

$$
T_{\exp(-i\alpha\bar{\Lambda})}\,\hat{H}_{\Lambda}\,(T_{\exp(-i\alpha\bar{\Lambda})})^{-1}\ ,
$$

where $\hat{H}_{\Lambda}$ is a self-adjoint extension of $\hat{H}_{\Lambda 0}$.

For the proof, we note that $T_{\exp(i\alpha\bar{\Lambda})}$ is a unitary linear operator on $L^2_{\mathbb{C}}(\kappa\Omega)$, with inverse $T_{\exp(-i\alpha\bar{\Lambda})}$, that maps $C_0^2(\kappa\Omega, \mathbb{C})$ onto itself. Further, for every $f \in C_0^2(\kappa\Omega, \mathbb{C})$, it follows that

$$
\begin{aligned}
& T_{\exp(i\alpha\bar{\Lambda})}\,\hat{H}_{00}\,T_{\exp(-i\alpha\bar{\Lambda})}\,f \\
&= T_{\exp(i\alpha\bar{\Lambda})}\,\frac{(\hbar\kappa)^2}{2m}\left[\sum_{k=1}^{3}\left(\frac{1}{i}\frac{\partial}{\partial u_k} - \alpha\bar{\vec{A}}_k\right)^2 + \bar{\phi}\right]\exp(-i\alpha\bar{\Lambda})\,f \\
&= \frac{(\hbar\kappa)^2}{2m}\left[\sum_{k=1}^{3}\exp(i\alpha\bar{\Lambda})\left(\frac{1}{i}\frac{\partial}{\partial u_k} - \alpha\bar{\vec{A}}_k\right)^2\exp(-i\alpha\bar{\Lambda}) + \bar{\phi}\right] f\,.
\end{aligned}
$$

Since for every $k \in \{1, 2, 3\}$

$$\begin{aligned}
&\exp\big(i\alpha\bar{\Lambda}\big)\left(\frac{1}{i}\,\frac{\partial}{\partial u_k} - \alpha\vec{\bar{A}}_k\right)^2 \exp\big(-i\alpha\bar{\Lambda}\big)\, f \\
&= \exp\big(i\alpha\bar{\Lambda}\big)\left(\frac{1}{i}\,\frac{\partial}{\partial u_k} - \alpha\vec{\bar{A}}_k\right)\exp\big(-i\alpha\bar{\Lambda}\big) \\
&\quad \cdot \exp\big(i\alpha\bar{\Lambda}\big)\left(\frac{1}{i}\,\frac{\partial}{\partial u_k} - \alpha\vec{\bar{A}}_k\right)\exp\big(-i\alpha\bar{\Lambda}\big)\, f \\
&= \left(\exp\big(i\alpha\bar{\Lambda}\big)\,\frac{1}{i}\,\frac{\partial}{\partial u_k}\exp\big(-i\alpha\bar{\Lambda}\big) - \alpha\vec{\bar{A}}_k\right) \\
&\quad \cdot \left(\exp\big(i\alpha\bar{\Lambda}\big)\,\frac{1}{i}\,\frac{\partial}{\partial u_k}\exp\big(-i\alpha\bar{\Lambda}\big) - \alpha\vec{\bar{A}}_k\right) f \\
&= \left(\frac{1}{i}\,\frac{\partial}{\partial u_k} - \alpha\,\frac{\partial\bar{\Lambda}}{\partial u_k} - \alpha\vec{\bar{A}}_k\right)\left(\frac{1}{i}\,\frac{\partial\bar{\Lambda}}{\partial u_k} - \alpha\,\frac{\partial\bar{\Lambda}}{\partial u_k} - \alpha\vec{\bar{A}}_k\right) f\ ,
\end{aligned}$$

this implies that

$$\begin{aligned}
&T_{\exp(i\alpha\bar{\Lambda})}\hat{H}_{00}T_{\exp(-i\alpha\bar{\Lambda})}f \\
&= \frac{(\hbar\kappa)^2}{2m}\left[\sum_{k=1}^{3}\left(\frac{1}{i}\,\frac{\partial}{\partial u_k} - \alpha\bar{\Lambda}_{,k} - \alpha\vec{\bar{A}}_k\right)^2 + \bar{\phi}\right] f = \hat{H}_{\Lambda 0} f\ .
\end{aligned}$$

In particular, if $\hat{H}_\Lambda$ is a self-adjoint extension of $\hat{H}_{\Lambda 0}$, then

$$T_{\exp(-i\alpha\bar{\Lambda})}\hat{H}_\Lambda T_{\exp(i\alpha\bar{\Lambda})}$$

is a self-adjoint extension of $\hat{H}_{\Lambda 0}$. Hence,

$$\hat{H}_\Lambda = T_{\exp(i\alpha\bar{\Lambda})}[\,T_{\exp(-i\alpha\bar{\Lambda})}\hat{H}_\Lambda T_{\exp(i\alpha\bar{\Lambda})}]\,T_{\exp(-i\alpha\bar{\Lambda})}\ .$$

Further, if $\hat{H}$ is a self-adjoint extension of $\hat{H}_0$, then

$$T_{\exp(i\alpha\bar{\Lambda})}\,\hat{H}\,(T_{\exp(i\alpha\bar{\Lambda})})^{-1}\ ,$$

is a self-adjoint extension of $\hat{H}_{\Lambda 0}$. Hence,

$$\hat{H} = T_{\exp(-i\alpha\bar{\Lambda})}\,[\,T_{\exp(i\alpha\bar{\Lambda})}\,\hat{H}\,(T_{\exp(i\alpha\bar{\Lambda})})^{-1}]\,T_{\exp(i\alpha\bar{\Lambda})}\ .$$

Simple Quantum Systems in 1 Space Dimension 3

3.1 Auxiliary Results About Perturbations of the Free Hamilton Operator in 1D

In Sect. 1.6, we studied perturbations of the free Hamiltonian in $n \in \mathbb{N}^*$ space dimensions. In the following, we state these results for 1 space dimension again and derive more detailed information about the domains of the involved operators.

In particular, we showed in Sect. 1.6 that the densely-defined, linear and symmetric operator

$$\hat{H}_{V0} : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$$

in $L^2_{\mathbb{C}}(\mathbb{R})$, defined by

$$\hat{H}_{V0} f := -\frac{\hbar^2 \kappa^2}{2m} f'' + Vf = \frac{\hbar^2 \kappa^2}{2m} \left(-f'' + \frac{2m}{\hbar^2 \kappa^2} Vf \right) ,$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, where $V \in L^2(\mathbb{R}) + L^\infty(\mathbb{R})$, is essentially self-adjoint. In addition,

$$\overline{\hat{H}_{V0}} = \hat{H} + T_V ,$$

where $\hat{H}$ is the free Hamiltonian from Sect. 1.4, and T_V denotes the maximal multiplication operator with V in $L^2_{\mathbb{C}}(\mathbb{R})$, and

$$D\left(\overline{\hat{H}_{V0}}\right) = D(\hat{H}) \subset C_\infty(\mathbb{R}, \mathbb{C}).$$

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_3.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_3

Also, we showed there that the essential spectrum $\sigma_e(\hat{H})$ of the free Hamiltonian $\hat{H}$ and the essential spectrum, $\sigma_e(\overline{\hat{H}_{V0}})$, of $\overline{\hat{H}_{V0}}$ coincide and are given by the interval $[0, \infty)$:

$$\sigma_e(\overline{\hat{H}_{V0}}) = \sigma_e(\hat{H}) = [0, \infty),$$

if V is such that there is a sequence $V_1, V_2, \ldots$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ satisfying

$$\lim_{\nu \to \infty} \|V_\nu - V\|_\infty = 0.$$

In the following, we are going to derive further information on $D(\hat{H})$. For this purpose, we recall from Sect. 1.4 that

$$A : C^2_0(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}), \tag{3.1}$$

defined for every $f \in C^2_0(\mathbb{R}, \mathbb{C})$ by

$$Af := -f'',$$

is a densely-defined, linear, positive symmetric and essentially self-adjoint operator in $L^2_{\mathbb{C}}(\mathbb{R})$, whose closure $\bar{A}$ has the spectrum $\sigma(\bar{A}) = [0, \infty)$, such that

$$\begin{aligned}(\bar{A}+1)^{-1} f = F_2^{-1}(1+|\ |^2)^{-1} F_2 f &= F_2\,(1+|\ |^2)^{-1} F_2^{-1} f \\ &= \frac{1}{(2\pi)^{1/2}}\, F_1\,(1+|\ |^2)^{-1} F_2^{-1} f \\ &= \frac{1}{(2\pi)^{1/2}}\, [F_2\,(1+|\ |^2)^{-1}] * f,\end{aligned} \tag{3.2}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$. Using,

$$F_1 \frac{1}{1+|\ |^2} = \pi\, e^{-|\ |},$$

which implies that

$$\frac{1}{(2\pi)^{1/2}} \frac{1}{1+|\ |^2} = F_2^{-1} \frac{1}{2}\, e^{-|\ |},$$

we arrive at a further representation of $(\bar{A}+1)^{-1}$

$$(\bar{A}+1)^{-1} f = \frac{1}{2}\, e^{-|\ |} * f,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$. Subsequently, we arrived at the following Sobolev inequality

$$\|f\|_\infty \leqslant c_1\, \|(\bar{A}+1) f\|_2 \leqslant c_1 \left(\|\bar{A} f\|_2 + \|f\|_2 \right), \tag{3.3}$$

for every $f \in D(\bar{A})$. In the following, we add to the analysis from Sect. 1.6. Since

$$(\bar{A}+1)^{-1}f = \frac{1}{(2\pi)^{1/2}}\, F_1\,(1+|\ |^2)^{-1}F_2^{-1}f\,,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$, see (3.2), and

$$\frac{1}{1+\mathrm{id}_{\mathbb{R}}^2}\,,\ \frac{\mathrm{id}_{\mathbb{R}}}{1+\mathrm{id}_{\mathbb{R}}^2} \in L^2_{\mathbb{C}}(\mathbb{R}),$$

it follows that

$$(\bar{A}+1)^{-1}f \in \{g \in C_\infty(\mathbb{R},\mathbb{C}) \cap C^1(\mathbb{R},\mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R}) : g' \in C_\infty(\mathbb{R},\mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})\},$$

where it is used that for every $f \in L^1_{\mathbb{C}}(\mathbb{R})$ such that $\mathrm{id}_{\mathbb{R}} \cdot f \in L^1_{\mathbb{C}}(\mathbb{R})$, it follows the differentiability of $F_1 f$ and that $(F_1 f)' = F_1(-i.\mathrm{id}_{\mathbb{R}} \cdot f)$. Hence, we arrive at the following result, concerning the regularity or "smoothness" of the members of the domain of $\bar{A}$.

$$D(\bar{A}) \subset \{f \in C^1(\mathbb{R},\mathbb{C}) \cap C_\infty(\mathbb{R},\mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R}) : f' \in C_\infty(\mathbb{R},\mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})\}.$$

Here it has been used that for every $f \in L^1_{\mathbb{C}}(\mathbb{R})$ such that $\mathrm{id}_{\mathbb{R}} \cdot f \in L^1_{\mathbb{C}}(\mathbb{R})$, it follows the differentiability of $F_1 f$ and that $(F_1 f)' = F_1(-i.\mathrm{id}_{\mathbb{R}} \cdot f)$. Further, we conclude that

$$\begin{aligned}
&\|((\bar{A}+1)^{-1}g)'\|_2 = \|\frac{1}{\sqrt{2\pi}}\,F_1\,(-i.\mathrm{id}_{\mathbb{R}})\frac{(F_2 g)\circ(-\mathrm{id}_{\mathbb{R}})}{1+\mathrm{id}_{\mathbb{R}}^2}\|_2 \\
&= \|F_2^{-1}\,(-i.\mathrm{id}_{\mathbb{R}})\frac{F_2 g}{1+\mathrm{id}_{\mathbb{R}}^2}\|_2 \leqslant \frac{1}{2}\|g\|_2 = \frac{1}{2}\|(\bar{A}+1)(\bar{A}+1)^{-1}g\|_2 \\
&\leqslant \frac{1}{2}\|\bar{A}\,(\bar{A}+1)^{-1}g\|_2 + \frac{1}{2}\|(\,\bar{A}+1)^{-1}g\|_2
\end{aligned}$$

as well as that

$$\begin{aligned}
&\|((\bar{A}+1)^{-1}g)'\|_\infty = \|\frac{1}{\sqrt{2\pi}}\,F_1\,(-i.\mathrm{id}_{\mathbb{R}})\frac{(F_2 g)\circ(-\mathrm{id}_{\mathbb{R}})}{1+\mathrm{id}_{\mathbb{R}}^2}\|_\infty \\
&\leqslant \frac{1}{\sqrt{2\pi}}\,\|\mathrm{id}_{\mathbb{R}}\,\frac{(F_2 g)\circ(-\mathrm{id}_{\mathbb{R}})}{1+\mathrm{id}_{\mathbb{R}}^2}\|_1 \leqslant \frac{1}{\sqrt{2\pi}}\,\|\frac{\mathrm{id}_{\mathbb{R}}}{1+\mathrm{id}_{\mathbb{R}}^2}\|_2 \cdot \|g\|_2 \\
&= \frac{1}{\sqrt{2\pi}}\,\|\frac{\mathrm{id}_{\mathbb{R}}}{1+\mathrm{id}_{\mathbb{R}}^2}\|_2 \cdot \|(\bar{A}+1)(\bar{A}+1)^{-1}g\|_2 \\
&\leqslant \frac{1}{\sqrt{2\pi}}\,\|\frac{\mathrm{id}_{\mathbb{R}}}{1+\mathrm{id}_{\mathbb{R}}^2}\|_2\left(\|\bar{A}\,(\bar{A}+1)^{-1}g\|_2 + \|(\,\bar{A}+1)^{-1}g\|_2\right)
\end{aligned}$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R})$, where Hoelder's inequality has been used, and finally the Sobolev inequalities

$$\|f'\|_2 \leqslant \frac{1}{2}\left(\|\bar{A}f\|_2 + \|f\|_2\right), \quad \|f'\|_\infty \leqslant c_2\left(\|\bar{A}\,f\|_2 + \|f\|_2\right), \tag{3.4}$$

for every $f \in D(\bar{A})$, where
$$c_2 := \frac{1}{(2\pi)^{1/2}}\,\|\frac{\mathrm{id}_{\mathbb{R}}}{1+\mathrm{id}_{\mathbb{R}}^2}\|_2.$$

We show an auxiliary result needed for the proof of Lemma 3.1.3 that is necessary to deal with perturbations of $\hat{H}$ by piecewise continuous potentials.

Lemma 3.1.1 *If $f \in C^1([0,\infty),\mathbb{C}) \cap L^1_{\mathbb{C}}((0,\infty))$ is such that $f' \in L^1_{\mathbb{C}}((0,\infty))$, then*

$$\lim_{x\to\infty} f(x) = 0, \;\; f(0) = -\int_0^\infty f'\,dv^1. \tag{3.5}$$

If $g \in C^1((-\infty,0],\mathbb{C}) \cap L^1_{\mathbb{C}}((-\infty,0))$ is such that $g' \in L^1_{\mathbb{C}}((-\infty,0))$, then

$$\lim_{x\to-\infty} g(x) = 0, \;\; g(0) = \int_{-\infty}^0 g'\,dv^1. \tag{3.6}$$

Proof For the proof, let such f, g be given, then

$$f(x) = f(0) + \int_0^x f'\,dv^1, \;\; g(y) = g(0) - \int_y^0 g'\,dv^1,$$

for $x > 0$ and $y < 0$. Hence, it follows the existence of

$$a_+ := \lim_{x\to\infty} f(x), \;\; a_- := \lim_{x\to-\infty} g(x).$$

If $a_+ \neq 0$, there is $x_0 > 0$ such that $|f(x)| \geqslant |a_+|/2$ for all $x \geqslant x_0$. Hence,

$$\int_0^x |f|\,dv^1 \geqslant \frac{|a_+|}{2}\,(x - x_0)$$

for every $x \in [x_0,\infty)$, which contradicts the existence of

$$\lim_{x\to\infty}\int_0^x |f|\,dv^1. \lightning$$

If $a_- \neq 0$, there is $x_0 < 0$ such that $|g(x)| \geqslant |a_-|/2$ for all $x \leqslant x_0$. Hence,

$$\int_x^0 |g|\,dv^1 \geqslant \frac{|a_-|}{2}\,(x_0 - x)$$

for every $x \in (-\infty, x_0]$, which contradicts the existence of

$$\lim_{x \to -\infty} \int_x^0 |g|\,dv^1 . \lightning$$

Hence, it follows the validity of (3.5) and (3.6). □

Lemma 3.1.2 (A core for $\bar{\mathbf{A}}$)

$$D := \{f \in C^2(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R}) : f', f'' \in L^2_{\mathbb{C}}(\mathbb{R})\}$$

is a core for $\bar{A}$. *In particular,*

$$\bar{A} f = -f'',$$

for every $f \in D$.

Proof For the proof, we define $A_0 : D \to X$ in $X := L^2_{\mathbb{C}}(\mathbb{R})$ by

$$A_0 f := -f'',$$

for every $f \in D$. The operator A_0 is densely-defined, since $C_0^\infty(\mathbb{R}, \mathbb{C}) \subset D$. Further, with the help of Lemma 3.1.1, it follows that

$$\begin{aligned}\langle f|A_0 g\rangle_2 &= -\int_{\mathbb{R}} f^* \cdot g''\,dv^1 = -\int_{\mathbb{R}} \left[(f^* \cdot g')' - f'^* g'\right] dv^1 = \int_{\mathbb{R}} f'^* g'\,dv^1 \\ &= \left(\int_{\mathbb{R}} g'^* f'\,dv^1\right)^* = \langle g|A_0 f\rangle_2^* = \langle A_0 f|g\rangle_2\end{aligned}$$

for all $f, g \in D$ and hence that A_0 is symmetric. Hence A_0 is a symmetric linear extension of A. Since, A is essentially self-adjoint, this implies that $\bar{A}_0 = \bar{A}$. □

The following Lemma provides the information needed for dealing with perturbations of $\hat{H}$ by piecewise continuous potentials.

Lemma 3.1.3 *The subspace D of $X := L^2_{\mathbb{C}}(\mathbb{R})$, defined by*

$$D := \{f \in C^1(\mathbb{R}, \mathbb{C}) \cap X : f' \in X,\ f \text{ is piecewise } C^2 \text{ such that } f'' \in X\},$$

is contained in $D(\bar{A})$, *and*

$$\bar{A}f = -f'',$$

for every $f \in D$.

Proof For $f \in D$, there is $n \in \mathbb{N}$ such that $n \geqslant 2$ and $a_1, \ldots, a_n \in \mathbb{R}$ satisfying $a_1 < \cdots < a_n$ as well as such that

$$f|_{(-\infty,a_1)} \in C^2((-\infty, a_1], \mathbb{C}), \ldots, f|_{(a_n,\infty)} \in C^2([a_n, \infty), \mathbb{C}).$$

In particular, it follows with the help of Lemma 3.1.1 and for $g \in D(A_0)$, where A_0 is defined as in the proof of Lemma 3.1.2, that

$$\begin{aligned}
\langle f|A_0 g\rangle_2 &= -\int_{\mathbb{R}} f^* g'' dv^1 \\
&= -\int_{(-\infty,a_1)} f^* g'' dv^1 - \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} f^* g'' dv^1 - \int_{(a_n,\infty)} f^* g'' dv^1 \\
&= \int_{(-\infty,a_1)} [\, f'^* g' - (f^* g')' \,] dv^1 + \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} [\, f'^* g' - (f^* g')' \,] dv^1 \\
&\quad + \int_{(a_n,\infty)} [\, f'^* g' - (f^* g')' \,] dv^1 \\
&= \int_{(-\infty,a_1)} f'^* g' dv^1 + \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} f'^* g' dv^1 + \int_{(a_n,\infty)} f'^* g' dv^1 \\
&\quad - f^*(a_1) g'(a_1) - \sum_{k=1}^{n-1} [f^*(a_{k+1}) g'(a_{k+1}) - f^*(a_k) g'(a_k)] \\
&\quad + f^*(a_n) g'(a_n) \\
&= \int_{(-\infty,a_1)} f'^* g' dv^1 + \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} f'^* g' dv^1 + \int_{(a_n,\infty)} f'^* g' dv^1 \\
&= \int_{(-\infty,a_1)} [\, (f'^* g)' - f''^* g \,] dv^1 + \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} [\, (f'^* g)' - f''^* g \,] dv^1 \\
&\quad + \int_{(a_n,\infty)} [\, (f'^* g)' - f''^* g \,] dv^1 \\
&= -\int_{(-\infty,a_1)} f''^* g dv^1 - \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} f''^* g dv^1 - \int_{(a_n,\infty)} f''^* dv^1
\end{aligned}$$

$$
\begin{aligned}
&+ f'^*(a_1)g(a_1) + \sum_{k=1}^{n-1}[f'^*(a_{k+1})g(a_{k+1}) - f'^*(a_k)g(a_k)] \\
&- f'^*(a_n)g(a_n) \\
= &- \int_{(-\infty,a_1)} f''^* g dv^1 - \sum_{k=1}^{n-1} \int_{(a_k,a_{k+1})} f''^* g dv^1 - \int_{(a_n,\infty)} f''^* dv^1 \\
= &\langle -f''|g\rangle_2 .
\end{aligned}
$$

As a consequence, $f \in D(A_0^*)$ and $A_0^* f = -f''$. Since

$$A_0^* = (A_0^*)^{**} = \bar{A}^* = \bar{A},$$

this implies that $f \in D(\bar{A})$ and $\bar{A} f = -f''$. □

3.2 Quantum Tunneling

We consider the densely-defined, linear and symmetric operator

$$\hat{H}_0 : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$$

in $L^2_{\mathbb{C}}(\mathbb{R})$, defined by[1]

$$\hat{H}_0 f := -\frac{\hbar^2\kappa^2}{2m} f'' + V_0 \left(\chi_{(-\infty,-1]} + \chi_{[1,\infty)}\right) f = \frac{\hbar^2\kappa^2}{2m} \left(-f'' + V f\right) ,$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, where $V_0 > 0$ has the dimension of an energy,

$$V := \alpha \left(\chi_{(-\infty,-1]} + \chi_{[1,\infty)}\right) ,$$

and

$$\alpha := \frac{2mV_0}{\hbar^2\kappa^2} > 0$$

is dimensionless. Since $V_0 \left(\chi_{(-\infty,-1]} + \chi_{[1,\infty)}\right) \in L^\infty(\mathbb{R})$, $\hat{H}_0$ is essentially self-adjoint (Figs. 3.1 and 3.2).

No physical potential exhibits such an abrupt or sudden change. In reality, a smoother change in potentials is to be expected. For example, free electrons in a metal experience a smooth change of potential near the metal surface. On the other hand, the use of this idealized potential simplifies the mathematical treatment, and its results are applicable to actual cases, as an indication of the physical situation.

---

[1] We note that $V_0 \left(\chi_{(-\infty,-1]} + \chi_{[1,\infty)}\right)$ coincides with the classical potential function only up to a scale factor. The classical potential function is given by $V_0 \left(\chi_{(-\infty,-\kappa^{-1}]} + \chi_{[\kappa^{-1},\infty)}\right)$.

Fig. 3.1 Graph of V

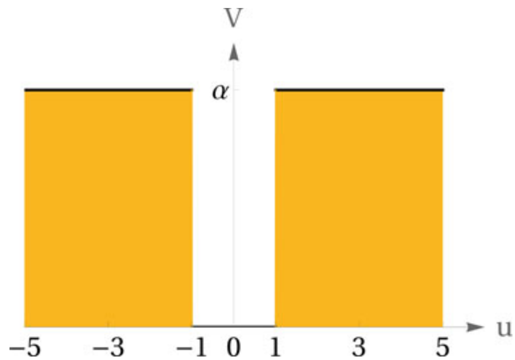
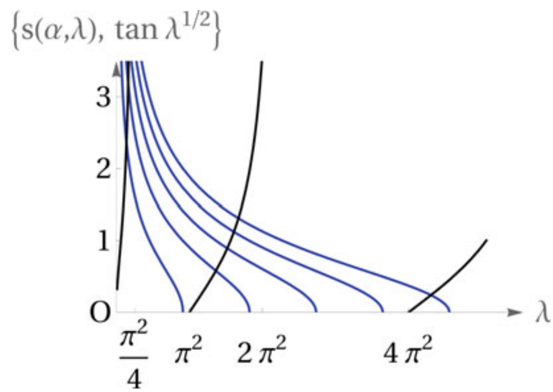


Fig. 3.2 Graphs of $s(9,\cdot), s(18,\cdot), s(27,\cdot), s(36,\cdot), s(45,\cdot)$, coming from the top (blue, left to right), where $s(\alpha,\lambda) := \sqrt{(\alpha/\lambda)-1}$ for every $\lambda > 0$, and the crossing graph of $([0,\infty) \to \mathbb{R}, \lambda \mapsto \tan(\sqrt{\lambda}))$ (black). The abscissas of the intersections are the eigenvalues of $\bar{A}_V$



In the following, we are going to determine the spectrum $\sigma(\hat{H})$ of the closure $\hat{H}$ of $\hat{H}_0$. In a first step, we note that

$$\sigma(\hat{H}) \subset [0, \infty),$$

as consequence of the positivity of the free Hamiltonian in 1-space dimension and the positivity of V. In this, we use Theorem 12.5.4 from the Appendix. In a second step, we note, see Sect. 3.1, that the essential spectrum $\sigma_e(\hat{H} - V_0)$ of $\hat{H} - V_0$ is given by

$$\sigma_e(\hat{H} - V_0) = [0, \infty).$$

As a consequence,

$$\sigma(\hat{H} - V_0) = [0, \infty) \cup \sigma_d(\hat{H} - V_0),$$

where $\sigma_d(\hat{H} - V_0)$ denotes the discrete spectrum of $\hat{H} - V_0$, consisting of isolated points in $\sigma(\hat{H} - V_0)$ that are eigenvalues of finite multiplicity. As a consequence,

$$\boxed{\sigma(\hat{H}) = [V_0, \infty) \cup \sigma_d(\hat{H})\ ,} \tag{3.7}$$

Table 3.1 Discrete eigenvalues λ of $\bar{A}_V$ and corresponding discrete eigenvalues ε of $\hat{H}$, for $\alpha =$ 9, 18, 27, 36 and 45

α	9	18	27	36	45
λ	1.369	1.606 13.455	1.729 14.990	1.808 15.887	1.865 16.500 42.515
$\varepsilon/V_0 = \lambda/\alpha$	0.152	0.089 0.747	0.064 0.555	0.050 0.441	0.041 0.367 0.945

where $\sigma_d(\hat{H})$ denotes the discrete spectrum of $\hat{H}$, which we are going to determine in the following. For this purpose, we use Lemma 3.1.3 from Sect. 3.1. For simplicity of notation, we apply the process to the closure $\bar{A}_V$ of the symmetric and essentially self-adjoint DLO $A_V : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$, given by

$$A_V f := -f'' + Vf \ ,$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$.[2] Hence,

$$\sigma(\bar{A}_V) = [\alpha, \infty) \cup \sigma_d(\bar{A}_V),$$

where $\sigma_d(\bar{A}_V)$ denotes the discrete spectrum of $\bar{A}_V$. For $\lambda \in [0, \alpha)$, it is straightforward to find a candidate for a corresponding eigenvector satisfying $f \in C^1(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$, $f' \in L^2_{\mathbb{C}}(\mathbb{R})$ and such that f is piecewise C^2 with $f'' \in L^2_{\mathbb{C}}(\mathbb{R})$. Such candidate is given by

$$f(u) = \begin{cases} e^{(1+u)\sqrt{\alpha-\lambda}} & \text{if } u \leqslant -1 \\ \cos\left[(1+u)\sqrt{\lambda}\right] + \frac{\sqrt{\alpha-\lambda}\,\sin\left[(1+u)\sqrt{\lambda}\right]}{\sqrt{\lambda}} & \text{if } -1 < u \leqslant 0 \\ \cos\left[(-1+u)\sqrt{\lambda}\right] - \frac{\sqrt{\alpha-\lambda}\,\sin\left[(-1+u)\sqrt{\lambda}\right]}{\sqrt{\lambda}} & \text{if } 0 < u \leqslant 1 \\ e^{(1-u)\sqrt{\alpha-\lambda}} & \text{if } u > 1 \end{cases}, \tag{3.8}$$

for every $u \in \mathbb{R}$, but $f \in C^1(\mathbb{R}, \mathbb{C})$ if and only if $\lambda > 0$ and

$$\tan(\sqrt{\lambda}) = \sqrt{\frac{\alpha}{\lambda} - 1}. \tag{3.9}$$

For every value of α, there is at least 1 corresponding eigenvalue of $\bar{A}_V$ in $[0, \alpha)$.

Rounded to 3 decimal places, we arrive to the Table 3.1 where the last line of the table gives the corresponding eigenvalues ε of $\hat{H}$. We note that the energies in $[0, V_0)$ are classically

[2] The operator $\hat{H}$ is a multiple of $\bar{A}_V$, $\hat{H} = \frac{\hbar^2\kappa^2}{2m}\,\bar{A}_V$.

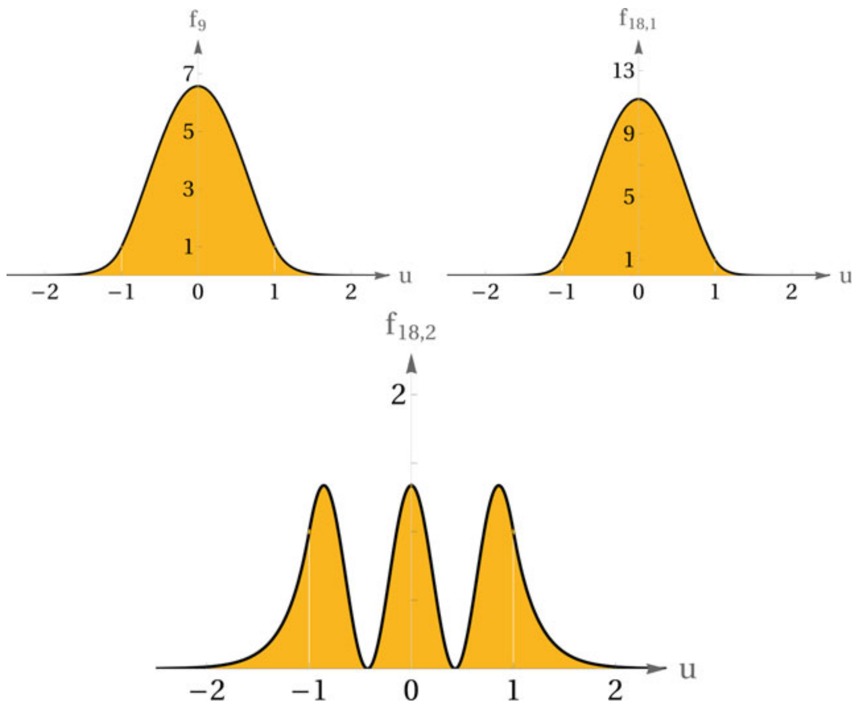


Fig. 3.3 Graph of the absolute squares of the "tunneling" eigenfunction corresponding to $\alpha = 9$ and the "tunneling" eigenfunctions corresponding to $\alpha = 18$

forbidden energies. Classical particles would be confined to the interval $[-1, 1]$. On the other hand, a "quantum particle" can penetrate or "tunnel through" the potential barrier, indicated by an exponential decay of the square of the eigenfunction beyond the ends of $[-1, 1]$ (Fig. 3.3).

Penetration of a potential barrier has no analog in classical mechanics. It has been observed in many situations, e.g., in trigonal pyramidal shaped molecule of ammonia, NH_3, with 3 hydrogen atoms situated on an equilateral triangle plane and the position of the nitrogen atom tunneling between 2 positions of lowest energy, in "field electron emission" from material surfaces under the influence of strong electric fields and the emission of α-particles, composite particles consisting of two protons and two neutrons, from nuclei by tunneling through the atomic shell (Fig. 3.4).

Still the question remains, whether all the discrete eigenfunctions of $\bar{A}_V$ are of the form (3.8). Indeed, this is the case. For the proof, we need to investigate the regularity or "smoothness" of the eigenfunctions of $\bar{A}_V$. If λ is an eigenvalue of $\bar{A}_V$ and $f \in D(\bar{A}_V)$ a corresponding eigenfunction, we note that $f \in D(\bar{A}_V)$ implies according to Sect. 3.1 that $f \in C^1(\mathbb{R}, \mathbb{C}) \cap C_\infty(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$ such that $f' \in C_\infty(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$, then

$$\lambda f = \bar{A}_V f = \bar{A} f + V f = (\bar{A} + 1) f + (V - 1) f,$$

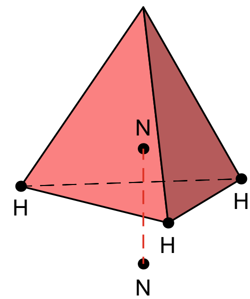


Fig. 3.4 Trigonal pyramidal shaped molecule of ammonia, with 2 positions of lowest energy of the Nitrogen atom, relative to the plane determined the hydrogen atoms

where $\bar{A}$ is the closure of the operator A, defined by (3.1) in Sect. 3.1, and hence

$$f(u) = [(\bar{A}+1)^{-1}(1+\lambda-V)f](u) = \frac{1}{2}\,[e^{-|\,|} * (1+\lambda-V)f](u)$$
$$= \frac{1}{2}\left[e^{-u}\int_{-\infty}^{u} e^{\bar{u}}\,[(1+\lambda-V)f](\bar{u})\,d\bar{u} + e^{u}\int_{u}^{\infty} e^{-\bar{u}}\,[(1+\lambda-V)f](\bar{u})\,d\bar{u}\right],$$

for every $u \in \mathbb{R}$. Therefore

$$f'(u)$$
$$= \frac{1}{2}\left[e^{u}\int_{u}^{\infty} e^{-\bar{u}}\,[(1+\lambda-V)f](\bar{u})\,d\bar{u} - e^{-u}\int_{-\infty}^{u} e^{\bar{u}}\,[(1+\lambda-V)f](\bar{u})\,d\bar{u}\right],$$

for every $u \in \mathbb{R}$, and

$$f''(u) = f(u) - [(1+\lambda-V)f](u),$$

for every $u \in \mathbb{R} \setminus \{-1, 1\}$. In particular, f is piecewise C^2, with possible jumps in the second derivative only in $\{-1, 1\}$, such that $f'' \in L^2_{\mathbb{C}}(\mathbb{R})$.

Finally, it might be asked, whether the non-vanishing of the potential $V_0\,(\chi_{(-\infty,-1]} + \chi_{[1,\infty)})$ at infinity is somehow responsible for the tunneling effect. It is easy to see that this is not the case, since the potential well $-V_0\,\chi_{(-1,1)}$ vanishes at infinity, the operators $\hat{H}$ and $\hat{H} - V_0$ share the same eigenvectors. If ε is a discrete eigenvalue of $\hat{H}$ and f a corresponding eigenvector, then $\varepsilon - V_0$ (< 0) is a discrete eigenvalue of $\hat{H} - V_0$ and f a corresponding eigenvector.

3.3 Potential Wells and Potential Barriers

We consider the densely-defined, linear and symmetric operator

$$\hat{H}_0 : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$$

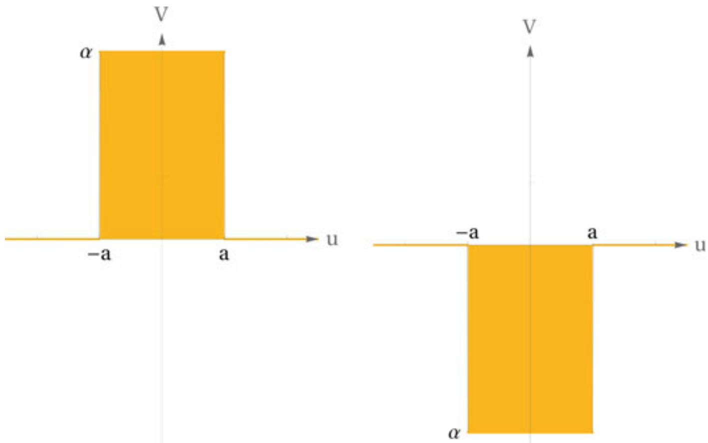


Fig. 3.5 Graph of V if $\alpha > 0$ and $\alpha < 0$, respectively

in $L^2_{\mathbb{C}}(\mathbb{R})$, defined by[3]

$$\hat{H}_0 f := -\frac{\hbar^2\kappa^2}{2m}\,f'' + V_0\,\chi_{[-a,a]} f = \frac{\hbar^2\kappa^2}{2m}\left(-f'' + Vf\right) ,$$

for every $f \in C^2_0(\mathbb{R},\mathbb{C})$, where $a > 0$ is dimensionless, $V_0 \in \mathbb{R}^*$ has the dimension of an energy,

$$V := \alpha\,\chi_{[-a,a]},$$

and

$$\alpha := \frac{2mV_0}{\hbar^2\kappa^2} \in \mathbb{R}^*$$

is dimensionless (Fig. 3.5).

Since $V_0\,\chi_{[-a,a]} \in L^\infty(\mathbb{R})$, $\hat{H}_0$ is essentially self-adjoint. In a second step, we note, see Sect. 3.1, that the essential spectrum $\sigma_e(\hat{H})$ of the closure $\hat{H}$ of $\hat{H}_0$ is given by

$$\sigma_e(\hat{H}) = [0,\infty).$$

As a consequence,

$$\sigma(\hat{H}) = [0,\infty) \,\dot\cup\, \sigma_d(\hat{H}),$$

where $\sigma_d(\hat{H})$ denotes the discrete spectrum of $\hat{H}$. Further, as a consequence of partial integration, see Lemma 1.2.1, and since $V_0\,\chi_{[-a,a]} \geqslant V_0$, $\hat{H}_0$ is semi-bounded from below with the lower bound V_0. Hence the closure $\hat{H}$ of $\hat{H}_0$ is semi-bounded from below with the lower bound V_0, too, implying that the spectrum $\sigma(\hat{H})$ of $\hat{H}$ satisfies

[3] We note that $V_0\,\chi_{[-a,a]}$ coincides with the classical potential function only up to a scale factor. The classical potential function is given by $V_0\,\chi_{[-\kappa^{-1}a,\kappa^{-1}a]}$.

$$\sigma(\hat{H}) \subset [V_0, \infty),$$

where we use Theorem 12.5.4 from the Appendix. Hence, we arrive at the following result.

The Spectrum $\sigma(\hat{H})$ of $\hat{H}$

☞ If $V_0 > 0$, then

$$\sigma(\hat{H}) = [0, \infty).$$

Further, the discrete spectrum $\sigma_d(\hat{H})$ of $\hat{H}$ is empty

$$\sigma_d(\hat{H}) = \phi.$$

☞ If $V_0 < 0$, then

$$\sigma(\hat{H}) = [0, \infty) \cup \sigma_d(\hat{H}),$$

and

$$\sigma_d(\hat{H}) \subset [V_0, 0).$$

In the following, we are going to calculate the resolvent of $\hat{H}$. For simplicity of notation, we apply the process to the closure $\bar{A}_V$ of the symmetric and essentially self-adjoint DLO $A_V : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$, given by

$$A_V f := -f'' + Vf \ ,$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$.[4] Hence, the spectrum $\sigma(\bar{A}_V)$ of $\bar{A}_V$ satisfies

$$\sigma(\bar{A}_V) = [0, \infty) \cup \sigma_d(\bar{A}_V), \ \ \sigma_d(\bar{A}_V) = \begin{cases} \phi & \text{if } \alpha > 0 \\ \subset [\alpha, 0) & \text{if } \alpha < 0 \end{cases},$$

where $\sigma_d(\bar{A}_V)$ denotes the discrete spectrum of $\bar{A}_V$.

For the construction of the resolvent for $\bar{A}_V$, let $\lambda \in \mathbb{C}\backslash[0, \infty)$. Also, for the case that $\alpha \leqslant \lambda < 0$, we define

$$\sqrt{\alpha - \lambda} := i\sqrt{\lambda - \alpha},$$

and in the following we understand implicitly the use of the holomorphic extension of $\sinh/\mathrm{id}_{\mathbb{C}}$ for the case that $\lambda = \alpha$. Then $f_{\lambda l} : \mathbb{R} \to \mathbb{C}$, where $f_{\lambda l}(u)$ is defined for every $u \in \mathbb{R}$ by

[4] The operator $\hat{H}$ is a multiple of $\bar{A}_V$, $\hat{H} = \frac{\hbar^2\kappa^2}{2m}\,\bar{A}_V$.

$$\begin{cases} e^{\sqrt{-\lambda}\,(u+a)} & \text{if } u \leqslant -a \\ \cosh\big[\sqrt{\alpha-\lambda}\,(u+a)\big] + \frac{\sqrt{-\lambda}\,\sinh\big[\sqrt{\alpha-\lambda}\,(u+a)\big]}{\sqrt{\alpha-\lambda}} & \text{if } u \in (-a,a] \\ [\cosh(2a\sqrt{\alpha-\lambda}\,) + \frac{\sqrt{-\lambda}\,\sinh(2a\sqrt{\alpha-\lambda}\,)}{\sqrt{\alpha-\lambda}}] & \\ \cdot\cosh\big[\sqrt{-\lambda}\,(u-a)\big] & \\ +[\sqrt{\alpha-\lambda}\,\sinh(2a\sqrt{\alpha-\lambda}\,) + \sqrt{-\lambda}\,\cosh(2a\sqrt{\alpha-\lambda}\,)] & \\ \cdot\frac{\sinh\big[\sqrt{-\lambda}\,(u-a)\big]}{\sqrt{-\lambda}} & \text{if } u > a\ , \end{cases}$$

is continuously differentiable, piecewise C^2 with bounded second order derivatives, such that

$$-f_{\lambda l}''(u) + (V-\lambda)f_{\lambda l}(u) = 0,$$

for every $u \in (-\infty,-a) \cup (-a,a) \cup (a,\infty)$ and square integrable close to $-\infty$. The same is true for $f_{\lambda r} : \mathbb{R} \to \mathbb{C}$, where $f_{\lambda r}(u) := f_{\lambda l}(-u)$ for every $u \in \mathbb{R}$, but instead being square integrable close to $-\infty$, $f_{\lambda r}$ is square integrable close to ∞. Further, the Wronski determinant of $f_{\lambda l}$ and $f_{\lambda r}$ is given by

$$\begin{aligned}
[W(f_{\lambda l}, f_{\lambda r})](u) &= f_{\lambda l}(u)\, f_{\lambda r}'(u) - f_{\lambda l}'(u)\, f_{\lambda r}(u) \\
&= -\left[2\sqrt{-\lambda}\cosh(2a\sqrt{\alpha-\lambda}\,) + \frac{\alpha-2\lambda}{\sqrt{\alpha-\lambda}}\,\sinh(2a\sqrt{\alpha-\lambda}\,)\right],
\end{aligned}$$

for every $u \in \mathbb{R}$. From Lemma 3.1.3 and since $\bar{A}_V$ has no non-real eigenvalues, it follows that

$$W(f_{\lambda l}, f_{\lambda r}) \neq 0,$$

for all non-real λ. Further, for non-real λ, $f_{\lambda l}$ satisfies an estimate of the form

$$|f_{\lambda l}(u)| \leqslant C\, e^{\mathrm{Re}(\sqrt{-\lambda}\,)\, u}, \tag{3.10}$$

for every $u \in \mathbb{R}$, were C is some positive number. As a consequence, $f_{\lambda r}$ satisfies the estimate

$$|f_{\lambda r}(u)| \leqslant C\, e^{-\,\mathrm{Re}(\sqrt{-\lambda}\,)\, u}, \tag{3.11}$$

for every $u \in \mathbb{R}$. We define the continuous function $G_\lambda : \mathbb{R}^2 \to \mathbb{C}$ by

$$G_\lambda(u,\bar{u}) = \frac{1}{[-W(f_{\lambda l}, f_{\lambda r})]} \begin{cases} f_{\lambda r}(u) f_{\lambda l}(\bar{u}) & \bar{u} \leqslant u \\ f_{\lambda l}(u) f_{\lambda r}(\bar{u}) & u < \bar{u} \end{cases},$$

for all $(u, \bar{u}) \in \mathbb{R}^2$. We note for $u \in \mathbb{R}$ that

$$\begin{aligned} \int_{-\infty}^{\infty} |G_\lambda(u,\bar{u})|\, d\bar{u} &= \int_{-\infty}^{u} |G_\lambda(u,\bar{u})|\, d\bar{u} + \int_{u}^{\infty} |G_\lambda(u,\bar{u})|\, d\bar{u} \\ &\leqslant \frac{C^2}{|W(f_{\lambda l}, f_{\lambda r})|} \Bigg[e^{-\operatorname{Re}(\sqrt{-\lambda})\, u} \int_{-\infty}^{u} e^{\operatorname{Re}(\sqrt{-\lambda})\, \bar{u}}\, d\bar{u} \\ &\qquad + e^{\operatorname{Re}(\sqrt{-\lambda})\, u} \int_{u}^{\infty} e^{-\operatorname{Re}(\sqrt{-\lambda})\, \bar{u}}\, d\bar{u} \Bigg] \\ &= \frac{2C^2}{|W(f_{\lambda l}, f_{\lambda r})|} \frac{1}{\operatorname{Re}(\sqrt{-\lambda})} \end{aligned}$$

and for $\bar{u} \in \mathbb{R}$ that

$$\begin{aligned} \int_{-\infty}^{\infty} |G_\lambda(u,\bar{u})|\, du &= \int_{-\infty}^{\bar{u}} |G_\lambda(u,\bar{u})|\, du + \int_{\bar{u}}^{\infty} |G_\lambda(u,\bar{u})|\, du \\ &\leqslant \frac{C^2}{|W(f_{\lambda l}, f_{\lambda r})|} \Bigg[e^{-\operatorname{Re}(\sqrt{-\lambda})\, \bar{u}} \int_{-\infty}^{\bar{u}} e^{\operatorname{Re}(\sqrt{-\lambda})\, u}\, du \\ &\qquad + e^{\operatorname{Re}(\sqrt{-\lambda})\, \bar{u}} \int_{\bar{u}}^{\infty} e^{-\operatorname{Re}(\sqrt{-\lambda})\, u}\, du \Bigg] \\ &= \frac{2C^2}{|W(f_{\lambda l}, f_{\lambda r})|} \frac{1}{\operatorname{Re}(\sqrt{-\lambda})}. \end{aligned}$$

Hence the function G_λ induces a bounded linear integral operator $\operatorname{Int}(G_\lambda)$ on $L^2_{\mathbb{C}}(\mathbb{R})$, with kernel function G_λ. In particular, the operator norm $\|\operatorname{Int}(G_\lambda)\|$ satisfies

$$\|\operatorname{Int}(G_\lambda)\| \leqslant \frac{2C^2}{|W(f_{\lambda l}, f_{\lambda r})|} \frac{1}{\operatorname{Re}(\sqrt{-\lambda})}.$$

Further for $h \in C_0(\mathbb{R}, \mathbb{C})$, the corresponding function $\bar{h} : \mathbb{R} \to \mathbb{C}$, defined by

$$\begin{aligned} \bar{h}(u) &:= [\operatorname{Int}(G_\lambda)h](u) \\ &= \frac{1}{[-W(f_{\lambda l}, f_{\lambda r})]} \left[f_{\lambda r}(u) \int_{-\infty}^{u} f_{\lambda l}(\bar{u}) h(\bar{u}) d\bar{u} + f_{\lambda l}(u) \int_{u}^{\infty} f_{\lambda r}(\bar{u}) h(\bar{u}) d\bar{u} \right], \end{aligned}$$

for every $u \in \mathbb{R}$, satisfies $\bar{h} \in C^1(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$, $\bar{h}' \in L^2_{\mathbb{C}}(\mathbb{R})$ and is piecewise C^2 with $\bar{h}'' \in L^2_{\mathbb{C}}(\mathbb{R})$. Further,

$$-\bar{h}'' + (V - \lambda)\,\bar{h} = h.$$

Hence according to Lemma 3.1.3, $\bar{h} \in D(\bar{A}_V)$ and

$$(\bar{A}_V - \lambda)\,\bar{h} = h.$$

The latter implies that, $(\bar{A}_V - \lambda)^{-1}h = \mathrm{Int}(G_\lambda)h$ and, since $C_0(\mathbb{R}, \mathbb{C})$ is dense in $L^2_{\mathbb{C}}(\mathbb{R})$ that

$$\boxed{(\bar{A}_V - \lambda)^{-1} = \mathrm{Int}(G_\lambda).}$$

3.3.1 Eigenvalues of $\hat{H}$ for $V_0 < 0$

In the following, we try to find eigenvalues λ of $\bar{A}_V$ in the half-open interval

$$[\alpha, 0).$$

Our main focus in the following is going to show that there is always such an eigenvalue, that the number of eigenvalues is finite and to give an estimate of the number of eigenvalues in terms of the parameters that are present in the potential.

For this purpose, we look for a non-trivial $f \in C^1(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$ such that

$$f|_{(-\infty,-a)} \in C^2((-\infty, -a], \mathbb{C}),\ \ f|_{(-a,a)} \in C^2([-a, a], \mathbb{C}),$$
$$f|_{(a,\infty)} \in C^2([a, \infty), \mathbb{C})$$

and such that

$$\begin{cases} -f''(u) - \lambda f(u) = 0 & \text{if } u < -a, \\ -f''(u) + (\alpha - \lambda) f(u) = 0 & \text{if } -a < u < a, \\ -f''(u) - \lambda f(u) = 0 & \text{if } a < u. \end{cases}$$

In the following, we define

$$\gamma_1 := \sqrt{-\lambda} > 0,\ \ \gamma_2 := \sqrt{\lambda - \alpha} \in [0, c_0),$$

where

$$c_0 := \sqrt{-\alpha} > 0\ .$$

We note that

$$\gamma_1^2 + \gamma_2^2 = -\lambda + \lambda - \alpha = -\alpha = c_0^2.$$

Then

$$f(u) = \begin{cases} A_1 e^{\gamma_1(u+a)} & \text{if } u < -a, \\ \sin[\gamma_2(u + a) + \beta] & \text{if } -a < u < a, \\ A_3 e^{-\gamma_1(u+a)} & \text{if } a < u, \end{cases} \tag{3.12}$$

where $A_1, A_3, \beta \in \mathbb{R}$[5] are such that

$$A_1 = \sin\beta, \;\; \gamma_1 A_1 = \gamma_2 \cos\beta,$$
$$\sin(2\gamma_2 a + \beta) = A_3 e^{-2\gamma_1 a}, \;\; \gamma_2 \cos(2\gamma_2 a + \beta) = -\gamma_1 A_3 e^{-2\gamma_1 a}.$$

Note that this implies that $\gamma_2 \neq 0$. The latter system is equivalent to the system

$$A_1 = \sin\beta, \;\; A_3 = \sin(2\gamma_2 a + \beta) e^{2\gamma_1 a},$$
$$\gamma_1 \sin\beta = \gamma_2 \cos\beta, \;\; \gamma_2 \cos(2\gamma_2 a + \beta) = -\gamma_1 \sin(2\gamma_2 a + \beta), \tag{3.13}$$

which itself is equivalent to the system

$$A_1 = \sin\beta, \;\; A_3 = \sin(2\gamma_2 a + \beta) e^{2\gamma_1 a},$$
$$0 = \frac{\gamma_2}{c_0}\cos\beta - \frac{\gamma_1}{c_0}\sin\beta = \sin\left[\arcsin\left(\frac{\gamma_2}{c_0}\right) - \beta\right],$$
$$0 = \frac{\gamma_2}{c_0}\cos(2\gamma_2 a + \beta) + \frac{\gamma_1}{c_0}\sin(2\gamma_2 a + \beta) = \sin\left[2\gamma_2 a + \beta + \arcsin\left(\frac{\gamma_2}{c_0}\right)\right],$$

where it has been used that

$$\cos x = \sqrt{1 - \sin^2 x}$$

for every $x \in [0, \pi/2]$. Also, we note that

$$\frac{\gamma_2}{c_0} \in (0, 1).$$

Hence (3.13) is equivalent to the system

$$A_1 = \sin\beta, \;\; A_3 = \sin(2\gamma_2 a + \beta) e^{2\gamma_1 a},$$
$$\beta = \arcsin\left(\frac{\gamma_2}{c_0}\right) + n_1\pi, \;\; \beta + 2\gamma_2 a = -\arcsin\left(\frac{\gamma_2}{c_0}\right) + n_2\pi,$$

where $n_1, n_2 \in \mathbb{Z}$, which itself is equivalent to the system

$$A_1 = \sin\beta, \;\; A_3 = \sin(2\gamma_2 a + \beta) e^{2\gamma_1 a},$$
$$\beta = \arcsin\left(\frac{\gamma_2}{c_0}\right) + n_1\pi, \;\; 2\gamma_2 a = (n_2 - n_1)\pi - 2\arcsin\left(\frac{\gamma_2}{c_0}\right),$$

where $n_1, n_2 \in \mathbb{Z}$. Hence there is a function f of the required type if and only if

$$2\gamma_2 a = n\pi - 2\arcsin\left(\frac{\gamma_2}{c_0}\right),$$

[5] Note that there is no loss of generality in considering only real-valued f. For complex-valued also the corresponding real and imaginary parts, $\mathrm{Re} f$ and $\mathrm{Im} f$, respectively, satisfy the requirements.

for some $n \in \mathbb{N}^*$. For $n \in \mathbb{N}^*$, we consider the auxiliary functions $h_1, h_2 : (0, c_0) \to \mathbb{R}$ defined by

$$h_1(\gamma_2) := 2a\gamma_2, \ \ h_2(\gamma_2) := n\pi - 2 \arcsin\left(\frac{\gamma_2}{c_0}\right),$$

for every $\gamma_2 \in (0, c_0)$. The function h_1 is strictly increasing, whereas h_2 is strictly decreasing. Hence there is at most one $\gamma_2 \in (0, c_0)$ such that $h_1(\gamma_2) = h_2(\gamma_2)$. Further,

$$\operatorname{Ran} h_1 = (0, 2ac_0), \ \ \operatorname{Ran} h_2 = \left(n\pi - 2 \arcsin\left(\frac{\gamma_2}{c_0}\right), \ n\pi\right)$$

and hence, taking into account that

$$n\pi - 2 \arcsin\left(\frac{\gamma_2}{c_0}\right) > 0,$$

$h_1(\gamma_2) = h_2(\gamma_2)$ for $\gamma_2 \in (0, c_0)$ if and only if

$$(n-1)\pi < 2ac_0,$$

As a consequence, if $N \in \mathbb{N}$ is the largest number satisfying

$$N < 1 + \frac{2a}{\pi}\sqrt{|\alpha|}$$

then there are precisely N values of $\lambda \in [\alpha, 0)$ for which there are corresponding f of the required type. Since N is the largest such element of $\mathbb{N}$, we conclude that $N \geqslant 1$, i.e., indicating that $\bar{A}_V$ always has an eigenvalue, and that

$$N - 1 < \frac{2a}{\pi}\sqrt{|\alpha|} \leqslant N.$$

Again, the question remains, whether all the discrete eigenfunctions of $\bar{A}_V$ are of the form (3.12). Indeed, this is the case. If λ is an eigenvalue of $\bar{A}_V$ and $f \in D(\bar{A}_V)$ a corresponding eigenfunction, we note that $f \in D(\bar{A}_V)$ implies according to Sect. 3.1 that $f \in C^1(\mathbb{R}, \mathbb{C}) \cap C_\infty(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$ such that $f' \in C_\infty(\mathbb{R}, \mathbb{C}) \cap L^2_{\mathbb{C}}(\mathbb{R})$. In addition, it follows as in Sect. 3.2 that f is in particular piecewise C^2, with possible jumps in the second derivative only in $\{-a, a\}$, such that $f'' \in L^2_{\mathbb{C}}(\mathbb{R})$.

Hence, we arrive at the following result.

The Eigenvalues of $\hat{H}$ in $(V_0, 0)$ if $V_0 < 0$

If $V_0 < 0$, then $(V_0, 0)$ contains at least 1 eigenvalue. Further, the number $N \in \mathbb{N}^*$ of eigenvalues in $(V_0, 0)$ satisfies

$$N - 1 < \frac{2a}{\pi}\sqrt{\frac{2m|V_0|}{\hbar^2\kappa^2}} \leqslant N.$$

Finally, V_0 is not an eigenvalue.[a]

[a] As said above, the length $\bar{a}$ corresponding to a in the classical potential is given by $\bar{a} = a\kappa^{-1}$. The introduction of $\bar{a}$ into this inequality, leads to the scale independent inequality

$$N - 1 < \frac{2\bar{a}}{\pi}\sqrt{\frac{2m|V_0|}{\hbar^2}} \leqslant N.$$

3.3.2 Motion in a "δ-Function" Potential

On first sight, the concept of a "δ-function" does not appear of any use for quantum theory.[6] A δ-function is supposed to have its support in 1-point. Now, every subset of $\mathbb{R}^n$, $n \in \mathbb{N}^*$, containing countably many points, is a set of Lebesgue measure 0. Hence, a δ-function on $\mathbb{R}^n$ is a.e. equal to the function of value 0 on $\mathbb{R}^n$, and the equivalence class in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ corresponding to the δ-function is given by 0-vector of that space. Therefore multiplication of an element of $L^2_{\mathbb{C}}(\mathbb{R}^n)$ by the δ-function can only lead to the 0-vector of that space, and the corresponding multiplication operator is the 0 operator on that space.

On the other hand, the δ-function has a proper definition in distribution theory, and in this context, the δ-distribution can be represented as a limit of functions (regular distributions). For instance, if $n = 1$, the δ-distribution and the negative δ-distribution are limits of the sequence of step functions

$$\left(\frac{1}{2\nu}\,\chi_{[-\nu,\nu]}\right)_{\nu\in\mathbb{N}^*} \quad \text{and} \quad \left(-\frac{1}{2\nu}\,\chi_{[-\nu,\nu]}\right)_{\nu\in\mathbb{N}^*},$$

respectively, for $\nu \to \infty$, where we note that the corresponding sequence of integrals over $\mathbb{R}$ is constant of value 1 and -1, respectively (Fig. 3.6).

Hence, it might be asked if the operators $\bar{A}_{V_a}$ for $a \to 0+$ approach in some sense a densely-defined, linear and self-adjoint operator $A_{\beta\delta}$ in $L^2_{\mathbb{C}}(\mathbb{R})$, where $\beta \in \mathbb{R}^*$ and

$$V_a := \frac{\beta}{2a}\,\chi_{[-a,a]},$$

[6] Operators in the resolvent of operators, induced by formal partial differential operators D, are usually integral operators. The corresponding kernel functions K can be interpreted as solutions of inhomogeneous PDE with a δ-distribution inhomogeneity. On the other hand, there are usually more direct ways for obtaining these kernel functions, without involving the theory of distributions.

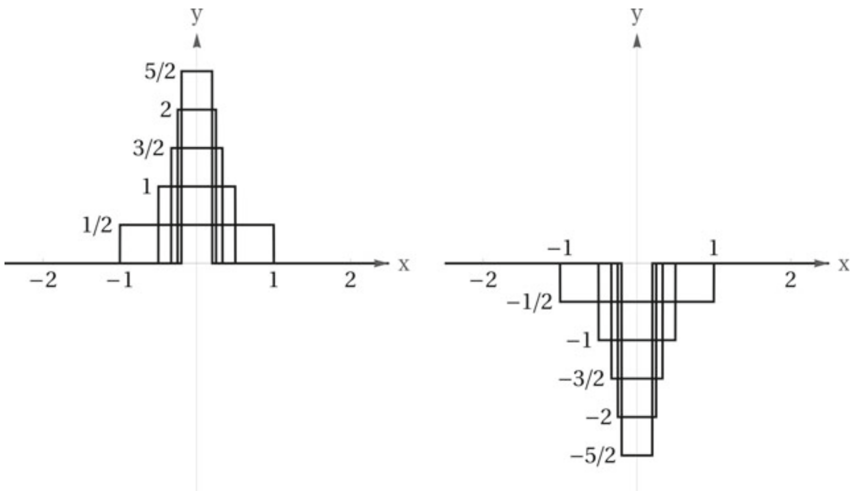


Fig. 3.6 Graphs of $\frac{1}{2\nu}\,\chi_{[-\nu,\nu]}$ and $-\frac{1}{2\nu}\,\chi_{[-\nu,\nu]}$ for $\nu = 1, \ldots, 5$

for every $a > 0$. Indeed, this is the case. This follows from the fact that for every non-real λ

$$\lim_{a\to 0+} (\bar{A}_{V_a} - \lambda)^{-1} f = \mathrm{Int}(K_\lambda) f ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$, where for every non-real λ as well as for every $\lambda < 0$ such that $2\sqrt{-\lambda} + \beta \neq 0$, $K_\lambda : \mathbb{R}^2 \to \mathbb{C}$ is the continuous function defined by

$$K_\lambda(u, \bar{u}) = \frac{1}{2\sqrt{-\lambda} + \beta} \begin{cases} \mathrm{f}_{\lambda r}(u)\, \mathrm{f}_{\lambda l}(\bar{u}) & \bar{u} \leqslant u \\ \mathrm{f}_{\lambda l}(u)\, \mathrm{f}_{\lambda r}(\bar{u}) & u < \bar{u} \end{cases} ,$$

the continuous functions $\mathrm{f}_{\lambda l} : \mathbb{R} \to \mathbb{C}$ and $\mathrm{f}_{\lambda r} : \mathbb{R} \to \mathbb{C}$ are defined by

$$\mathrm{f}_{\lambda l}(u) := e^{\sqrt{-\lambda}\,u} + \beta\, \chi_{(0,\infty)}(u)\, \frac{\sinh(\sqrt{-\lambda}\,u)}{\sqrt{-\lambda}},$$
$$\mathrm{f}_{\lambda r}(u) := e^{-\sqrt{-\lambda}\,u} - \beta\, \chi_{(-\infty,0)}(u)\, \frac{\sinh(\sqrt{-\lambda}\,u)}{\sqrt{-\lambda}},$$

for every $u \in \mathbb{R}$, as well as

$$
\begin{aligned}
&\mathrm{Int}(K_\lambda) f \\
&= \left(\begin{array}{c} \mathbb{R} \to \mathbb{C} \\ u \mapsto \frac{1}{2\sqrt{-\lambda}+\beta} \left[\mathsf{f}_{\lambda r}(u) \int_{-\infty}^{u} \mathsf{f}_{\lambda l}(\bar{u}) f(\bar{u})\, d\bar{u} + \mathsf{f}_{\lambda l}(u) \int_{u}^{\infty} \mathsf{f}_{\lambda r}(\bar{u}) f(\bar{u})\, d\bar{u} \right] \end{array} \right) \\
&= \left(\begin{array}{c} \mathbb{R} \to \mathbb{C} \\ t \mapsto \int_{\mathbb{R}} K_\lambda(\lambda, u, \bar{u}) f(\bar{u})\, d\bar{u} \end{array} \right),
\end{aligned}
$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$. The proof of this fact is left to the reader.

Exercise 5

For every non-real λ, show that

$$
\lim_{a \to 0+} (\bar{A}_{V_a} - \lambda)^{-1} f = \mathrm{Int}(K_\lambda) f,
$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$.

For later use in an equivalent definition of $A_{\beta\delta}$ in Sect. 3.3.2.1, we note that $\mathsf{f}_{\lambda l}, \mathsf{f}_{\lambda l}$ are continuous, C^2 on $(-\infty, 0)$ and $(0, \infty)$, with derivatives that have continuous extensions to the boundaries of these intervals. In addition, $\mathsf{f}_{\lambda l}|_{(-\infty,0)}, \mathsf{f}_{\lambda r}|_{(0,\infty)}$ and their derivatives are L^2. Further, they satisfy the characteristic jump condition

$$
\begin{aligned}
\lim_{u \to 0+} \mathsf{f}'_{\lambda l}(u) - \lim_{u \to 0-} \mathsf{f}'_{\lambda l}(u) &= \beta \lim_{u \to 0} \mathsf{f}_{\lambda l}(u), \\
\lim_{u \to 0+} \mathsf{f}'_{\lambda r}(u) - \lim_{u \to 0-} \mathsf{f}'_{\lambda r}(u) &= \beta \lim_{u \to 0} \mathsf{f}_{\lambda r}(u).
\end{aligned}
$$

Since, in analogy to the estimates (3.10), (3.11) for $f_{\lambda l}$ and $f_{\lambda r}$, $\mathsf{f}_{\lambda l}$ and $\mathsf{f}_{\lambda r}$, satisfy

$$
|\mathsf{f}_{\lambda l}(u)| \leqslant \left(1 + \frac{|\beta|}{|\sqrt{-\lambda}|}\right) e^{\mathrm{Re}(\lambda) u} \quad \text{and} \quad |\mathsf{f}_{\lambda r}(u)| \leqslant \left(1 + \frac{|\beta|}{|\sqrt{-\lambda}|}\right) e^{-\mathrm{Re}(\lambda) u},
$$

respectively, for every $u \in \mathbb{R}$, and hence the function K_λ induces a bounded linear integral operator $\mathrm{Int}(K_\lambda)$ on $L^2_{\mathbb{C}}(\mathbb{R})$, with kernel function K_λ. In particular, the operator norm $\|\mathrm{Int}(K_\lambda)\|$ satisfies

$$\|\mathrm{Int}(K_\lambda)\| \leqslant \frac{2\left(1+\frac{|\beta|}{|\sqrt{-\lambda}|}\right)^2}{|2\sqrt{-\lambda}+\beta|\,\mathrm{Re}(\sqrt{-\lambda}\,)}.$$

Further,

$$\begin{aligned}
&\mathsf{f}_{\lambda l}(u)\mathsf{f}'_{\lambda r}(u) - \mathsf{f}'_{\lambda l}(u)\mathsf{f}_{\lambda r}(u)\\
&= [e^{\sqrt{-\lambda}\,u} + \beta\,\chi_{(0,\infty)}(u)\,\frac{\sinh(\sqrt{-\lambda}\,u)}{\sqrt{-\lambda}}]\\
&\quad \cdot [-\sqrt{-\lambda}e^{-\sqrt{-\lambda}\,u} - \beta\,\chi_{(-\infty,0)}(u)\,\cosh(\sqrt{-\lambda}\,u)]\\
&\quad - [\sqrt{-\lambda}e^{\sqrt{-\lambda}\,u} + \beta\,\chi_{(0,\infty)}(u)\,\cosh(\sqrt{-\lambda}\,u)]\\
&\qquad \cdot [e^{-\sqrt{-\lambda}\,u} - \beta\,\chi_{(-\infty,0)}(u)\,\frac{\sinh(\sqrt{-\lambda}\,u)}{\sqrt{-\lambda}}]\\
&= -2\sqrt{-\lambda}\\
&\quad - \beta\,\chi_{(-\infty,0)}(u)e^{\sqrt{-\lambda}\,u}\cosh(\sqrt{-\lambda}\,u) + \beta\,\chi_{(-\infty,0)}(u)e^{\sqrt{-\lambda}\,u}\sinh(\sqrt{-\lambda}\,u)\\
&\quad - \beta\,\chi_{(0,\infty)}(u)e^{-\sqrt{-\lambda}\,u}\sinh(\sqrt{-\lambda}\,u) - \beta\,\chi_{(0,\infty)}(u)e^{-\sqrt{-\lambda}\,u}\cosh(\sqrt{-\lambda}\,u)\\
&= -2\sqrt{-\lambda} - \beta\,\chi_{(-\infty,0)}(u) - \beta\,\chi_{(0,\infty)}(u) = -(2\sqrt{-\lambda}+\beta) \neq 0,
\end{aligned}$$

for every $u \in \mathbb{R}^*$, and, for $f \in L^2_{\mathbb{C}}(\mathbb{R})$ and almost all $u \in \mathbb{R}$, that

$$\begin{aligned}
&[\mathrm{Int}(K_\lambda)f](u)\\
&= \frac{1}{2\sqrt{-\lambda}+\beta}\left[\mathsf{f}_{\lambda r}(u)\int_{-\infty}^{u}\mathsf{f}_{\lambda l}(\bar u)\,f(\bar u)\,d\bar u + \mathsf{f}_{\lambda l}(u)\int_{u}^{\infty}\mathsf{f}_{\lambda r}(\bar u)\,f(\bar u)\,d\bar u\right],\\
&[\mathrm{Int}(K_\lambda)f]'(u)\\
&= \frac{1}{2\sqrt{-\lambda}+\beta}\left[\mathsf{f}'_{\lambda r}(u)\int_{-\infty}^{u}\mathsf{f}_{\lambda l}(\bar u)\,f(\bar u)\,d\bar u + \mathsf{f}'_{\lambda l}(u)\int_{u}^{\infty}\mathsf{f}_{\lambda r}(\bar u)\,f(\bar u)\,d\bar u\right],\\
&[\mathrm{Int}(K_\lambda)f]''(u)\\
&= \frac{1}{2\sqrt{-\lambda}+\beta}\left[\mathsf{f}''_{\lambda r}(u)\int_{-\infty}^{u}\mathsf{f}_{\lambda l}(\bar u)\,f(\bar u)\,d\bar u + \mathsf{f}''_{\lambda l}(u)\int_{u}^{\infty}\mathsf{f}_{\lambda r}(\bar u)\,f(\bar u)\,d\bar u\right]\\
&\quad + \frac{1}{2\sqrt{-\lambda}+\beta}\,[\mathsf{f}_{\lambda l}(u)\mathsf{f}'_{\lambda r}(u) - \mathsf{f}'_{\lambda l}(u)\mathsf{f}_{\lambda r}(u)]\,f(u)\\
&= -\lambda\,[\mathrm{Int}(K_\lambda)f](u) - f(u).
\end{aligned}$$

Hence, for $f \in L^2_{\mathbb{C}}(\mathbb{R})$ and almost all $u \in \mathbb{R}$ (Fig. 3.7),

$$-[\mathrm{Int}(K_\lambda)f]''(u) - \lambda\,[\mathrm{Int}(K_\lambda)f](u) = f(u).$$

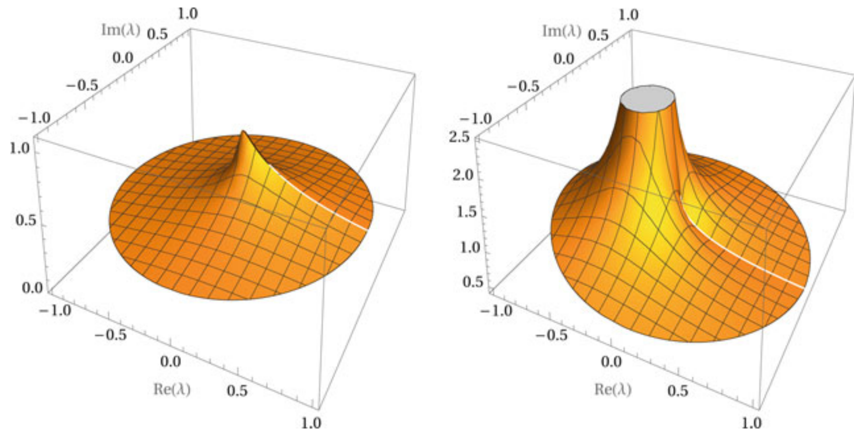


Fig. 3.7 Graphs of the continuous extension of $(\mathbb{C}\backslash\mathbb{R} \to \mathbb{R}, \lambda \mapsto (1/|2\sqrt{-\lambda} + \beta|)$, for the case of a delta function barrier $\beta = 1$ and the case of a delta function well $\beta = -1$. The former is everywhere continuous on $\mathbb{C}$, whereas the latter is continuous on $\mathbb{C}\backslash\{-1/4\}$ and singular at $\lambda = -1/4$

The latter implies that $\mathrm{Int}(K_\lambda)$ is injective and, since

$$[\mathrm{Int}(K_\lambda)]^* = \mathrm{Int}(K_{\lambda^*}),$$

it follows from Theorem 12.4.7 in the Appendix that

$$\{0\} = \ker\ \mathrm{Int}(K_{\lambda^*}) = \ker\,[\mathrm{Int}(K_\lambda)]^* = (\mathrm{Ran}\,\mathrm{Int}(K_\lambda))^\perp,$$

i.e., the range of $\mathrm{Int}(K_\lambda))$ is dense in $L^2_{\mathbb{C}}(\mathbb{R})$. Hence, it follows from Theorem VIII.22 of Vol. I of [60] that the operators $\bar{A}_{V_a}$ for $a \to 0+$ converge in the strong resolvent sense to a self-adjoint operator $A_{\beta\delta}$ in $L^2_{\mathbb{C}}(\mathbb{R})$. As a consequence, we obtain that

$$\boxed{(A_{\beta\delta} - \lambda)^{-1} = \mathrm{Int}(K_\lambda),}$$

for every non-real λ. In the following, if not stated otherwise, we assume that λ is non-real. After some calculation, we arrive at a representation $(A_{\beta\delta} - \lambda)^{-1}$ that connects the resolvent of $A_{\beta\delta}$ to the resolvent of the closure $\bar{A}$ of the negative second order derivative A, see (1.29)

$$\begin{aligned}(A_{\beta\delta} - \lambda)^{-1} f &= \frac{1}{2\sqrt{-\lambda} + \beta}\,[\,e^{-\sqrt{-\lambda}|\,|} * f\,] \\ &+ \frac{\beta}{2\sqrt{-\lambda}\,(2\sqrt{-\lambda} + \beta)}\Big\{\chi_{(0,\infty)} \cdot \big(e^{-\sqrt{-\lambda}|\,|} * [P_r f - (P_r f) \circ (-\mathrm{id}_{\mathbb{R}})]\big) \\ &\qquad + \chi_{(-\infty,0)} \cdot \big(e^{-\sqrt{-\lambda}|\,|} * [P_l f - (P_l f) \circ (-\mathrm{id}_{\mathbb{R}})]\big)\Big\},\end{aligned}$$

where

$$P_r f := \chi_{(0,\infty)} \cdot f, \quad P_l f := \chi_{(-\infty,0)} \cdot f.$$

Hence, for every non-real λ and $f \in L^2_{\mathbb{C}}(\mathbb{R})$, we have

$$\begin{aligned}(A_{\beta\delta} - \lambda)^{-1} f &= \frac{2\sqrt{-\lambda}}{2\sqrt{-\lambda} + \beta} (\bar{A} - \lambda)^{-1} f \\ &+ \frac{\beta}{2\sqrt{-\lambda} + \beta} \big\{ \chi_{(0,\infty)} \cdot (\bar{A} - \lambda)^{-1} [P_r f - (P_r f) \circ (-\mathrm{id}_{\mathbb{R}})] \\ &\quad + \chi_{(-\infty,0)} \cdot (\bar{A} - \lambda)^{-1} [P_l f - (P_l f) \circ (-\mathrm{id}_{\mathbb{R}})] \big\},\end{aligned} \tag{3.14}$$

where

$$P_r f := \chi_{(0,\infty)} \cdot f, \quad P_l f := \chi_{(-\infty,0)} \cdot f.$$

We note that the latter representation implies that the domain $D(A_{\beta\delta})$ of $A_{\beta\delta}$ and $D(\bar{A})$ of $\bar{A}$ differ because the domain of $A_{\beta\delta}$ contains functions that are not continuously differentiable in $u = 0$, whereas all elements in the domain of $\bar{A}$ are continuously differentiable, see Sect. 3.1.

In particular, $A_{\beta\delta}$ is not a relatively bounded perturbation of $\bar{A}$.

Further, it follows from (3.14) that

$$(A_{\beta\delta} - \lambda)^{-1} g = (\bar{A} - \lambda)^{-1} g, \tag{3.15}$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R})$ that is a.e. antisymmetric. If $f \in D(A)$ is antisymmetric, then $(A - \lambda) f$ is also antisymmetric. Hence, in this case $f \in D(A_{\beta\delta})$,

$$(A_{\beta\delta} - \lambda)^{-1} (\bar{A} - \lambda) f = f = (A_{\beta\delta} - \lambda)^{-1} (A_{\beta\delta} - \lambda) f,$$

and $A_{\beta\delta} f = \bar{A} f$.

If $f \in D(A)$ is antisymmetric, then $f \in D(A_{\beta\delta})$ and $A_{\beta\delta} f = Af$.

We note that this indicates a kind of semi-transparency of the δ-potential. From (3.15) and Corollary 12.9.11, it follows that the time-evolution generated by $A_{\beta\delta}$ coincides with the "free" time evolution generated by A, for data that are antisymmetric. In addition, from (3.15) it follows that $[0, \infty)$ is part of the spectrum $\sigma(A_{\beta\delta})$

$$\boxed{\sigma(A_{\beta\delta}) \supset [0, \infty).}$$

For the proof, let $\lambda \in [0, \infty)$, φ a non-trivial antisymmetric element of $C_0^2(\mathbb{R}, \mathbb{C})$. We define for $\nu \in \mathbb{N}^*$, $f_\nu^\pm \in C_0^2(\mathbb{R}, \mathbb{C})$ by

$$f_\nu^\pm(u) := \frac{1}{\|\varphi\|_2}\, \nu^{-1/2} \varphi(u/\nu)\, e^{\pm i\sqrt{\lambda} u},$$

for every $u \in \mathbb{R}$. It follows for $\nu \in \mathbb{N}^*$ that

$$\begin{aligned}
&\|f_\nu^\pm\|_2^2 = \frac{1}{\|\varphi\|_2^2}\, \nu^{-1} \int_{\mathbb{R}} |\varphi(u/\nu)|^2\, du = \frac{1}{\|\varphi\|_2^2} \int_{\mathbb{R}} |\varphi(u)|^2\, du = 1,\\
&(Af_\nu^\pm)(u)\\
&= \frac{1}{\|\varphi\|_2}\, \nu^{-1/2} \left[-\nu^{-2}\varphi''(u/\nu) \mp 2i\nu^{-1}\sqrt{\lambda}\,\varphi'(u/\nu) + \lambda\varphi(u/\nu)\right] e^{\pm i\sqrt{\lambda}u}\\
&= -\frac{1}{\|\varphi\|_2}\, \nu^{-3/2} \left[\nu^{-1}\varphi''(u/\nu) \pm 2i\sqrt{\lambda}\,\varphi'(u/\nu)\right] e^{\pm i\sqrt{\lambda}u} + \lambda f_\nu^\pm(u),
\end{aligned}$$

for every $u \in \mathbb{R}$. Hence,

$$\begin{aligned}
&\|(A - \lambda) f_\nu^\pm\|_2 \leqslant\\
&\frac{1}{\|\varphi\|_2}\, \nu^{-3/2} \left[\nu^{-1} \left(\int_{\mathbb{R}} |\varphi''(u/\nu)|^2 du\right)^{1/2} + 2\sqrt{\lambda} \left(\int_{\mathbb{R}} |\varphi'(u/\nu)|^2 du\right)^{1/2}\right]\\
&= \frac{1}{\|\varphi\|_2} \left(\nu^{-3/2}\|\varphi''\|_2 + 2\nu^{-1/2}\sqrt{\lambda}\,\|\varphi'\|_2\right).
\end{aligned}$$

As a consequence, $\|f_\nu^\pm\|_2 = 1$ for every $\nu \in \mathbb{N}^*$ and

$$\lim_{\nu \to \infty} \|(A - \lambda) f_\nu^\pm\|_2 = 0. \tag{3.16}$$

We note that f_ν^+ and f_ν^- are antisymmetric for $\lambda = 0$. For $\lambda \neq 0$ and $\nu \in \mathbb{N}^*$, it follows that $f_\nu^+ - f_\nu^-$ is antisymmetric and that

$$\begin{aligned}\|f_\nu^+ - f_\nu^-\|_2^2 &= \frac{4}{\|\varphi\|_2^2}\,\nu^{-1}\int_{\mathbb{R}} |\varphi(u/\nu)|^2\,\sin^2(\sqrt{\lambda}\,u)\,du \\ &= \frac{2}{\|\varphi\|_2^2}\,\nu^{-1}\int_{\mathbb{R}} |\varphi(u/\nu)|^2\,[1-\cos(2\sqrt{\lambda}\,u)]\,du \\ &= \frac{2}{\|\varphi\|_2^2}\int_{\mathbb{R}} |\varphi(u)|^2\,[1-\cos(2\sqrt{\lambda}\,\nu\,u)]\,du \\ &= \frac{2}{\|\varphi\|_2^2}\left[\|\varphi\|_2^2 - \int_{\mathbb{R}} \cos(2\sqrt{\lambda}\,\nu\,u)\cdot|\varphi(u)|^2\,du\right].\end{aligned}$$

Since, $|\varphi|^2 \in L^1_{\mathbb{C}}(\mathbb{R})$, it follows that

$$\lim_{\nu\to\infty}\int_{\mathbb{R}} \cos(2\sqrt{\lambda}\,\nu\,u)\cdot|\varphi(u)|^2\,du = 0$$

and hence that

$$\lim_{\nu\to\infty}\|f_\nu^+ - f_\nu^-\|_2 = \sqrt{2} > 0.$$

Therefore, we conclude from (3.16), the fact that

$$A_{\beta\delta}(f_\nu^+ - f_\nu^-) = A(f_\nu^+ - f_\nu^-),$$

for every $\nu \in \mathbb{N}^*$, and Theorem 12.5.3 that

$$[0,\infty) \subset \sigma(A_{\beta\delta}).$$

In the following, we are going to use the following convolution products. If $\mathrm{Re}(a) > 0$ and $\mathrm{Re}(b) > 0$, then

$$e^{-a|\,|} * e^{-b|\,|} = \begin{cases} \frac{2}{a^2-b^2}\left(ae^{-b|\,|} - be^{-a|\,|}\right) & \text{if } a \neq b \\ \frac{1}{a}\,(1+a|\,|)\,e^{-a|\,|} & \text{if } a = b \end{cases},$$

$$\begin{aligned}&\left\{e^{-a|\,|} * [(\chi_{(0,\infty)} - \chi_{(-\infty,0)})\cdot e^{-b|\,|}]\right\}(u) \\ &= \begin{cases} \frac{2a}{a^2-b^2}\left(e^{-b|u|} - e^{-a|u|}\right) & \text{if } a \neq b \text{ and } u > 0 \\ -\frac{2a}{a^2-b^2}\left(e^{-b|u|} - e^{-a|u|}\right) & \text{if } a \neq b \text{ and } u < 0 \\ |u|\,e^{-a|u|} & \text{if } a = b \text{ and } u > 0 \\ -|u|\,e^{-a|u|} & \text{if } a = b \text{ and } u < 0 \end{cases}.\end{aligned}$$

Hence, if $b \neq \sqrt{-\lambda}$, then

$$\begin{aligned}&(A_{\beta\delta} - \lambda)^{-1} e^{-b|\,|} \\ &= \frac{1}{(\beta + 2\sqrt{-\lambda}\,)(\lambda + b^2)}\,[(\beta + 2b)\,e^{-\sqrt{-\lambda}|\,|} - \left(\beta + 2\sqrt{-\lambda}\right)e^{-b|\,|}].\end{aligned}$$

In particular, if $\beta < 0$ and $b = |\beta|/2$, then

$$(A_{\beta\delta} - \lambda)^{-1} e^{-\frac{|\beta|}{2}|\,|} = -\frac{1}{\lambda + \frac{\beta^2}{4}} e^{-\frac{|\beta|}{2}|\,|},$$

i.e., $e^{-\frac{|\beta|}{2}|\,|}$ is an eigenvector of $(A_{\beta\delta} - \lambda)^{-1}$ to the eigenvalue $-(\lambda + \frac{\beta^2}{4})^{-1}$.

Therefore, if $\beta < 0$, then $e^{-\frac{|\beta|}{2}\cdot|\,|}$ is an eigenfunction of $A_{\beta\delta}$ to the eigenvalue $-\frac{\beta^2}{4}$. For the normalization of this eigenfunction, we note that (Fig. 3.8)

$$\|e^{-\frac{|\beta|}{2}|\,|}\|_2 = \left(\frac{2}{|\beta|}\right)^{1/2}.$$

3.3.2.1 An Equivalent Definition of $A_{\beta\delta}$

We observe for non-real λ as well as for every $\lambda < 0$ such that $2\sqrt{-\lambda} + \beta \neq 0$ and $g \in C_0(\mathbb{R}, \mathbb{C})$ that

$$\lim_{u \to 0} [\mathrm{Int}(K_\lambda)g](u) = \frac{1}{2\sqrt{-\lambda} + \beta} \left[\int_{-\infty}^{0} \mathsf{f}_{\lambda l}(\bar{u})\, g(\bar{u})\, d\bar{u} + \int_{0}^{\infty} \mathsf{f}_{\lambda r}(\bar{u})\, g(\bar{u})\, d\bar{u} \right],$$

$$\lim_{u \to 0-} [\mathrm{Int}(K_\lambda)g]'(u) =$$

$$\frac{1}{2\sqrt{-\lambda} + \beta} \left[-(\sqrt{-\lambda} + \beta) \int_{-\infty}^{0} \mathsf{f}_{\lambda l}(\bar{u})\, g(\bar{u})\, d\bar{u} + \sqrt{-\lambda} \int_{0}^{\infty} \mathsf{f}_{\lambda r}(\bar{u})\, g(\bar{u})\, d\bar{u} \right],$$

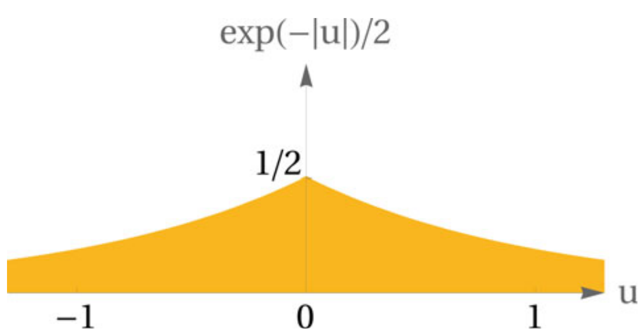


Fig. 3.8 Graph of the probability distribution corresponding to the normalized eigenfunction of $A_{\beta\delta}$ above, for the case $\beta = -1$

$$\lim_{u\to 0+}[\mathrm{Int}(K_\lambda)g]'(u) =$$
$$\frac{1}{2\sqrt{-\lambda}+\beta}\left[-\sqrt{-\lambda}\int_{-\infty}^{0}\mathsf{f}_{\lambda l}(\bar{u})\,g(\bar{u})\,d\bar{u}+(\sqrt{-\lambda}+\beta)\int_{0}^{\infty}\mathsf{f}_{\lambda r}(\bar{u})\,g(\bar{u})\,d\bar{u}\right],$$

and hence that

$$\lim_{u\to 0+}[\mathrm{Int}(K_\lambda)g]'(u)-\lim_{u\to 0-}[\mathrm{Int}(K_\lambda)g]'(u)=\beta\lim_{u\to 0}[\mathrm{Int}(K_\lambda)g](u).$$

This observation opens an equivalent more direct definition of $A_{\beta\delta}$. For this purpose, we define the linear subspace $D(A_{\beta\delta 0})$ of $L^2_{\mathbb{C}}(\mathbb{R})$ by

$$\begin{aligned}
D(A_{\beta\delta 0}) := \{f\in C(\mathbb{R},\mathbb{C}) :\ & \\
& f|_{(0,\infty)}\in C^2([0,\infty),\mathbb{C})\cap L^2_{\mathbb{C}}((0,\infty)) \\
& \wedge (f|_{(0,\infty)})',(f|_{(0,\infty)})''\in L^2_{\mathbb{C}}((0,\infty)) \\
& \wedge f|_{(-\infty,0)}\in C^2((-\infty,0],\mathbb{C})\cap L^2_{\mathbb{C}}((-\infty,0)) \\
& \wedge (f|_{(-\infty,0)})',(f|_{(-\infty,0)})''\in L^2_{\mathbb{C}}((-\infty,0)) \\
& \wedge \big[\lim_{u\to 0+}f'(u)\big]-\big[\lim_{u\to 0-}f'(u)\big]=\beta f(0)\ \}
\end{aligned}$$

and the linear map $A_{\beta\delta 0} : D(A_{\beta\delta 0})\to L^2_{\mathbb{C}}(\mathbb{R})$ by

$$A_{\beta\delta 0}f := -f'',$$

for every $f\in D(A_{\beta\delta 0})$. We note that $D(A_{\beta\delta 0})$ is dense in $L^2_{\mathbb{C}}(\mathbb{R})$, since containing the subspace

$$\{\hat{f_1}+\hat{f_2} : f_1\in C^2_0((-\infty,0),\mathbb{C})\wedge f_2\in C^2_0((0,\infty),\mathbb{C})\},$$

where the wedge symbol denotes the extension of a function to a function on $\mathbb{R}$, assuming the value 0 in the complement of the domain of the original function. The latter space is dense in $L^2_{\mathbb{C}}(\mathbb{R})$, since $C^2_0((-\infty,0),\mathbb{C})$ is dense in $L^2_{\mathbb{C}}((-\infty,0))$ and $C^2_0((0,\infty),\mathbb{C})$ is dense in $L^2_{\mathbb{C}}((0,\infty))$. Further, if $f,g\in D(A_{\beta\delta 0})$, then it follows from Lemma 3.1.1 that

$$\begin{aligned}
\langle f|A_{0\beta}g\rangle &= -\int_{-\infty}^{\infty}f^*(u)g''(u)\,du \qquad (3.17)\\
&= -\int_{-\infty}^{0}f^*(u)g''(u)\,du-\int_{0}^{\infty}f^*(u)g''(u)\,du \\
&= -\int_{-\infty}^{0}[\,(f^*g')'-f'^*g'\,](u)\,du-\int_{0}^{\infty}[\,(f^*g')'-f'^*g'\,](u)\,du \\
&= f^*(0)\cdot\left(\big[\lim_{u\to 0+}g'(u)\big]-\big[\lim_{u\to 0-}g'(u)\big]\right)+\int_{-\infty}^{\infty}f'^*(u)g'(u)\,du \\
&= \langle f'|g'\rangle+\beta f^*(0)g(0)=\big[\langle g'|f'\rangle+\beta g^*(0)f(0)\big]^*=\langle A_{0\beta}g|f\rangle\,.
\end{aligned}$$

Hence, $A_{\beta\delta 0}$ is a densely-defined, linear and symmetric operator in $L^2_{\mathbb{C}}(\mathbb{R})$. Further, for non-real λ as well as for every $\lambda < 0$ such that $2\sqrt{-\lambda} + \beta \neq 0$ and $g \in C_0(\mathbb{R}, \mathbb{C})$

$$\mathrm{Int}(K_\lambda)g \in D(A_{\beta\delta 0}), \tag{3.18}$$

and

$$(A_{\beta\delta 0} - \lambda)\mathrm{Int}(K_\lambda)g = g. \tag{3.19}$$

Hence, it follows from Theorem 12.4.9 that $A_{\beta\delta 0}$ is essentially self-adjoint. Further, for every non-real λ, $(\bar{A}_{\lambda\delta 0} - \lambda)^{-1}$ and $\mathrm{Int}(K_\lambda)$, where $\bar{A}_{\lambda\delta 0}$ denotes the closure of $A_{\beta\delta 0}$, coincide on a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R})$, and hence

$$(\bar{A}_{\beta\delta 0} - \lambda)^{-1} = \mathrm{Int}(K_\lambda).$$

The latter implies that

$$\bar{A}_{\beta\delta 0} = A_{\beta\delta}.$$

Also, for every $\lambda < 0$ such that $2\sqrt{-\lambda} + \beta \neq 0$, since (3.18) and (3.19) are true for every g from the dense subspace $C_0(\mathbb{R}, \mathbb{C})$, and since $\mathrm{Int}(K_\lambda) \in L(L^2_{\mathbb{C}}(\mathbb{R}), L^2_{\mathbb{C}}(\mathbb{R}))$, it follows from Lemma 12.4.8 that[7]

$$\sigma(A_{\beta\delta}) \cap \{\lambda < 0 : 2\sqrt{-\lambda} + \beta \neq 0\} = \phi,$$

and

$$(\bar{A}_{\beta\delta 0} - \lambda)^{-1} = \mathrm{Int}(K_\lambda),$$

for non-real λ as well as for every $\lambda < 0$ such that $2\sqrt{-\lambda} + \beta \neq 0$. Summarizing the information about $\sigma(A_{\beta\delta})$, we arrive at the following statements.

- ☞ If $\beta > 0$, then $\sigma(A_{\beta\delta}) = [0, \infty)$.
- ☞ If $\beta < 0$, then $\sigma(A_{\beta\delta}) = [0, \infty) \cup \{-\frac{\beta^2}{4}\}$.

The physical Hamilton operator $\hat{H}$ corresponding to $A_{\beta\delta}$ is given by

$$\hat{H} = \frac{\hbar^2 \kappa^2}{2m} A_{\beta\delta},$$

where

$$\beta = \frac{2m V_0}{\hbar^2 \kappa^2} \in \mathbb{R}^*$$

[7] We note for $\beta > 0$, the subsequent result can also be obtained from (3.17), since the latter implies that $A_{\beta\delta 0}$ is positive. Hence, it follows from Theorem 12.5.4 that $A_{\beta\delta}$ is positive and that $\sigma(A_{\beta\delta}) \subset [0, \infty)$.

and $V_0 \in \mathbb{R}^*$ has the dimension of an energy.[8] Hence the spectrum of $\sigma(\hat{H})$ of $\hat{H}$ is given by

☞ If $V_0 > 0$, then $\sigma(\hat{H}) = [0, \infty)$.
☞ If $V_0 < 0$, then $\sigma(\hat{H}) = [0, \infty) \cup \{-\frac{m}{2\hbar^2}(\kappa^{-1}V_0)^2\}$.

Exercise 6

Calculate the resonances of $\hat{H}$ for $V_0 > 0$, and use Remark 12.9.12 and contour integration to obtain an estimate for the corresponding time evolution operators.

3.4 Weyl's Limit Point/Limit Circle Criterion

Weyl's criterion is an appropriate tool for the determination of the deficiency indices

$$\dim\Big([\mathrm{Ran}(A+i)]^{\perp}\Big),\ \dim\Big([\mathrm{Ran}(A-i)]^{\perp}\Big),$$

of symmetric DLO's A that are induced by formal second order ordinary differential operators, called Sturm-Liouville operators. In these cases, the deficiency indices coincide and are both either equal to 0, 1 or 2, respectively. If the deficiency indices are both equal to 0, A is essentially self-adjoint. If the deficiency indices are both equal to $n \in \{1, 2\}$, to every element of the unitary group

$$U(n) := \{U \in \mathrm{GL}(n \times n, \mathbb{C}) : U^* = U^{-1}\}$$

in n dimensions there corresponds precisely 1 densely-defined, linear and self-adjoint extension of A. Such extensions of A corresponding to different elements of $U(n)$ are different.[9]

Definition 3.4.1 (*Weyl's Limit Point/Limit Circle Cases*) Let $a \in \mathbb{R} \cup \{-\infty\}$, $b \in \mathbb{R} \cup \{+\infty\}$ be such that $a < b$, $J := (a, b)$, $p \in C^1(J, \mathbb{R})$ such that $p > 0$ and $q \in C(J, \mathbb{R})$. Further, let $D^2_{p,q}$ be the ordinary linear differential operator, defined by

$$D^2_{p,q} := \Big(C^2(J, \mathbb{C}) \to C(J, \mathbb{C}),\ f \mapsto -\big(p \cdot f'\big)' + q \cdot f\Big). \tag{3.20}$$

---

[8] We note that the "potential" $V_0\,\delta$ present in $\hat{H}$ coincides with the classical potential function only up to a scale factor. The classical potential function is given by $\kappa^{-1}V_0\delta$. The latter "δ-function" has the dimension $1/\text{length}$.

[9] If A_1 and A_2 are (densely-defined, linear and) self-adjoint extensions of A corresponding to different elements of $U(n)$, then neither $A_2 \supset A_1$ nor $A_1 \supset A_2$. In this context, it needs to be remembered that DSLO's have no proper (densely-defined, linear and) symmetric extensions.

We say that

$$D^2_{p,q} \text{ is of } \left\{ \begin{array}{l} \text{limit point type at } a \text{ (at } b) \\ \text{limit circle type at } a \text{ (at } b) \end{array} \right\} ,$$

if there is $(c, z) \in J \times \mathbb{C}$

$$\left\{ \begin{array}{l} \text{and } f \in \ker(D^2_{p,q} - z) \text{ such that } \chi_{(a,c]} f \notin L^2_{\mathbb{C}}(J)\big(\chi_{[c,b)} f \notin L^2_{\mathbb{C}}(J)\big) \\ \text{such that } \chi_{(a,c]} f \in L^2_{\mathbb{C}}(J)\big(\chi_{[c,b)} f \in L^2_{\mathbb{C}}(J)\big) \text{ for all } f \in \ker(D^2_{p,q} - z) \end{array} \right\} .$$

We arrive at the following

Theorem 3.4.2 *Let a, b, J, p, q and $D^2_{p,q}$ as in Definition 3.4.1. In addition, we define the modified Wronskian determinant W for $D^2_{p,q}$ by*

$$W := \left(\left(C^1(J, \mathbb{C})\right)^2 \to C(J, \mathbb{C}), (u, v) \mapsto p \cdot \left(u\, v' - u' v\right) \right).$$

Then

(i) by

$$A_0 := \begin{pmatrix} C^2_0(J, \mathbb{C}) \to L^2_{\mathbb{C}}(J) \\ f \mapsto D^2_{p,q} f \end{pmatrix},$$

there is defined a densely-defined, linear and symmetric operator in $L^2_C(J)$,

(ii) for every $z \in \mathbb{C} \backslash (\mathbb{R} \times \{0\})$:

$$[\text{Ran}\,(A_0 - z)]^{\perp} = \left\{ v \in \ker\left(D^2_{p,q} - z^*\right) \cap L^2_{\mathbb{C}}(J) \right\},$$

(iii) the deficiency indices of A_0 are both equal to

$$\begin{cases} 0 & \text{if } D^2_{p,q} \text{ is of limit point type at } a \text{ and } b, \\ 1 & \text{if the types of } D^2_{p,q} \text{ differ at } a \text{ and } b, \\ 2 & \text{if } D^2_{p,q} \text{ is of limit circle type at } a \text{ and } b, \end{cases}$$

(iv) A_0 is essentially self-adjoint if and only if $D^2_{p,q}$ is of the limit point type at a and b. If this is the case, then

$$\begin{aligned} &(\bar{A}_0 - z)^{-1} f \\ &= \begin{pmatrix} J \to \mathbb{C} \\ t \mapsto -\left[u_2(t) \int_a^t u_1(\tau) f(\tau) d\tau + u_1(t) \int_t^b u_2(\tau) f(\tau) d\tau\right] \end{pmatrix} \\ &= \begin{pmatrix} J \to \mathbb{C} \\ t \mapsto \int_J G(t, \tau) f(\tau) d\tau \end{pmatrix}, \end{aligned} \tag{3.21}$$

for every $L^2_C(J)$*, where*

$$G(t,\tau) = \begin{cases} -u_2(t)u_1(\tau) & a < \tau < t \\ -u_1(t)u_2(\tau) & t < \tau < b \end{cases}$$

and u_1, u_2 *are existing elements of* $\ker\left(D^2_{p,q} - z\right)$ *satisfying* $W(u_1, u_2)(c) = 1, u_1\big|_{(a,c]} \in L^2_{\mathbb{C}}((a,c])$ *and* $u_2\big|_{[c,b)} \in L^2_{\mathbb{C}}([c,b))$*, for some* $c \in J$*.*

The proof will not be given here, see [42], [60] Vol. II.

3.4.1 The Free Hamiltonian in 1 Space Dimension, a Simple Application

According to Theorem 3.4.2, by

$$A_0 := \begin{pmatrix} C^2_0(\mathbb{R},\mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}) \\ f \mapsto -f'' \end{pmatrix},$$

there is defined a densely-defined, linear and symmetric operator in $L^2_{\mathbb{C}}(\mathbb{R})$. For $\lambda \in \mathbb{C} \setminus [0,\infty)$, the C^2-solutions of the differential equation

$$-f'' - \lambda f = -[f'' - (\sqrt{-\lambda})^2 f] = 0,$$

are given by the linear combinations of $f_1, f_2 \in C^2(\mathbb{R},\mathbb{C})$, defined by

$$f_l(u) := e^{\sqrt{-\lambda}\,u}, \;\; f_r(u) := e^{-\sqrt{-\lambda}\,u},$$

for every $u \in \mathbb{R}$, where $\sqrt{} : \mathbb{C}\setminus(-\infty,0] \to \mathbb{C}$ is the principal branch of the complex square root function. Since f_l is not L^2 in a neighborhood of $+\infty$ and f_r is not L^2 in a neighborhood of $-\infty$, A_0 is essentially self-adjoint.

The free Hamiltonian $\hat{H}$ in 1-space dimension is given by

$$\hat{H} := \varepsilon_0\,\bar{A}_0,$$

where $\bar{A}_0$ denotes the closure of A_0, and

$$\varepsilon_0 := \frac{\hbar^2\kappa^2}{2m}.$$

Further, the Wronski determinant of f_l and f_r is given by

$$\begin{aligned}[W(f_l, f_r)](u) &= f_l(u)\,f_r'(u) - f_l'(u) f_r(u) \\ &= -\sqrt{-\lambda}\,e^{\sqrt{\lambda}\,u}e^{-\sqrt{-\lambda}\,u} - \sqrt{-\lambda}\,e^{\sqrt{-\lambda}\,u}e^{-\sqrt{-\lambda}\,u} = -2\sqrt{-\lambda},\end{aligned}$$

for every $u \in \mathbb{R}$, and for every $\lambda \in \mathbb{C}\backslash\mathbb{R}$

$$
\begin{aligned}
&(\bar{A}_0 - \lambda)^{-1} f \\
&= \left(\begin{array}{c} \mathbb{R} \to \mathbb{C} \\ u \mapsto \frac{1}{2\sqrt{-\lambda}} \left[f_r(u) \int_{-\infty}^{u} f_l(\bar{u}) f(\bar{u})\, d\bar{u} + f_l(u) \int_u^{\infty} f_r(\bar{u}) f(\bar{u})\, d\bar{u} \right] \end{array} \right) \\
&= \left(\begin{array}{c} \mathbb{R} \to \mathbb{C} \\ t \mapsto \int_{\mathbb{R}} G(\lambda, u, \bar{u}) f(\bar{u})\, d\bar{u} \end{array} \right),
\end{aligned}
$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$, where

$$
\begin{aligned}
G(\lambda, u, \bar{u}) &= \frac{1}{2\sqrt{-\lambda}} \begin{cases} f_r(u) f_l(\bar{u}) & \bar{u} < u \\ f_l(u) f_r(\bar{u}) & u < \bar{u} \end{cases} \\
&= \frac{1}{2\sqrt{-\lambda}} \begin{cases} e^{-\sqrt{-\lambda}\, u} e^{\sqrt{-\lambda}\, \bar{u}} & \bar{u} < u \\ e^{\sqrt{-\lambda}\, u} e^{-\sqrt{-\lambda}\, \bar{u}} & u < \bar{u} \end{cases} = \frac{e^{-\sqrt{-\lambda}\, |u - \bar{u}|}}{2\sqrt{-\lambda}},
\end{aligned}
$$

for all $u, \bar{u} \in \mathbb{R}$.

Hence for $\lambda \in \mathbb{C}\backslash\mathbb{R}$ and $f \in L^2_{\mathbb{C}}(\mathbb{R})$,

$$
\begin{aligned}
&[(\bar{A}_0 - \lambda)^{-1} f](u) \\
&= \frac{1}{2\sqrt{-\lambda}} \left[e^{-\sqrt{-\lambda}\, u} \int_{-\infty}^{u} e^{\sqrt{-\lambda}\, \bar{u}} f(\bar{u})\, d\bar{u} + e^{\sqrt{-\lambda}\, u} \int_u^{\infty} e^{-\sqrt{-\lambda}\, \bar{u}} f(\bar{u})\, d\bar{u} \right] \\
&= \left(\frac{e^{-\sqrt{-\lambda}\, |\,|}}{2\sqrt{-\lambda}} * f \right)(u),
\end{aligned} \tag{3.22}
$$

for almost all $u \in \mathbb{R}$.

3.5 Further Results About the Hamilton Operator of the Harmonic Oscillator

The harmonic oscillator has already been studied in detail in [7]. There, we defined the Hamiltonian $\hat{H}$ of the system by an explicitly given self-adjoint extension of the densely-defined, linear and symmetric operator $\hat{H}_0$, given by

$$
\hat{H}_0 f = \hbar\omega \left(-f'' + \frac{1}{4} u^2 f \right),
$$

for every $f \in D_0$, where u denotes the identical function on $\mathbb{R}$ and the Schwartz space D_0 is defined by

$$D_0 := \{f \in C^\infty(\mathbb{R}, \mathbb{C}) \cap X : f^{(n)} \in X \wedge u^n f \in X \ , \ \text{for every } n \in \mathbb{N}^*\},$$

where $X := L^2_{\mathbb{C}}(\mathbb{R})$. In the following, we are going to show that $\hat{H}_0$ is indeed essentially self-adjoint. More generally, we have the following result.

> The operator $\hat{H}_0$ and the densely-defined, linear and symmetric operator $\mathcal{H}_0 : C^2_0(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$ in $L^2_{\mathbb{C}}(\mathbb{R})$, defined by
>
> $$\mathcal{H}_0 f := \hbar\omega \left(-f'' + \frac{1}{4}\, u^2 f\right),$$
>
> for every $f \in C^2_0(\mathbb{R}, \mathbb{C})$, are essentially self-adjoint and
>
> $$\hat{H} = \bar{\hat{H}}_0 = \bar{\mathcal{H}}_0.$$

According to Weyl's limit point criterion, for the proof that the densely-defined, linear and symmetric operator in $L^2_{\mathbb{C}}(\mathbb{R})$, $\mathcal{H}_0$, is essentially self-adjoint, it is sufficient to show that the ordinary linear differential operator $D_{1_{\mathbb{R}}, u^2/4}$, defined by (3.20), where $J = \mathbb{R}$, $1_{\mathbb{R}}$ denotes the constant function of value 1 on $\mathbb{R}$ and u denotes the identical function on $\mathbb{R}$, is of limit point type at $\pm\infty$. For this purpose, we investigate the solutions $f \in C^2(\mathbb{R}, \mathbb{C})$ of the ordinary differential equation

$$-f'' + \left(\frac{1}{2} + \frac{u^2}{4}\right) f = 0.$$

The latter differential equation has the solution $f \in C^2(\mathbb{R}, \mathbb{C})$, defined by

$$f(u) := e^{u^2/4},$$

for every $u \in \mathbb{R}$, which is neither L^2 at $-\infty$ nor L^2 at ∞. Hence, $D_{1_{\mathbb{R}}, u^2/4}$ is of limit point type at $\pm\infty$.

For the proof that the closure of $\mathcal{H}_0$ coincides with $\hat{H}$, we note that it follows from the results of Sects. 1.2 and 1.4 that the closure of the densely-defined, linear and symmetric operator $\mathcal{H}_{00} : C^\infty_0(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$ in $L^2_{\mathbb{C}}(\mathbb{R})$, defined by

$$\mathcal{H}_{00} f := \hbar\omega \left(-f'' + \frac{1}{4}\, u^2 f\right),$$

for every $f \in C_0^\infty(\mathbb{R}, \mathbb{C})$, is an extension of $\hat{H}_0$ as well as that the closure of $\mathcal{H}_{00}$ is an extension of $\mathcal{H}_0$. As a consequence,

$$\bar{\mathcal{H}}_{00} \supset \hat{H}_0 \supset \mathcal{H}_0, \ \ \bar{\mathcal{H}}_{00} \supset \mathcal{H}_0,$$

implying that

$$\bar{\mathcal{H}}_{00} \supset \bar{\hat{H}}_0 \supset \bar{\mathcal{H}}_0, \ \ \bar{\mathcal{H}}_{00} \supset \bar{\mathcal{H}}_0.$$

Since $\bar{\mathcal{H}}_0$ is in particular self-adjoint, we conclude that $\bar{\mathcal{H}}_{00} = \bar{\mathcal{H}}_0$ as well as that $\hat{H}_0$ is in particular essentially self-adjoint with $\bar{\hat{H}}_0 = \bar{\mathcal{H}}_0$. Finally, since $\hat{H}$ is a self-adjoint extension of $\hat{H}_0$, it follows that $\hat{H}$ is a self-adjoint extension of $\bar{\hat{H}}_0$ and hence that $\hat{H} = \bar{\mathcal{H}}_0$.

3.6 Motion in a Repulsive Pöschl–Teller Potential and Resonances

We define the Hamiltonian of the system as the closure of the densely-defined, linear operator in $L^2_{\mathbb{C}}(\mathbb{R})$, $\hat{H}_0 : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$, defined by

$$\hat{H}_0 f := -\frac{\hbar^2 \kappa^2}{2m} f'' + V\left(\frac{u}{\kappa}\right) f = \frac{\hbar^2 \kappa^2}{2m} \left[-f'' + \frac{U_0}{\cosh^2(u)} f \right], \tag{3.23}$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, where u denotes the identical function on $\mathbb{R}$, the classical potential V is the Pöschl–Teller potential [58], defined by

$$V(q) := \frac{V_0}{\cosh^2(\kappa q)},$$

for every $q \in \mathbb{R}$, and

$$U_0 := \frac{2m V_0}{\hbar^2 \kappa^2}$$

is dimensionless. Here $V_0 > 0$ and $\kappa^{-1} > 0$ are the maximal value and the "width" of V, respectively. Since $U_0 \cosh^{-2}(u) \in L^\infty(\mathbb{R})$, it follows from the Rellich-Kato theorem, Theorem 1.6.1, that $A_0 : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$, defined by

$$A_0 f := -f'' + \frac{U_0}{\cosh^2} f, \tag{3.24}$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, is a densely-defined, linear, symmetric and essentially self-adjoint operator in $X := L^2_{\mathbb{C}}(\mathbb{R})$. Further, as a consequence of partial integration, see Lemma 1.2.1, and the positivity of $U_0 \cdot \cosh^{-2}$, A_0 is positive. Hence the closure A of A_0 is positive, too, implying that the spectrum $\sigma(A)$ of A satisfies

$$\sigma(A) \subset [0, \infty),$$

where we use Theorem 12.5.4 from the Appendix. In a further step, we note, see Sect. 3.1, that the essential spectrum $\sigma_e(A)$ is given by

$$\sigma_e(A) = [0, \infty).$$

Hence, we conclude that

$$\sigma(A) = [0, \infty)$$

and therefore also that the discrete spectrum of A, consisting of isolated points in $\sigma(A)$ that are eigenvalues of finite multiplicity, is empty. The same applies to the spectrum $\sigma(\hat{H})$ of $\hat{H}$, in particular,

$$\boxed{\sigma(\hat{H}) = [0, \infty),}$$

where $\hat{H}$ denotes the closure of $\hat{H}_0$.

3.6.1 Calculation of the Resolvent and the Resonances of A

In the next step, we are going to calculate the resolvent of A, using the results of Sect. 3.4. For this purpose, we introduce the linear differential operator

$$D_{1_{\mathbb{R}}, U_0 \cosh^{-2}} := \left(C^2(\mathbb{R}, \mathbb{C}) \to C(\mathbb{R}, \mathbb{C}), f \mapsto -f'' + \frac{U_0}{\cosh^2} \cdot f \right),$$

where $1_{\mathbb{R}}$ denotes the constant function of value 1 on $\mathbb{R}$ and consider the solutions of the ordinary differential equation

$$\left(D_{1_{\mathbb{R}}, U_0 \cosh^{-2}} + \mu^2 \right) f = \left[D_{1_{\mathbb{R}}, U_0 \cosh^{-2}} - (-\mu^2) \right] f = 0, \tag{3.25}$$

where $\mu \in \mathbb{C}$. We note that the map $pr := (\mathbb{C} \to \mathbb{C}, \mu \mapsto -\mu^2)$ is a covering of $\mathbb{C}$ with branch point 0. For every $\lambda \in \mathbb{C}^*$, the fiber $pr^{-1}(\lambda)$ over λ contains exactly 2 elements, whereas $pr^{-1}(0) = \{0\}$. Moreover, pr maps the open right half-plane, $(0, \infty) \times \mathbb{R}$, biholomorphically onto the slized plane $\mathbb{C} \setminus [0, \infty)$ (Fig. 3.9).

Further, if $g \in C^2(\mathbb{R}, \mathbb{C})$ is a solution of the hypergeometric differential equation

$$v(1-v)g'' + (1 + \mu - 2v)\, g' - U_0 g = 0,$$

where v denotes the identical function on $\mathbb{R}$, then $f \in C^2(\mathbb{R}, \mathbb{C})$, defined by

$$f(u) := e^{\mu u} g\left(\frac{1}{1 + e^{-2u}} \right),$$

for every $u \in \mathbb{R}$, is a solution of (3.25). Hence $f_l, f_r \in C^2(\mathbb{R}, \mathbb{C})$, defined by

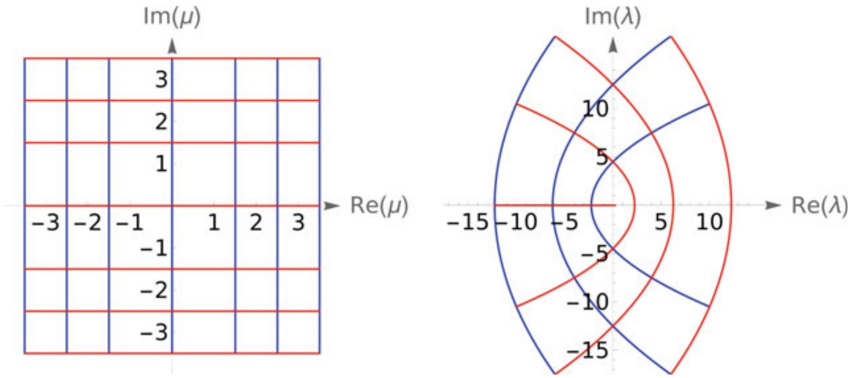


Fig. 3.9 Grid lines inside the covering space and corresponding projections onto the base ("spectral") space under pr

$$
\begin{aligned}
f_l(u) &:= e^{\mu u} \cdot \bar{F}\left(\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, 1 + \mu, \frac{1}{1 + e^{-2u}}\right), \\
&= [2\cosh(u)]^{-\mu}\, \bar{F}\left(\frac{1}{2} - \alpha + \mu, \frac{1}{2} + \alpha + \mu, 1 + \mu, \frac{1}{1 + e^{-2u}}\right), \\
f_r(u) &:= f_l(-u) = e^{-\mu u} \cdot \bar{F}\left(\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, 1 + \mu, \frac{1}{1 + e^{2u}}\right) \\
&= e^{-\mu u} \cdot \bar{F}\left(\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, 1 + \mu, 1 - \frac{1}{1 + e^{-2u}}\right),
\end{aligned}
$$

for every $u \in \mathbb{R}$, where [56] (15.8.1) has been used, and where

$$
\alpha := \begin{cases} \sqrt{\frac{1}{4} - U_0} & \text{for } U_0 \leqslant \frac{1}{4} \\ i\sqrt{U_0 - \frac{1}{4}} & \text{for } U_0 > \frac{1}{4} \end{cases},
$$

are solutions (3.25). Here $\bar{F} : \mathbb{C}^3 \times U_1(0) \to \mathbb{C}$ is the holomorphic extension of the function

$$
\left(\mathbb{C}^2 \times (\mathbb{C} \setminus (-\mathbb{N})) \times U_1(0) \to \mathbb{C}, (a, b, c, z) \mapsto F(a, b, c, z)/\Gamma(c)\right),
$$

where the hypergeometric function (Gauss series) F and the Gamma function Γ are defined according to [1] and $1/\Gamma$ denotes the extension of $(\mathbb{C} \setminus (-\mathbb{N}) \to \mathbb{C}, c \mapsto 1/\Gamma(c))$ to an entire analytic function. In particular, if $\mu = -n$, for $n \in \mathbb{N}^*$, then according to [56] (15.2.3.5)

$$
\begin{aligned}
f_l(u) &= e^{-nu} \cdot \bar{F}\left(\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, 1 - n, \frac{1}{1 + e^{-2u}}\right) \\
&= \frac{(\frac{1}{2} - \alpha)_n (\frac{1}{2} + \alpha)_n}{2^n\, n!\, \cosh^n(u)}\, F\left(\frac{1}{2} - \alpha + n, \frac{1}{2} + \alpha + n, n + 1, \frac{1}{1 + e^{-2u}}\right),
\end{aligned}
$$

for every $u \in \mathbb{R}$.

> We note that for $\mu \in (0, \infty) \times \mathbb{R}$, f_l is L^2 at $-\infty$ and f_r is L^2 at ∞. In particular, via Weyl's limit point / limit circle criterion, this fact provides another independent proof that A_0 is essentially self-adjoint.

In a first step towards the calculation of the resolvent of A, we are going to calculate the Wronski determinant $W(f_l, f_r)$ of f_l and f_r. For this purpose, we introduce the parameters

$$a := \frac{1}{2} - \alpha, \;\; b := \frac{1}{2} + \alpha = 1 - a, \;\; c := 1 + \mu. \tag{3.26}$$

According to (15.8.4) of [56], if $z \in U_1(0) \setminus (-1, 0]$, then

$$\begin{aligned}
&\frac{\sin(\pi(c-a-b))}{\pi}\, \bar{F}(a, b, c, z) \\
&= \frac{1}{\Gamma(c-a)\Gamma(c-b)}\, \bar{F}(a, b, a+b-c+1, 1-z) \\
&\quad - \frac{(1-z)^{c-a-b}}{\Gamma(a)\Gamma(b)}\, \bar{F}(c-a, c-b, c-a-b+1, 1-z).
\end{aligned}$$

As a consequence, it follows that

$$\begin{aligned}
&\frac{\sin(\pi(c-a-b))}{\pi}\, \bar{F}(a, b, c, 1-z) \\
&= \frac{1}{\Gamma(c-a)\Gamma(c-b)}\, \bar{F}(a, b, a+b-c+1, z) \\
&\quad - \frac{z^{c-a-b}}{\Gamma(a)\Gamma(b)}\, \bar{F}(c-a, c-b, c-a-b+1, z) \\
&= \frac{1}{\Gamma(c-a)\Gamma(c-b)}\, \bar{F}(a, b, a+b-c+1, z) \\
&\quad - \frac{1}{\Gamma(a)\Gamma(b)}\, z^{c-a-b}(1-z)^{1-c}\bar{F}(1-b, 1-a, c-a-b+1, z),
\end{aligned}$$

where we used (15.8.1) of [56]. Hence if $c - (a+b) = \mu \notin \mathbb{Z}$, then

$$\begin{aligned}
&\bar{F}(a, b, c, 1-z) \\
&= \frac{\pi/\sin(\pi(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\, \bar{F}(a, b, a+b-c+1, z) \\
&\quad - \frac{\pi/\sin(\pi(c-a-b))}{\Gamma(a)\Gamma(b)}\, z^{c-a-b}(1-z)^{1-c}\bar{F}(1-b, 1-a, c-a-b+1, z).
\end{aligned}$$

In particular, since

$$a + b = 1, \ \ c \notin \mathbb{Z},$$

we have

$$\begin{aligned} & z^{1-c}\,(1-z)^{c-a-b}\bar{F}(a,b,c,1-z) \\ &= -\frac{\pi/\sin(\pi c)}{\Gamma(c-a)\Gamma(c-b)}\,z^{1-c}\,(1-z)^{c-a-b}\,\bar{F}(1-a,1-b,2-c,z) \\ &\quad + \frac{\pi/\sin(\pi c)}{\Gamma(a)\Gamma(b)}\,\bar{F}(a,b,c,z). \end{aligned}$$

According to (15.10.2), (15.10.3) and (15.8.1) of [56], since none of the numbers c and $c-(a+b)$ is an integer, and if $a-b=-2\alpha$ is no integer, the latter only excludes the case that $U_0 = 1/4$, then g_1, g_2 defined by

$$\begin{aligned} g_1(z) &= \bar{F}(a,b,c,z), \\ g_2(z) &= z^{1-c}\bar{F}(a-c+1,b-c+1,2-c,z) \\ &= z^{1-c}\,(1-z)^{c-a-b}\bar{F}(1-a,1-b,2-c,z), \end{aligned}$$

for every $z \in U_1(0) \setminus (-1,0]$, satisfy the hypergeometric differential equation

$$z\,(1-z)g_j''(z) + [c-(a+b+1)z]g_j'(z) - ab g_j(z) = 0,$$

$j \in \{1,2\}$, as well as

$$\begin{aligned} & [W(g_1,g_2)](z) = g_1(z)g_2'(z) - g_1'(z)g_2(z) \\ &= \frac{1-c}{\Gamma(c)\Gamma(2-c)}\,z^{-c}\,(1-z)^{c-a-b-1} = \frac{\sin(\pi c)}{\pi}\,z^{-c}\,(1-z)^{c-a-b-1}, \end{aligned}$$

for every $z \in U_1(0) \setminus (-1,0]$. Hence,

$$[W(g_1,g_3)](z) = -\frac{1}{\Gamma(c-a)\Gamma(c-b)}\,z^{-c}\,(1-z)^{c-a-b-1},$$

where

$$g_3(z) := z^{1-c}\,(1-z)^{c-a-b}\bar{F}(a,b,c,1-z),$$

for every $z \in U_1(0) \setminus (-1,0]$. We note that since $a+b=1$

$$
\begin{aligned}
f_2(u) &:= e^{(c-1)u} g_3\left(\frac{1}{1+e^{-2u}}\right)\\
&= e^{(c-1)u}\left(\frac{1}{1+e^{-2u}}\right)^{1-c}\left(1-\frac{1}{1+e^{-2u}}\right)^{c-1}\bar{F}\left(a,b,c,1-\frac{1}{1+e^{-2u}}\right)\\
&= e^{(c-1)u}\left(\frac{1}{1+e^{-2u}}\right)^{1-c}\left(\frac{e^{-2u}}{1+e^{-2u}}\right)^{c-1}\bar{F}\left(a,b,c,1-\frac{1}{1+e^{-2u}}\right)\\
&= e^{(c-1)u}e^{-2(c-1)u}\bar{F}\left(a,b,c,1-\frac{1}{1+e^{-2u}}\right)\\
&= e^{-(c-1)u}\bar{F}\left(a,b,c,1-\frac{1}{1+e^{-2u}}\right) = f_r(u),
\end{aligned}
$$

for every $u \in \mathbb{R}$. Also, defining $f_1 : \mathbb{R} \to \mathbb{C}$ by

$$
f_1(u) := e^{(c-1)u} g_1\left(\frac{1}{1+e^{-2u}}\right) = f_l(u),
$$

for every $u \in \mathbb{R}$, it follows that

$$
\begin{aligned}
[W(f_1, f_2)](u) &= f_1(u) f_2'(u) - f_1'(u) f_2(u)\\
&= 2\,\frac{e^{2cu}}{(1+e^{2u})^2}\,[W(g_1,g_3)]\left(\frac{1}{1+e^{-2u}}\right)\\
&= -\frac{2}{\Gamma(c-a)\Gamma(c-b)}\,\frac{e^{2cu}}{(1+e^{2u})^2}\left(\frac{1}{1+e^{-2u}}\right)^{-c}\left[1-\left(\frac{1}{1+e^{-2u}}\right)\right]^{c-2}\\
&= -\frac{2}{\Gamma(c-a)\Gamma(c-b)}\,\frac{e^{2cu}}{(1+e^{2u})^2}\left(\frac{1}{1+e^{-2u}}\right)^{-c}\left(\frac{e^{-2u}}{1+e^{-2u}}\right)^{c-2}\\
&= -\frac{2}{\Gamma(c-a)\Gamma(c-b)}\,\frac{e^{2cu}}{(1+e^{2u})^2}\left(\frac{e^{-2u}}{1+e^{-2u}}\right)^{-2}\left(\frac{1}{1+e^{-2u}}\right)^{-c}\left(\frac{e^{-2u}}{1+e^{-2u}}\right)^{c}\\
&= -\frac{2}{\Gamma(c-a)\Gamma(c-b)}\,\frac{1}{(1+e^{2u})^2}\left(\frac{1}{1+e^{2u}}\right)^{-2} = -\frac{2}{\Gamma(c-a)\Gamma(c-b)}\\
&= -\frac{2}{\Gamma\left(\frac{1}{2}+\alpha+\mu\right)\Gamma\left(\frac{1}{2}-\alpha+\mu\right)}.
\end{aligned}
$$

As a consequence, using analytic extension, we arrive at the following result:

The Wronski determinant $W(f_l, f_r)$ of f_l and f_r is given by

$$[W(f_l, f_r)](u) = f_l(u) f_r'(u) - f_l'(u) f_r(u)$$
$$= -\frac{2}{\Gamma\left(\frac{1}{2}+\alpha+\mu\right)\Gamma\left(\frac{1}{2}-\alpha+\mu\right)},$$

for every $u \in \mathbb{R}$. In particular, f_l and f_r are linearly independent, if and only if

$$\mu \notin r(A) := \bigcup_{n\in\mathbb{N}} \{\mu_n^-, \mu_n^+\},$$

where for each $n \in \mathbb{N}$,

$$\mu_n^- := -\left(n + \frac{1}{2} - \alpha\right), \quad \mu_n^+ := -\left(n + \frac{1}{2} + \alpha\right).$$

Since $0 \leqslant \mathrm{Re}(\alpha) < 1/2$,

$$r(A) \subset (-\infty, 0) \times \mathbb{R}.$$

The elements of $r(A)$ are called *resonances of* A (Fig. 3.10).

We note that the functions f_l^- and f_r^-, corresponding to μ_n^-, for $n \in \mathbb{N}$, satisfy

$$f_l^-(u) = e^{-\left(n+\frac{1}{2}-\alpha\right)u} \cdot \bar{F}\left(\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, \frac{1}{2}+\alpha-n, \frac{1}{1+e^{-2u}}\right)$$
$$= 2^{n+\frac{1}{2}-\alpha} \cosh^{n+\frac{1}{2}-\alpha}(u)\, \bar{F}\left(-n, 2\alpha-n, \frac{1}{2}+\alpha-n, \frac{1}{1+e^{-2u}}\right)$$
$$= \frac{2^{n+\frac{1}{2}-\alpha}}{\Gamma(\frac{1}{2}+\alpha-n)} \cosh^{n+\frac{1}{2}-\alpha}(u)\, F\left(-n, 2\alpha-n, \frac{1}{2}+\alpha-n, \frac{1}{1+e^{-2u}}\right)$$

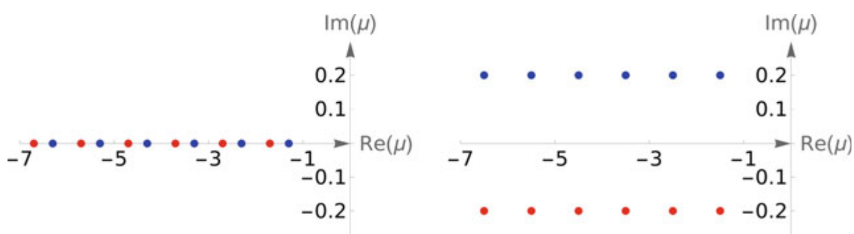


Fig. 3.10 List plot of μ_n^- (blue) and μ_n^+ (red) for $n = 1$ to 6. The left drawing corresponds to $U_0 = 21/100 < 1/4$, and the right corresponds to $U_0 = 29/100 > 1/4$

$$= \frac{2^{n+\frac{1}{2}-\alpha}}{\Gamma(\frac{1}{2}+\alpha-n)} \cosh^{n+\frac{1}{2}-\alpha}(u)\, \frac{(\frac{1}{2}-\alpha)_n}{(\frac{1}{2}+\alpha-n)_n}$$
$$F\left(-n, 2\alpha-n, \frac{1}{2}+\alpha-n, \frac{1}{1+e^{2u}}\right)$$
$$= \frac{(\frac{1}{2}-\alpha)_n}{(\frac{1}{2}+\alpha-n)_n}\, f_l^-(-u) = \frac{\Gamma(\frac{1}{2}-\alpha+n)\,\Gamma(\frac{1}{2}+\alpha-n)}{\Gamma(\frac{1}{2}-\alpha)\,\Gamma(\frac{1}{2}+\alpha)}\, f_r^-(u)$$
$$= \frac{\sin(\pi(\frac{1}{2}-\alpha))}{\sin(\pi(\frac{1}{2}-\alpha+n))}\, f_r^-(u) = (-1)^n\, f_r^-(u),$$

for every $u \in \mathbb{R}$, where (15.8.1) and (15.8.7) of [56] have been used. Further, we note that the functions f_l^+ and f_r^+, corresponding to μ_n^+, for $n \in \mathbb{N}$, satisfy

$$f_l^+(u) = e^{-\left(n+\frac{1}{2}+\alpha\right)u} \cdot \bar{F}\left(\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, \frac{1}{2}-\alpha-n, \frac{1}{1+e^{-2u}}\right)$$
$$= 2^{n+\frac{1}{2}+\alpha} \cosh^{n+\frac{1}{2}+\alpha}(u)\, \bar{F}\left(-n, -2\alpha-n, \frac{1}{2}-\alpha-n, \frac{1}{1+e^{-2u}}\right)$$
$$= \frac{2^{n+\frac{1}{2}+\alpha}}{\Gamma(\frac{1}{2}-\alpha-n)} \cosh^{n+\frac{1}{2}+\alpha}(u)\, F\left(-n, -2\alpha-n, \frac{1}{2}-\alpha-n, \frac{1}{1+e^{-2u}}\right)$$
$$= \frac{2^{n+\frac{1}{2}+\alpha}}{\Gamma(\frac{1}{2}-\alpha-n)} \cosh^{n+\frac{1}{2}+\alpha}(u)\, \frac{(\frac{1}{2}+\alpha)_n}{(\frac{1}{2}-\alpha-n)_n}$$
$$F\left(-n, -2\alpha-n, \frac{1}{2}-\alpha-n, \frac{1}{1+e^{2u}}\right)$$
$$= \frac{(\frac{1}{2}+\alpha)_n}{(\frac{1}{2}-\alpha-n)_n}\, f_l^+(-u) = \frac{\Gamma(\frac{1}{2}-\alpha-n)\,\Gamma(\frac{1}{2}+\alpha+n)}{\Gamma(\frac{1}{2}-\alpha)\,\Gamma(\frac{1}{2}+\alpha)}\, f_r^+(u)$$
$$= \frac{\sin(\pi(\frac{1}{2}+\alpha))}{\sin(\pi(\frac{1}{2}+\alpha+n))}\, f_r^+(u) = (-1)^n\, f_r^+(u),$$

for every $u \in \mathbb{R}$, where again (15.8.1) and (15.8.7) of [56] have been used. As a consequence, we arrive at the following result:

The functions f_l^- and f_l^+, corresponding to the resonances μ_n^- and μ_n^+, respectively, where $n \in \mathbb{N}$, satisfy

$$f_l^-(u) = [2\cosh(u)]^{n+\frac{1}{2}-\alpha}\, \bar{F}\left(-n, 2\alpha-n, \frac{1}{2}+\alpha-n, \frac{1}{1+e^{-2u}}\right),$$

$$f_l^+(u) = [2\cosh(u)]^{n+\frac{1}{2}+\alpha}\,\bar{F}\left(-n, -2\alpha - n, \frac{1}{2} - \alpha - n, \frac{1}{1+e^{-2u}}\right),$$

$$f_l^-(-u) = (-1)^n f_l^-(u), \;\; f_l^+(-u) = (-1)^n f_l^+(u),$$

for every $u \in \mathbb{R}$. In particular, these so called *resonance modes* grow exponentially at $-\infty$ and $+\infty$ and therefore are no elements of $L^2_{\mathbb{C}}(\mathbb{R})$.

From Theorem 3.4.2, it follows for $\mu \in (0,\infty) \times \mathbb{R}^*$ that

$$\begin{aligned} R(-\mu^2)f &= (A+\mu^2)^{-1}f = \frac{1}{2}\,\Gamma\left(\frac{1}{2}+\alpha+\mu\right)\Gamma\left(\frac{1}{2}-\alpha+\mu\right) \\ &\quad\cdot \begin{pmatrix} \mathbb{R} \to \mathbb{C} \\ u \mapsto f_r(u)\int_{-\infty}^{u} f_l(v)f(v)dv + f_l(u)\int_u^{\infty} f_r(v)f(v)dv \end{pmatrix} \\ &= \begin{pmatrix} \mathbb{R} \to \mathbb{C} \\ u \mapsto \int_{\mathbb{R}} K(\mu,u,v)f(v)dv \end{pmatrix}, \end{aligned}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$, where $K \in (\mathbb{C}\backslash r(A)) \times \mathbb{R}^2 \to \mathbb{C}$ is defined by

$$\begin{aligned} K(\mu,u,v) &:= \frac{1}{2}\,\Gamma\left(\frac{1}{2}+\alpha+\mu\right)\Gamma\left(\frac{1}{2}-\alpha+\mu\right)\begin{cases} f_r(u)f_l(v) & v \leqslant u \\ f_l(u)f_r(v) & u < v \end{cases} \\ &= \frac{1}{2}\,\Gamma\left(\frac{1}{2}+\alpha+\mu\right)\Gamma\left(\frac{1}{2}-\alpha+\mu\right)e^{-\mu|u-v|} \\ &\quad\cdot \begin{cases} \bar{F}\left(\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, 1+\mu, \frac{1}{1+e^{2u}}\right)\bar{F}\left(\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, 1+\mu, \frac{1}{1+e^{-2v}}\right) & v \leqslant u \\ \bar{F}\left(\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, 1+\mu, \frac{1}{1+e^{-2u}}\right)\bar{F}\left(\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, 1+\mu, \frac{1}{1+e^{2v}}\right) & u < v \end{cases}, \end{aligned}$$

for every $\mu \in \mathbb{C}\backslash r(A)$ and all $u, v \in \mathbb{R}$. It follows from Theorem 12.9.31 that K is continuous and for $f, g \in C^2_0(\mathbb{R}, \mathbb{C})$, by differentiation under the integral sign, that $\mathcal{R}_{g,f} : \mathbb{C}\backslash r(A) \to \mathbb{C}$, defined by

$$\mathcal{R}_{g,f}(\mu) := \int_{\mathbb{R}^2} g^*(u)K(\mu,u,v)f(v)\,dudv,$$

for every $\mu \in \mathbb{C}\backslash r(A)$, is a holomorphic extension of $((0,\infty)\times\mathbb{R}^* \to \mathbb{C}, \mu \mapsto \langle g|(A+\mu^2)^{-1}f\rangle)$.

The resonances of A, which coincide with the zeros of the Wronskian determinant function $W(f_l, f_r)$, are poles of $\mathcal{R}_{g,f}$. These poles are simple for the case $\alpha \neq 0$ and second order for the case $\alpha = 0$. It should be noted that in fact these resonances depend not only on the operator A, but also on the choice of a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R})$.[10] This subspace is

[10] It can be shown that A and the closure of the negative second order derivative (1.29), are unitarily equivalent, but the analogous analysis shows that the latter operator, for the same subspace, has no

the space where the data for the Schrödinger equation are going to be taken from, here the space of complex-valued C^2-functions on the real line with compact support.

3.6.2 Calculation of the Functional Calculus for A

For the calculation of the Functional Calculus for A, we use Stone's formula, Theorem 12.9.8 (ii).

Theorem 3.6.1 *The following is true.*

(i) For $f, g \in C_0^2(\mathbb{R}, \mathbb{C})$, by $h_{f,g}(\lambda) := 0$, for every $\lambda < 0$, and

$$h_{f,g}(\lambda) := \frac{1}{2\pi i} \cdot \int_{\mathbb{R}^2} \left[K\left(-i\sqrt{\lambda}, u, v\right) - K\left(i\sqrt{\lambda}, u, v\right)\right] \cdot f^*(u)g(v)\, du dv,$$

for every $\lambda \geqslant 0$, there is defined a continuous complex-valued function $h_{f,g} : \mathbb{R} \to \mathbb{C}$. In particular, if $f = g$, then $h_{f,g}$ is positive real-valued.

(ii) The spectrum $\sigma(A) = [0, \infty)$ of A is purely absolutely continuous.[11]

(iii) For $k \in \overline{U^s_{\mathbb{C}}([0, \infty))}$

$$\langle f | k(A) g \rangle = \int_{\mathbb{R}} \hat{k}(\lambda)\, h_{f,g}(\lambda)\, d\lambda,$$

for all $f, g \in C_0^2(\mathbb{R}, \mathbb{C})$, where $\hat{k}$ denotes the extension of k to a function on $\mathbb{R}$ that vanishes on $(-\infty, 0)$.

Proof For the proof, let $f, g \in C_0^2(\mathbb{R}, \mathbb{C})$. We note that by

$$\mathfrak{F}(\lambda, u, v) := \left[K\left(-i\sqrt{\lambda}, u, v\right) - K\left(i\sqrt{\lambda}, u, v\right)\right] \cdot f^*(u)g(v),$$

for every $(\lambda, u, v) \in [0, \infty) \times \mathbb{R}^2$, there is defined a continuous function $\mathfrak{F} : [0, \infty) \times \mathbb{R}^2 \to \mathbb{C}$. Hence, if $\lambda \in [0, \infty)$ and $\lambda_1, \lambda_2, \dots$ is a sequence in $[0, \infty)$ that is convergent to λ, then $\mathfrak{F}(\lambda_1, \cdot), \mathfrak{F}(\lambda_2, \cdot), \dots$ is a sequence of continuous complex-valued functions with a compact support contained in $\operatorname{supp}(f) \times \operatorname{supp}(g)$ that is everywhere on $\mathbb{R}^2$ pointwise convergent to $\mathfrak{F}(\lambda, \cdot)$ and whose component functions are dominated by the integrable function

$$\left[\sup_{(\lambda', u, v) \in B_R(\lambda) \times \operatorname{supp}(f) \times \operatorname{supp}(g)} |\mathfrak{F}(\lambda', u, v)|\right] \chi_{\operatorname{supp}(f) \times \operatorname{supp}(g)},$$

resonances. On the other hand, using the results of this Section, a dense subspace of the domain of that operator can be given that leads to resonances.

[11] The latter means that every set of Lebesgue measure 0 is also a set of measure 0 for every spectral measure of A. In particular, as a consequence, A has no eigenvalues.

where $R > 0$ is such that $\lambda_\nu \in B_R(\lambda)$, for every $\nu \in \mathbb{N}^*$. Hence, it follows from Lebesgue's dominated convergence that $h_{f,g}$ is well-defined as well as continuous on $[0, \infty)$. Since $h_{f,g}$ is continuous on $(-\infty, 0)$ and since $h_{f,g}(0) = 0$, it follows that $h_{f,g}$ is continuous.

According to Stone's formula, Theorem 12.9.8 (ii), for $\alpha, \beta \in \mathbb{R}$ such that $\alpha < \beta$ and $\varepsilon > 0$,

$$
\begin{aligned}
&= \frac{1}{\pi} \left\langle f \middle| \left[\arctan\left(\frac{1}{\varepsilon} \left(\mathrm{id}_{[0,\infty)} - \alpha \right) \right) - \arctan\left(\frac{1}{\varepsilon} \left(\mathrm{id}_{[0,\infty)} - \beta \right) \right) \right] (A) g \right\rangle \\
&= \frac{1}{2\pi i} \int_\alpha^\beta \langle f | \left[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon) \right] g \rangle \, d\lambda \\
&= \frac{1}{2\pi i} \int_\alpha^\beta \left\langle f \middle| \left[R(-[\sqrt{-(\lambda + i\varepsilon)}\,]^2) - R(-[\sqrt{-(\lambda - i\varepsilon)}\,]^2) \right] g \right\rangle d\lambda \\
&= \frac{1}{2\pi i} \int_\alpha^\beta \left\{ \int_{\mathbb{R}^2} \left[K(\sqrt{-(\lambda + i\varepsilon)}\,, u, v) - K(\sqrt{-(\lambda - i\varepsilon)}\,, u, v) \right] \right. \\
&\qquad\qquad \left. \cdot f^*(u) g(v) \, du dv \right\} d\lambda \\
&= \frac{1}{2\pi i} \int_{[\alpha,\beta] \times \mathbb{R}^2} \left[K(\sqrt{-(\lambda + i\varepsilon)}\,, u, v) - K(\sqrt{-(\lambda - i\varepsilon)}\,, u, v) \right] \\
&\qquad\qquad \cdot f^*(u) g(v) \, d\lambda du dv,
\end{aligned}
$$

where we used Fubini's theorem and that the integrand of the last integral is a continuous function with a compact support. Also, we use that $G_+ : (\mathbb{R} \times (0, \infty)) \times \mathbb{R}^2 \to \mathbb{C}$ and $G_- : (\mathbb{R} \times (-\infty, 0)) \times \mathbb{R}^2 \to \mathbb{C}$, defined by

$$G_+(\lambda, u, v) := K(\sqrt{-\lambda}, u, v) f^*(u) g(v),$$

for all $(\lambda, u, v) \in (\mathbb{R} \times (0, \infty)) \times \mathbb{R}^2$ and

$$G_-(\lambda, u, v) := K(\sqrt{-\lambda}, u, v) f^*(u) g(v),$$

for all $(\lambda, u, v) \in (\mathbb{R} \times (-\infty, 0)) \times \mathbb{R}^2$, respectively, have an extension to continuous functions on the closed upper half-plane and closed lower half-plane, respectively. Further, for $\lambda \in \mathbb{R}$, it follows that

$$\sqrt{-(\lambda \pm i\varepsilon)} = \frac{1}{\sqrt{2}} \cdot \left(\sqrt{\sqrt{\lambda^2 + \varepsilon^2} + (-\lambda)} \mp i \sqrt{\sqrt{\lambda^2 + \varepsilon^2} - (-\lambda)} \right)$$

and hence that

$$\lim_{\varepsilon \to 0} \sqrt{-(\lambda \pm i\varepsilon)} = \frac{1}{\sqrt{2}} \cdot \left(\sqrt{|\lambda| - \lambda} \mp i \sqrt{|\lambda| + \lambda} \right) = \begin{cases} \mp i \sqrt{\lambda} & \text{if } \lambda \geqslant 0 \\ \sqrt{|\lambda|} & \text{if } \lambda < 0 \end{cases}.$$

Hence it follows from the spectral theorem, Theorem 12.6.4, see Remark 12.9.9, and Lebesgue's dominated convergence theorem that

$$
\begin{aligned}
&\frac{1}{2}\left\langle f\right|\left[\left(\chi_{(\alpha,\beta)}\big|_{[0,\infty)}\right)(A)+\left(\chi_{[\alpha,\beta]}\big|_{[0,\infty)}\right)(A)\right]g\Big\rangle \\
&= \frac{1}{2\pi i}\int_{\mathbb{R}^3}\chi_{[\alpha,\beta]}(\lambda)\,\chi_{[0,\infty)}(\lambda)\left[K(-i\sqrt{\lambda},u,v)-K(i\sqrt{\lambda},u,v)\right]\cdot f^*(u)g(v) \\
&\qquad d\lambda du dv \\
&= \int_{\mathbb{R}}\chi_{[\alpha,\beta]}(\lambda)\cdot h_{f,g}(\lambda)\,d\lambda,
\end{aligned}
$$

where Fubini's theorem has been used. With the help of the spectral theorem, Theorem 12.6.4, we conclude further that

$$
\begin{aligned}
&s-\lim_{\nu\to\infty}\frac{1}{2}\left[\left(\chi_{(\alpha,\alpha+\frac{1}{\nu})}\big|_{[0,\infty)}\right)(A)+\left(\chi_{[\alpha,\alpha+\frac{1}{\nu}]}\big|_{[0,\infty)}\right)(A)\right] \\
&= \frac{1}{2}\left(\chi_{[\alpha,\alpha]}\big|_{[0,\infty)}\right)(A)
\end{aligned}
$$

and with the help of Lebesgue's dominated convergence theorem that

$$
\lim_{\nu\to\infty}\int_{\mathbb{R}}\chi_{[\alpha,\alpha+\frac{1}{\nu}]}(\lambda)\cdot h_{f,g}(\lambda)\,d\lambda = 0,
$$

implying that

$$
\left\langle f\right|\left(\chi_{[\alpha,\alpha]}\big|_{[0,\infty)}\right)(A)g\Big\rangle = 0.
$$

Hence, we conclude that

$$
\left\langle f\right|\left(\chi_J\big|_{[0,\infty)}\right)(A)g\Big\rangle = \int_{\mathbb{R}}\chi_J(\lambda)\cdot h_{f,g}(\lambda)\,d\lambda,
$$

as well as that

$$
\psi_f(J) = \int_{\mathbb{R}}\chi_J(\lambda)\cdot h_{f,f}(\lambda)\,d\lambda,
$$

for every bounded interval J of $\mathbb{R}$, where ψ_f denotes the spectral measure corresponding to A and f. Since $h_{f,f}$ is continuous, the latter also implies that $h_{f,f}$ is positive real-valued. Further, from the Radon-Nikodym theorems, it follows that ψ_f is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$ and, for every $k \in \overline{U^s_{\mathbb{C}}([0,\infty))}$, since according to the spectral theorem, Theorem 12.6.4, $\hat{k}$ is ψ_f-integrable such that

$$
\langle f|k(A)f\rangle = \int_{\mathbb{R}}\hat{k}\,d\psi_f,
$$

that $\hat{k}\,h_{f,f}$ is Lebesgue measurable such that

$$\langle f|k(A)f\rangle = \int_{\mathbb{R}} \hat{k}(\lambda)\, h_{f,f}(\lambda)\, d\lambda.$$

Since the latter is true for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, with the help of the polarization identities for $\mathbb{C}$-Sesquilinear forms on complex vector spaces, see Theorem 12.3.3 (ii) in the Appendix, this implies that

$$\langle f|k(A)g\rangle = \int_{\mathbb{R}} \hat{k}(\lambda)\, h_{f,g}(\lambda)\, d\lambda,$$

for all $f, g \in C_0^2(\mathbb{R}, \mathbb{C})$. Finally, since for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, ψ_f is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$ and since $C_0^2(\mathbb{R}, \mathbb{C})$ is dense in $L^2_{\mathbb{C}}(\mathbb{R})$, the closed subspace of $L^2_{\mathbb{C}}(\mathbb{R})$, consisting of elements whose spectral measures are absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$, coincides with $L^2_{\mathbb{C}}(\mathbb{R})$, and hence the spectrum $\sigma(A) = [0, \infty)$ of A is purely absolutely continuous. □

Exercise 7 (Motion in an attractive Pöschl–Teller potential)

Show that $\hat{H}_0 : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$, defined by

$$\hat{H}_0 f := -\frac{\hbar^2\kappa^2}{2m}\, f'' + V\left(\frac{u}{\kappa}\right) f = \frac{\hbar^2\kappa^2}{2m}\left[-f'' - \frac{U_0}{\cosh^2(u)}\, f\right],$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, where u denotes the identical function on $\mathbb{R}$, the classical potential V is the attractive Pöschl–Teller potential [58], defined by

$$V(q) := -\frac{V_0}{\cosh^2(\kappa q)},$$

for every $q \in \mathbb{R}$, where $V_0 > 0$, $\kappa > 0$ has the dimension l^{-1} and

$$U_0 := \frac{2mV_0}{\hbar^2\kappa^2}$$

is dimensionless, is essentially self-adjoint. In addition, determine the spectrum of this operator.

Exercise 8 (Motion in a Rosen–Morse potential)

Show that $\hat{H}_0 : C_0^2(\mathbb{R}, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R})$, defined by

$$\begin{aligned} \hat{H}_0 f &:= -\frac{\hbar^2 \kappa^2}{2m} f'' + V\left(\frac{u}{\kappa}\right) f \\ &= \frac{\hbar^2 \kappa^2}{2m} \left\{ -f'' + \left[U_{01} \tanh(u) - \frac{U_{02}}{\cosh^2(u)} \right] f \right\}, \end{aligned}$$

for every $f \in C_0^2(\mathbb{R}, \mathbb{C})$, is the Rosen–Morse potential [64], defined by

$$V(q) := V_{01} \tanh(\kappa q) - \frac{V_{02}}{\cosh^2(\kappa q)},$$

for every $q \in \mathbb{R}$, where $V_{01} \in \mathbb{R}^*$, $V_{02} \in \mathbb{R}$, $\kappa > 0$ has the dimension l^{-1} and

$$U_{01} := \frac{2m V_{01}}{\hbar^2 \kappa^2}, \;\; U_{02} := \frac{2m V_{02}}{\hbar^2 \kappa^2},$$

are dimensionless, is essentially self-adjoint. In addition, determine the spectrum of this operator.

4 Motion in a Central Force Field

Frequently, the Hamiltonians in quantum mechanics are representations of formal[1] partial differential operators, restricted to an open subset Ω of $\mathbb{R}^n$, $n \in \mathbb{N}^*$, with singular coefficients, i.e., either the coefficients of the principal part of the operator vanish "on" the boundary of Ω or the potential is unbounded. For instance, in the case of the harmonic oscillator, the potential is unbounded. Also in the case of an electron in the electric field of an atomic nucleus, the so called "Coulomb-potential" is unbounded.[2] In such cases, the domain of the Hamiltonian is not a priori clear, but has to determined, if necessary, employing additional physical boundary conditions.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_4.

[1] In operator theory, the term "formal" indicates that the operator in question does not come together with a representation (function) space and a natural domain in that space, both crucial in determining the spectral properties of the later operator. The domain of a DSLO is critical. Neither proper extensions nor proper restrictions of a DSLO are self-adjoint. In this sense, domains of DSLO are "maximal." So, strictly speaking, a formal partial differential operator ("PDO") alone is of little significance in operator theory. This has to be seen in the context that the "operators" considered in the vast majority of quantum theory text books are formal PDOs.

[2] Such cases are rarely considered in the theory of partial differential equations. The fact of having singular coefficients complicates the analysis of these operators and lead to development of an area of operator theory studying extensions of operators, like von Neumann's extension theory of (densely-defined, linear and) symmetric operators in Hilbert spaces.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_4

In these cases, the determination of the corresponding Hamiltonian starts with a preliminary Hamiltonian $\hat{H}_0$, defined on a "minimal domain" D_0, like in the case of the harmonic oscillator.[3] Such "preliminary Hamiltonians" are densely-defined, linear and symmetric. In the next step, the self-adjoint extensions of $\hat{H}_0$ are studied. If there is such an extension,[4] such extensions are restrictions of the adjoint operator $\hat{H}_0^*$ of $\hat{H}_0$. If there is only 1 such extension, i.e., $\hat{H}_0$ is essentially self-adjoint, like in the case of the harmonic oscillator, then the Hamiltonian of the system is given by the closure of $\hat{H}_0$ which is equal to $\hat{H}_0^*$. If not, additional physical boundary conditions are needed that, on the one hand, should be trivially satisfied by the elements of D_0 and, on the other hand, restrict the domain of $\hat{H}_0^*$. In this case, the physical Hamiltonian is a *proper* restriction of $\hat{H}_0^*$.

In a position representation, the minimal Hamiltonian for a particle subject to a central potential $V \circ |\ |$ that might be singular in the origin, where $V : (0, \infty) \to \mathbb{R}$ is a continuous function, is given by

$$\hat{H}_0 = \begin{pmatrix} C_0^2(\mathbb{R}^3, \mathbb{C}) \to L_{\mathbb{C}}^2(\mathbb{R}^3) \\ f \mapsto -\frac{\hbar^2\kappa^2}{2m} \triangle f + (V \circ |\ |) \cdot f \end{pmatrix},$$

where we assume that $(V \circ |\ |) \cdot f \in L_{\mathbb{C}}^2(\mathbb{R}^3)$, for every $f \in C_0^2(\mathbb{R}^3, \mathbb{C})$.

With the help of Lemma 1.2.1, it follows that the operator $\hat{H}_0$ is densely-defined, linear and symmetric. In the following, we are going to use the spherical symmetry of the system to define the Hamiltonian as a direct sum of a countable number of Sturm–Liouville operators. For this, in a first step, we change the representation, using a unitary transformation U induced by spherical coordinates.

4.1 A Change of Representation Induced by Introduction of Spherical Coordinates

We repeat the steps from Sect. 2.4. First, we note the following Lemma.

Lemma 4.1.1 (Transformation of the Laplace Operator in 3 Dimensions into Spherical Coordinates) *For this, let* $\Omega \subset \mathbb{R}^3 \setminus (\{0\} \times \{0\} \times \mathbb{R})$ *be non-empty and open. In addition, let* $\Omega_{sph} \subset \mathbb{R}^3$ *be a non-empty open subset such*

$$g(\Omega_{sph}) = \Omega\ ,$$

[3] The domain is chosen "minimal," in order not to miss the physical extension.

[4] Preliminary Hamiltonians that have no self-adjoint extensions are easy to construct, but are usually of no physical relevance. On the other hand, frequently, preliminary Hamiltonians are semi-bounded from below, i.e, $\left\langle f|\hat{H}_0 f\right\rangle \geqslant \gamma \langle f|f\rangle$ for every $f \in D(\hat{H}_0)$ and some real γ. In these cases, there is always a self-adjoint extension of $\hat{H}_0$. One such extension is the so called "Friedrichs Extension." Often, it turns out that the "physical" extension coincides with the latter extension.

where $g \in C^{\infty}(\mathbb{R}^3, \mathbb{R}^3)$ *is defined by*

$$g(u, \theta, \varphi) := (u \sin(\theta) \cos(\varphi), u \sin(\theta) \sin(\varphi), u \cos(\theta))$$

for all $(u, \theta, \varphi) \in \mathbb{R}^3$*. Finally, let* $f \in C^2(\Omega, \mathbb{R})$*. Then*

$$\begin{aligned}(\triangle f)(g(u, \theta, \varphi)) &= \frac{\partial^2 \bar{f}}{\partial u^2}(u, \theta, \varphi) + \frac{2}{u}\frac{\partial \bar{f}}{\partial u}(u, \theta, \varphi) \\ &+ \frac{1}{u^2 \sin^2(\theta)}\left[\frac{\partial^2 \bar{f}}{\partial \varphi^2}(u, \theta, \varphi) + \sin^2(\theta)\frac{\partial^2 \bar{f}}{\partial \theta^2}(u, \theta, \varphi)\right. \\ &\left. + \sin(\theta)\cos(\theta)\frac{\partial \bar{f}}{\partial \theta}(u, \theta, \varphi)\right] \end{aligned} \tag{4.1}$$

for all $(u, \theta, \varphi) \in \Omega_{sph}$*, where* $\bar{f} \in C^2(\Omega_{sph}, \mathbb{R})$ *is defined by*

$$\bar{f}(u, \theta, \varphi) := (f \circ g)(u, \theta, \varphi) = f(u \sin(\theta) \cos(\varphi), u \sin(\theta) \sin(\varphi), u \cos(\theta))$$

for all $(u, \theta, \varphi) \in \Omega_{sph}$*.*

The proof of this Lemma is left to the reader.

Exercise 9

Prove Lemma 4.1.1.

Further, we define $U : L^2_{\mathbb{C}}(\mathbb{R}^3) \to L^2_{\mathbb{C}}(\Omega, u^2 \sin(\theta))$ by (2.7), where $\Omega := (0, \infty) \times (0, \pi) \times (-\pi, \pi)$. As a consequence of Lemma 4.1.1, $U\hat{H}_0 U^{-1}$ is given by

$$\begin{aligned} &U\hat{H}_0 U^{-1} f \\ &= -\frac{\hbar^2 \kappa^2}{2m}\left\{\frac{\partial^2}{\partial u^2} + \frac{2}{u}\frac{\partial}{\partial u} + \frac{1}{u^2 \sin^2(\theta)}\left[\frac{\partial^2}{\partial \varphi^2} + \sin(\theta)\frac{\partial}{\partial \theta}\sin(\theta)\frac{\partial}{\partial \theta}\right]\right\} f \\ &\quad + V(u) f \ , \end{aligned}$$

for every $f \in C^2_0(\Omega, \mathbb{C})$.

4.2 Reduction of $U\hat{H}_0 U^{-1}$

In the next step, we are going to use the spherical symmetry of the system to decompose into a countable number of densely-defined, linear, symmetric Sturm–Liouville operators. The basis for the reduction is Lemma 2.2.2. We define, $X := L^2_{\mathbb{C}}(\Omega, u^2 \sin(\theta))$, for every

$(\ell, m) \in \mathcal{I}$ a corresponding linear isometry $U_{\ell m} : L^2_{\mathbb{C}}(I, u^2) \to X$, where $I := (0, \infty)$, by (2.11) and the corresponding closed subspace $X_{\ell m}$ of X as the range of $U_{\ell m}$. Further, we define the dense subspaces $\mathcal{D}_{\ell m}$ of $X_{\ell m}$ by

$$\mathcal{D}_{\ell m} := U_{\ell m} C^2_0(I, \mathbb{C}),$$

for all $(\ell, m) \in \mathcal{I}$. For every $(\ell, m) \in \mathcal{I}$ and $f \in C^2_0(I, \mathbb{C})$, it follows that

$$\begin{aligned}
& U \hat{H}_0 U^{-1} f \otimes Y_{\ell m} \\
&= -\frac{\hbar^2 \kappa^2}{2m} \left\{ \frac{\partial^2}{\partial u^2} + \frac{2}{u} \frac{\partial}{\partial u} + \frac{1}{u^2 \sin^2(\theta)} \left[\frac{\partial^2}{\partial \varphi^2} + \sin(\theta) \frac{\partial}{\partial \theta} \sin(\theta) \frac{\partial}{\partial \theta} \right] \right\} f \otimes Y_{\ell m} \\
&\quad + V(u) f \otimes Y_{\ell m} \\
&= -\frac{\hbar^2 \kappa^2}{2m} \left\{ f'' + \frac{2}{u} f' - \left[\frac{\ell(\ell+1)}{u^2} + \frac{2m V(u)}{\hbar^2 \kappa^2} \right] f \right\} \otimes Y_{\ell m} \\
&= \frac{\hbar^2 \kappa^2}{2m} \left\{ -\left(f'' + \frac{2}{u} f' \right) + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2m V(u)}{\hbar^2 \kappa^2} \right] f \right\} \otimes Y_{\ell m} \in X_{\ell m} \ ,
\end{aligned}$$

where we used that

$$-\frac{1}{\sin^2(\theta)} \left\{ \frac{\partial^2}{\partial \varphi^2} + \left[\sin(\theta) \frac{\partial}{\partial \theta} \right]^2 \right\} Y_{\ell m} = \ell(\ell+1) \cdot Y_{\ell m}.$$

We note that the latter "invariance" is due the "spherical symmetry" of $\hat{H}_0$. This is going to explained in more detail in a separate chapter on symmetries.

4.3 Analysis of the Reduced Operators

The final step in the application of Lemma 2.2.2 consists in the analysis of the reduced operators that are unitarily equivalent to the, densely-defined, linear and symmetric, Sturm–Liouville operators $\hat{H}_{\ell m} : C^2_0(I, \mathbb{C}) \to L^2_{\mathbb{C}}(I, u^2)$, defined by

Reduced Operators

$$\hat{H}_{\ell m} f := \frac{\hbar^2 \kappa^2}{2m} \left\{ -\frac{1}{u^2} \left(u^2 f' \right)' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2m V(u)}{\hbar^2 \kappa^2} \right] f \right\},$$

for every $f \in C^2_0(I, \mathbb{C})$, where u denotes the the identity function on I, for all $(\ell, m) \in \mathcal{I}$. For this purpose, after applying another unitary transformation $\mathcal{U}$ to $\hat{H}_{\ell m}$, we are going to use Weyl's Limit Point/Limit Circle Criterion given below. The unitary transformation $\mathcal{U} : L^2_{\mathbb{C}}(I, u^2) \to L^2_{\mathbb{C}}(I)$ is given by

$$\mathcal{U} f := u f ,$$

for every $f \in L^2_{\mathbb{C}}(I)$. Then, $\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1}$ is given by

$$\begin{aligned}
\hat{H}_{\ell m}\mathcal{U}^{-1} f &= \frac{\hbar^2\kappa^2}{2m}\left\{-\frac{1}{u^2}\left[u^2\left(\frac{f}{u}\right)'\right]' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2mV(u)}{\hbar^2\kappa^2}\right]\frac{f}{u}\right\} \\
&= \frac{\hbar^2\kappa^2}{2m}\left\{-\frac{1}{u^2}\left[u^2\left(\frac{f'}{u} - \frac{f}{u^2}\right)\right]' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2mV(u)}{\hbar^2\kappa^2}\right]\frac{f}{u}\right\} \\
&= \frac{\hbar^2\kappa^2}{2m}\left\{-\frac{1}{u^2}\left(uf' - f\right)' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2mV(u)}{\hbar^2\kappa^2}\right]\frac{f}{u}\right\} \\
&= \frac{\hbar^2\kappa^2}{2m}\left\{-\frac{1}{u}\, f'' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2mV(u)}{\hbar^2\kappa^2}\right]\frac{f}{u}\right\} \\
&= \mathcal{U}^{-1}\,\frac{\hbar^2\kappa^2}{2m}\left\{-f'' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2mV(u)}{\hbar^2\kappa^2}\right] f\right\}
\end{aligned}$$

for every $f \in C^2_0(I, \mathbb{C})$ and hence $\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1} : C^2_0(I, \mathbb{C}) \to L^2_{\mathbb{C}}(I)$ is given by

Transformed Reduced Operators

$$\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1} f = \frac{\hbar^2\kappa^2}{2m}\left\{-f'' + \left[\frac{\ell(\ell+1)}{u^2} + \frac{2mV(u)}{\hbar^2\kappa^2}\right] f\right\},$$

for every $f \in C^2_0(I, \mathbb{C})$.

4.4 Motion in a Coulomb Field

4.4.1 An Application of Weyl's Criterion

In the following, we apply Weyl's Limit Point/Limit Circle Criterion to the case of an electron in the Coulomb field of an nucleus containing Z protons. In this case,

$$V = -\frac{Ze^2\kappa}{u},$$

where $e > 0$ denotes the charge of an electron. Then, for $(l, m) \in \mathcal{I}$

$$\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1}f = \frac{\hbar^2\kappa^2}{2m}\left[-f'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2}\right)f\right],$$

for every $f \in C_0^2(I, \mathbb{C})$, where

$$\nu := \frac{2mZe^2}{\hbar^2\kappa}, \quad \Lambda := \ell(\ell+1).$$

In a first step, we analyze the asymptotic of the solutions of

$$f'' + \left(\lambda + \frac{\nu}{u} - \frac{\Lambda}{u^2}\right)f = 0, \tag{4.2}$$

at 0, where $\lambda > 0$. In order to allow a direct application of Theorem 12.8.1, we use instead of f the auxiliary function $g := f \circ (-\mathrm{id}_{\mathbb{R}})$, which satisfies the differential equation

$$g'' + \left(\lambda - \frac{\nu}{u} - \frac{\Lambda}{u^2}\right)g = 0,$$

where now u denotes the identical function on $(-\infty, 0)$. In the next step, we define $g_1 := g/u$, $g_2 := g'$. Then

$$\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}' = \left[\frac{1}{-u}\begin{pmatrix} 1 & -1 \\ -\Lambda & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \nu - \lambda u & 0 \end{pmatrix}\right] \cdot \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}, \tag{4.3}$$

where

$$A_0 = \begin{pmatrix} 1 & -1 \\ -\Lambda & 0 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 0 & 0 \\ \nu - \lambda u & 0 \end{pmatrix}.$$

An application of Theorem 12.8.1 to (4.3) gives the existence of linearly independent solutions $f_1, f_2 \in C^2(I, \mathbb{C})$ of (4.2) and $R_1, R_2 \in C^1\left(I, \mathbb{C}^2\right)$ such that

$$\begin{aligned}
& f_1 = u^{-\ell}(1 + R_{11}), \quad f_1' = u^{-(\ell+1)}(-\ell + R_{12}), \\
& f_2 = u^{\ell+1}(1 + R_{21}), \quad f_2' = u^{\ell}(\ell + 1 + R_{22}), \\
& \lim_{u \to 0} |R_1(u)| = \lim_{u \to 0} |R_2(u)| = 0.
\end{aligned} \tag{4.4}$$

The details of this application are left to the reader.

Exercise 10

Use Theorem 12.8.1 to show that for every non-real λ

$$\lim_{a \to 0+} (\bar{A}_{V_a} - \lambda)^{-1} f = \mathrm{Int}(K_\lambda) f,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$.

Asymptotic of the Solutions of (4.2) at 0

We note in the case $\ell = 0$ that f_1 and f_2 are both square integrable close to 0, whereas in all other cases f_1 is not square integrable close to 0.

In a second step, we analyze the asymptotic of the solutions of (4.2) at ∞. For this purpose, we reparametrize f, with the help of an auxiliary function h, such that the resulting equation for $f \circ h$ allows the application of Theorem 12.8.1. The function h is defined by

$$h := \sqrt{u \cdot \left(u + \frac{\nu}{\lambda}\right)} + \frac{\nu}{\lambda} \cdot \operatorname{artanh}\left(\sqrt{\frac{u}{u + \frac{\nu}{\lambda}}}\right)$$
$$= \sqrt{u \cdot \left(u + \frac{\nu}{\lambda}\right)} + \ln\left\{\left[\frac{\lambda}{\nu}\left(\sqrt{u + \frac{\nu}{\lambda}} + \sqrt{u}\right)^2\right]^{\frac{\nu}{2\lambda}}\right\}. \tag{4.5}$$

Then

$$h' = \sqrt{1 + \frac{\nu/\lambda}{u}}, \;\; h'' = -\frac{\nu/\lambda}{2u^{3/2}\sqrt{u + (\nu/\lambda)}}, .$$

Since

$$h(0) = 0, \;\; h' \geqslant 1,$$

h is a strictly increasing C^2-diffeomorphism from $0, \infty)$ onto $(0, \infty)$. In addition, if $k : (0, \infty) \to \mathbb{R}$ is such that $k|_{[c,\infty)}$ is integrable, then it follows that $k \cdot |h'|\big|_{[c,\infty)}$ is integrable, since $|h'|$ is bounded measurable. Hence, it follows from Lebesgue's change of variable fomula that $k \circ h^{-1}|_{[h(c),\infty)}$ is integrable and that

$$\int_c^\infty k \cdot |h'|\, dv^1 = \int_{h(c)}^\infty k \circ h^{-1}\, dv^1.$$

Further,

$$g := f \circ h^{-1}$$

satisfies

$$f = g \circ h, \;\; f' = \left(g' \circ h\right) \cdot h', \;\; f'' = \left(g'' \circ h\right) \cdot h'^2 + \left(g' \circ h\right) \cdot h''$$

and, since

$$0 = f'' + \left(\lambda + \frac{\nu}{u} - \frac{\Lambda}{u^2}\right) f$$
$$= \left(g'' \circ h\right) \cdot h'^2 + \left(g' \circ h\right) \cdot h'' + \left(\lambda + \frac{\nu}{u} - \frac{\Lambda}{u^2}\right) (g \circ h),$$

it follows that

$$
\begin{aligned}
0 &= \left(g'' \circ h\right) + \frac{h''}{h'^2}\left(g' \circ h\right) + \frac{\lambda + \frac{\nu}{u} - \frac{\Lambda}{u^2}}{h'^2}\,(g \circ h) \\
&= \left(g'' \circ h\right) + \frac{h''}{h'^2}\left(g' \circ h\right) + \frac{\lambda \cdot (1 + \frac{\nu/\lambda}{u}) - \frac{\Lambda}{u^2}}{h'^2}\,(g \circ h) \\
&= \left(g'' \circ h\right) - \frac{\frac{\nu/\lambda}{2u^{3/2}\sqrt{u+(\nu/\lambda)}}}{1 + \frac{\nu/\lambda}{u}}\left(g' \circ h\right) + \frac{\lambda \cdot (1 + \frac{\nu/\lambda}{u}) - \frac{\Lambda}{u^2}}{h'^2}\,(g \circ h) \\
&= \left(g'' \circ h\right) - \frac{\nu/\lambda}{2u^2\left(1 + \frac{\nu/\lambda}{u}\right)^{3/2}}\left(g' \circ h\right) + \left(\lambda - \frac{\Lambda/u^2}{1 + \frac{\nu/\lambda}{u}}\right)(g \circ h)
\end{aligned}
$$

and hence that

$$
g'' - \left[\frac{(\nu/\lambda)/u^2}{2\left(1 + \frac{\nu/\lambda}{u}\right)^{3/2}} \circ h^{-1}\right] g' + \left[\lambda - \left(\frac{\Lambda/u^2}{1 + \frac{\nu/\lambda}{u}}\right) \circ h^{-1}\right] g = 0.
$$

Using the definitions

$$
a := \frac{(\nu/\lambda)/u^2}{2\left(1 + \frac{\nu/\lambda}{u}\right)^{3/2}} \circ h^{-1}, \;\; b := \left(\frac{\Lambda/u^2}{1 + \frac{\nu/\lambda}{u}}\right) \circ h^{-1},
$$

we arrive at the system

$$
\begin{pmatrix} g \\ g' \end{pmatrix}' = \left[\begin{pmatrix} 0 & 1 \\ -\lambda & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ b & a \end{pmatrix}\right]\begin{pmatrix} g \\ g' \end{pmatrix} = (\mathcal{A}_0 + \mathcal{A}_1)\begin{pmatrix} g \\ g' \end{pmatrix}, \tag{4.6}
$$

where

$$
\mathcal{A}_0 := \begin{pmatrix} 0 & 1 \\ -\lambda & 0 \end{pmatrix}, \;\; \mathcal{A}_1 = \begin{pmatrix} 0 & 0 \\ b & a \end{pmatrix}.
$$

We note that $a|_{[c,\infty)}$ and $b|_{[c,\infty)}$ are integrable for $c > 0$. Hence, Theorem 12.8.1 is applicable to (4.6) and gives the existence of linearly independent solutions $f_3, f_4 \in C^2(I, \mathbb{C})$ of (4.2) and $R_3, R_4 \in C^1\left(I, \mathbb{C}^2\right)$ such that

$$
\begin{aligned}
&f_3 = \exp(i\sqrt{\lambda}\,h) \cdot (1 + R_{31}), \;\; f_3' = \exp(i\sqrt{\lambda}\,h) \cdot (i\sqrt{\lambda} \cdot h' + R_{32}), \\
&f_4 = \exp(-i\sqrt{\lambda}\,h) \cdot (1 + R_{41}), \;\; f_4' = \exp(-i\sqrt{\lambda}\,h) \cdot (-i\sqrt{\lambda} \cdot h' + R_{42}), \\
&\lim_{u\to\infty} |R_3(u)| = \lim_{u\to\infty} |R_4(u)| = 0.
\end{aligned} \tag{4.7}
$$

The details of this application are left to the reader.

Exercise 11

Use Theorem 12.8.1 to show that there are linearly independent solutions $f_3, f_4 \in C^2(I, \mathbb{C})$ of (4.2) and $R_3, R_4 \in C^1\left(I, \mathbb{C}^2\right)$ such that (4.7) is satisfied.

Asymptotic of the Solutions of (4.2) at ∞

We note that in all cases f_3 and f_4 are both not square integrable close to ∞.

From the results on the asymptotic of the solutions of (4.2) at 0 and ∞, we conclude the following.

Extension Properties of the Reduced Operators

For the case that $\ell = m = 0$, the reduced operator $\hat{H}_{\ell m}$, i.e., the purely radial operator $\hat{H}_{00}$ is not essentially self-adjoint, with deficiency indices equal to 1. In all other cases, $\hat{H}_{\ell m}$ is essentially self-adjoint and hence the corresponding self-adjoint extension is given by $\hat{H}^*_{\ell m}$.

Since $\hat{H}_{\ell m}$ is essentially self-adjoint for $(\ell, m) \in \mathcal{I} \backslash \{(0,0)\}$, the corresponding self-adjoint extension is given by its adjoint $\hat{H}^*_{\ell m}$. From the general theory for Sturm–Liouville operators, see e.g. [80]), it follows that the following is true.

A Larger Core for $\hat{H}^*_{\ell m}$, $(\ell, m) \in \mathcal{I} \backslash \{(0,0)\}$

$$D_{\ell m} := \left\{ f \in C^2(I, C) \cap L^2_{\mathbb{C}}(I) : -f'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2}\right) f \in L^2_{\mathbb{C}}(I) \right\}$$

defines a core for $(\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1})^* = \mathcal{U}\hat{H}^*_{\ell m}\mathcal{U}^{-1}$.
For $f \in D_{\ell m}$, $(\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1})^* f$ is given by

$$(\mathcal{U}\hat{H}_{\ell m}\mathcal{U}^{-1})^* f = \frac{\hbar^2 \kappa^2}{2m} \left[-f'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2}\right) f \right].$$

Later, we are going to show that the eigenvectors of $\hat{H}^*_{\ell m}$, $(\ell, m) \in \mathcal{I} \setminus \{(0,0)\}$, are elements of $D_{\ell m}$.

4.4.2 Extensions of the Purely Radial Operator $\hat{H}_{00}$

For an application of Lemma 2.2.2, solely the radial operator $\hat{H}_{00}$ needs to be extended, such that the extended operator is in addition essentially self-adjoint. This is done in the following for the equivalent operator $A_{00} : C^2_0(I, \mathbb{C}) \to L^2_{\mathbb{C}}(I)$, defined by

$$A_{00} f := -f'' - \frac{\nu}{u} f ,$$

for every $f \in C^2_0(I, \mathbb{C})$, where $\lambda > 0$, by using a method which can be found in [41]. This method has the technical advantage over the von Neumann extension theory that it does not presuppose a detailed knowledge of the deficiency subspaces of A_{00}. For the application of this method, we let π denote the canonical projection of $D(A^*_{00})$ onto the quotient space $D(A^*_{00})/D(\bar{A}_{00})$ and define $\langle \, , \rangle : (D(A^*_{00})/D(\bar{A}_{00}))^2 \to \mathbb{C}$ by

$$\langle f + D(\bar{A}_{00}), g + D(\bar{A}_{00}) \rangle := i \, (\langle A^*_{00} f | g \rangle_2 - \langle f | A^*_{00} g \rangle_2) \ ,$$

for all $f, g \in D(A^*_{00})$, where $\langle \, | \, \rangle_2$ denotes the scalar product of $L^2_{\mathbb{C}}(J)$. Since both deficiency indices of A_{00} are equal to 1, $D(A^*_{00})/D(\bar{A}_{00})$ is a 2-dimensional complex vector space and $\langle \, , \rangle$ defines an inner product (i.e., a nondegenerate symmetric sesquilinear form) of signature $(1, 1)$ on $D(A^*_{00})/D(A_{00})$. A subspace D of $D(A^*_{00})$ "is" the domain of a linear self-adjoint extension of A_{00} if and only if $\pi(D)$ is a maximal null space of $(D(A^*_{00})/D(\bar{A}_{00}), \langle, \rangle)$, i.e., iff the equality

$$\begin{aligned} \pi(D) = \{ f + D(\bar{A}_{00}) \in D(A^*_{00})/D(\bar{A}_{00}) : \langle f + D(\bar{A}_{00}), g + D(\bar{A}_{00}) \rangle = 0, \\ \text{for all } g \in D \} \end{aligned}$$

is valid. Hence, given an orthonormal basis $f_1 + D(\bar{A}_{00})$, $f_2 + D(\bar{A}_{00})$ of $(D(A^*_{00})/D(\bar{A}_{00}), \langle \, , \rangle)$, i.e.,

$$\langle f_j + D(\bar{A}_{00}), f_k + D(\bar{A}_{00}) \rangle = \eta_{jk} \ ,$$

for $j, k \in \{1, 2\}$, where:

$$\eta_{11} = 1 \ , \ \eta_{22} = -1 \ , \ \eta_{12} = \eta_{21} = 0,$$

constructed below, the domains of linear self-adjoint extensions of A_{00} can be seen to be given by the sequence $(\mathcal{D}_\beta)_{\beta \in [0,\pi)}$ of pairwise different subspaces of $D(A^*_{00})$, where

$$\mathcal{D}_\beta := \{ f \in D(A^*_{00}) : i \, (\left\langle A^*_{00}(f_1 + e^{2i\beta} f_2) | f \right\rangle_2 - \left\langle f_1 + e^{2i\beta} f_2 | A^*_{00} f \right\rangle_2) = 0 \},$$

for $\beta \in [0, \pi)$. By the general theory for Sturm–Liouville operators (see, e.g., [80]),

$$D_0 := \{f : f \in C^2(I, C) \cap L^2_{\mathbb{C}}(I) \text{ and } -f'' - \frac{\nu}{u} f \in L^2_{\mathbb{C}}(I)\}$$

defines a core for A^*_{00}, and for $f \in D_0$ the corresponding $A^*_{00} f$ is given by

$$A^*_{00} f = -f'' - \frac{\nu}{u} f.$$

Hence for $f, g \in D_0$,

$$\begin{aligned}
&\langle f + D(\bar{A}_{00}), g + D(\bar{A}_{00})\rangle := i\,(\langle A^*_{00} f | g\rangle_2 - \langle f | A^*_{00} g\rangle_2) \\
&= i \int_0^\infty \left[\left(-f^{*\prime\prime} - \frac{\nu}{u} f^*\right) g - f^* \left(-g'' - \frac{\nu}{u} g\right)\right] du \\
&= i \int_0^\infty \left(-f^{*\prime\prime} g + f^* g''\right) du = i \int_0^\infty \left(-f^{*\prime} g + f^* g'\right)' du \\
&= i \int_0^\infty \left(f^* g' - f'^* g\right)' du.
\end{aligned}$$

We note that

$$g_1 := h \cdot [1 - \nu u \ln(u)], \;\; g_2 := hu,$$

where $h \in C^\infty(I, \mathbb{R})$ is an otherwise arbitrary auxiliary function which is equal to 1 on $(0, 1/4]$ and is equal to 0 on $[3/4, \infty)$ (such a function is of course easy to construct), are linearly independent elements of D_0 satisfying

$$\begin{aligned}
&\langle g_1 + D(\bar{A}_{00}), g_1 + D(\bar{A}_{00})\rangle = \langle g_2 + D(\bar{A}_{00}), g_2 + D(\bar{A}_{00})\rangle = 0, \\
&\langle g_1 + D(\bar{A}_{00}), g_2 + D(\bar{A}_{00})\rangle = -i, \;\; \langle g_2 + D(\bar{A}_{00}), g_1 + D(\bar{A}_{00})\rangle = i.
\end{aligned}$$

As a consequence, defining

$$f_1 := \frac{\sqrt{2}}{2}(g_1 + i g_2), \;\; f_2 := \frac{\sqrt{2}}{2}(g_1 - i g_2) = f_1^*,$$

we obtain

$$\begin{aligned}
&\langle f_1 + D(\bar{A}_{00}), f_1 + D(\bar{A}_{00})\rangle = 1, \;\; \langle f_2 + D(\bar{A}_{00}), f_2 + D(\bar{A}_{00})\rangle = -1, \\
&\langle f_1 + D(\bar{A}_{00}), f_2 + D(\bar{A}_{00})\rangle = \langle f_2 + D(\bar{A}_{00}), f_1 + D(\bar{A}_{00})\rangle = 0,
\end{aligned}$$

i.e., $f_1 + D\left(\bar{A}_{00}\right), f_2 + D\left(\bar{A}_{00}\right)$ is an orthonormal basis of $(D(A^*_{00})/D(\bar{A}_{00}), \langle\,,\,\rangle)$. (In particular, it follows that both f_1 and f_2 are not contained in the domain of $\bar{A}_{00}$.) Hence by $(A^*_{00}|_{\mathcal{D}_\beta})_{\beta \in [0,\pi)}$ it is given a sequence of pairwise different linear self-adjoint extensions of A^*_{00} which includes all linear self-adjoint extension of A_{00}. Furthermore, for any $\beta \in [0, \pi)$ the subspace $\mathcal{D}_\beta \cap D_0$ and $\mathcal{D}'_\beta$ defined below are cores for $A^*_{00}|_{\mathcal{D}_\beta}$. We note that

$$\begin{aligned}
&\mathcal{D}_\beta \cap D_0 \\
&= \Big\{ f \in C^2(I,\mathbb{C}) \cap L^2_{\mathbb{C}}(I) : -f'' - \frac{\nu}{u} f \in L^2_{\mathbb{C}}(I) \\
&\quad \text{and } \lim_{u\to 0} \left\{ [\cos(\beta) g_1 + \sin(\beta) g_2]^2 \left[\frac{f}{\cos(\beta) g_1 + \sin(\beta) g_2} \right]' \right\}(u) = 0 \Big\},
\end{aligned}$$

for $\beta \in [0,\pi)$. and $\mathcal{D}'_\beta \left(\subset \mathcal{D}_\beta \cap D_0\right)$ is given by

$$\mathcal{D}'_\beta := C^2_0(J,\mathbb{C}) + \mathbb{C}\,[\cos(\beta) g_1 + \sin(\beta) g_2]\,. \tag{4.8}$$

We note that for $\beta = \pi/2$ that

$$\cos(\beta) g_1 + \sin(\beta) g_2 = hu.$$

As a consequence,

$$\begin{aligned}
&\mathcal{D}_{\pi/2} \cap D_0 = \\
&\Big\{ f \in C^2(I,\mathbb{C}) \cap L^2_{\mathbb{C}}(I) : -f'' - \frac{\nu}{u} f \in L^2_{\mathbb{C}}(I) \wedge \lim_{u\to 0} u^2 (u^{-1} f)'(u) = 0 \Big\}, \\
&\mathcal{D}'_{\pi/2} = C^2_0(J,\mathbb{C}) + \mathbb{C}.hu.
\end{aligned}$$

The Appropriate Essentially Self-Adjoint Extension of $\hat{H}_{00}$

The extension $\mathcal{U}\hat{H}_{00e}\mathcal{U}^{-1}$ of $\mathcal{U}\hat{H}_{00}\mathcal{U}^{-1}$, given by

$$\mathcal{U}\hat{H}_{00e}\mathcal{U}^{-1} f := \frac{\hbar^2 \kappa^2}{2m} \left(-f'' - \frac{\nu}{u} f \right) \,,$$

for every $f \in C^2(I,\mathbb{C}) \cap L^2_{\mathbb{C}}(I)$ such that

$$- f'' - \frac{\nu}{u} f \in L^2_{\mathbb{C}}(I) \text{ and } \lim_{u\to 0} u^2 (u^{-1} f)'(u) = 0, \tag{4.9}$$

is essentially self-adjoint.

We note that the back transformation of hu gives

$$\mathcal{U}^{-1} hu = h.$$

Further,

$$U_{00}h = U\,\frac{1}{\sqrt{4\pi}}\,(h \circ |\;|).$$

where, see above, $h \in C^{\infty}(I, \mathbb{R})$ is an otherwise arbitrary auxiliary function which is equal to 1 on $(0, 1/4]$ and is equal to 0 on $[3/4, \infty)$. As a consequence,

$$\frac{1}{\sqrt{4\pi}}\,(h \circ |\;|) \in C_0^2(\mathbb{R}^3, \mathbb{C}).$$

In the following, we define

$$D_{00} := C_0^2(J, \mathbb{C}) + \mathbb{C}.hu.$$

From the previous analysis, we conclude that we cannot use Lemma 2.2.2, to conclude the essential self-adjointness of $\hat{H}_0$ for the case of an electron in the Coulomb field of an nucleus containing Z protons. For this reason, like in Sect. 1.6, we extend the minimal Hamiltonian $\hat{H}_0$ in this case to $\hat{H}_1 : C_0^2(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n)$ in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, defined by

$$\hat{H}_1 f := -\frac{\hbar^2\kappa^2}{2m}\,\triangle f - \frac{Ze^2\kappa}{|\;|} f = \frac{\hbar^2\kappa^2}{2m}\left(-\triangle f - \frac{\nu}{|\;|} f\right), \tag{4.10}$$

for every $f \in C_0^2(\mathbb{R}^n, \mathbb{C})$, where

$$\nu := \frac{2mZe^2}{\hbar^2\kappa}$$

is dimensionless. Then $\hat{H}_1$ is densely-defined, since $C_0^2(\mathbb{R}^n, \mathbb{C})$ is a dense subspace of $L^2_{\mathbb{C}}(\mathbb{R}^n)$. Further, as a consequence of the linearity of differentiation and outer multiplication of complex-valued functions by complex numbers, $\hat{H}_1$ is linear. As a consequence of “partial integration,” $\hat{H}_1$ is symmetric, see Lemma 1.2.1. In Sect. 1.6, we already proved that $\hat{H}_1$ is essentially self-adjoint. On the other hand, our previous analysis gives an independent proof of this fact. For this purpose, we use Lemma 2.2.2, where $A = U\hat{H}_1U^{-1}$.[5] Then,

$$(X_{\ell m})_{(\ell,m)\in\mathcal{I}}$$

gives a decomposition of $X = L^2_{\mathbb{C}}(\Omega, u^2\sin(\theta))$ into pairwise orthogonal subspaces. Further, the restrictions of A to the dense subspaces $U_{\ell m}\mathcal{U}^{-1}D_{\ell m}$, $(\ell, m) \in \mathcal{I}$ of $X_{\ell m}$ densely-defined, linear, symmetric and essentially self-adjoint operators in $X_{\ell m}$. Hence it follows from Lemma 2.2.2 that A is essentially self-adjoint. Further, we note that in Sect. 1.6, we proved that the essential spectrum $\sigma_e(\bar{\hat{H}}_1)$ of the closure of $\bar{\hat{H}}_1$ coincides with the essential spectrum of the free Hamiltonian, i.e., that

[5] We mention that in the definition of A we suppress a “trivial” unitary transformation. Strictly speaking, in the definition of A the unitary transformation U should be replaced by the unitary transformation $UV^{-1}_{\mathbb{R}^3\setminus\mathcal{H}}$. Similar is true for the operator $U\hat{H}_0U^{-1}$ above. Also there a trivial unitary transformation is suppressed.

The Essential Spectrum of $\bar{\hat{\bar{H}}}_1$

$$\sigma_e(\bar{\hat{\bar{H}}}_1) = [0, \infty). \tag{4.11}$$

4.4.3 Eigenvalues of $\hat{H}^*_{00e}$ and $\hat{H}^*_{\ell m}$ for $(\ell, m) \in \mathcal{I} \backslash \{(0, 0)\}$

In the next step, we are going to find the eigenvalues and corresponding eigenstates of $\hat{H}^*_{00e}$ and $\hat{H}^*_{\ell m}$ for $(\ell, m) \in \mathcal{I} \backslash \{(0, 0)\}$. For this purpose, we analyze the solutions of the equation

$$f'' + \left(-\sigma^2 + \frac{\nu}{u} - \frac{\Lambda}{u^2}\right) f = 0, \tag{4.12}$$

where $\sigma \in (0, \infty) \times \mathbb{R}$. The parameter $-\sigma^2$ may be regarded as a spectral parameter. [6,7] Using the ansatz

$$f(u) = u^{\ell+1} e^{-\sigma u} g(2\sigma u),$$

where g is a twice complex differentiable function, defined on open subset of $\mathbb{C}$, we arrive at the equation

$$2\sigma u\, g''(2\sigma u) + [2(\ell + 1) - 2\sigma u]\, g'(2\sigma u) - \left[(\ell + 1) - \frac{\nu}{2\sigma}\right] g(2\sigma u) = 0,$$

which is of the form of Kummer's equation. Hence, see [1, 56], solutions are given by

$$\begin{aligned}
f_1 &:= u^{\ell+1} e^{-\sigma u} M\Big((\ell + 1) - \frac{\nu}{2\sigma}, 2(\ell + 1), 2\sigma u\Big) \\
&= u^{\ell+1} e^{\sigma u} M\Big((\ell + 1) + \frac{\nu}{2\sigma}, 2(\ell + 1), -2\sigma u\Big) \\
&= (2\sigma)^{-(\ell+1)} M_{\frac{\nu}{2\sigma}, \ell+\frac{1}{2}}(2\sigma u)\ , \\
f_2 &:= u^{\ell+1} e^{-\sigma u} U\Big((\ell + 1) - \frac{\nu}{2\sigma}, 2(\ell + 1), 2\sigma u\Big) \\
&= (2\sigma)^{-(\ell+1)}\, W_{\frac{\nu}{2\sigma}, \ell+\frac{1}{2}}(2\sigma u)\ ,
\end{aligned} \tag{4.13}$$

where the Whittaker functions M and U are defined according to [1]. If

---

[6] We note that, as a consequence, $-\sigma^2 \in \mathbb{C} \backslash ([0, \infty) \times \{0\})$. On the other hand, according to the asymptotic analysis in Sect. 4.4.1, there are no eigenvalues in the interval $(0, \infty)$, where the below shown fact is used that eigenfunctions are C^∞. That 0 is no eigenvalue will be proved later.

[7] Of course, since the operators in question are self-adjoint, there are no non-real spectral values which include eigenvalues. On the other hand, considering the cases that $-\sigma^2$ is non-real does not involve more effort. In addition, we are going to need later the solutions of (4.12) corresponding to non-real values of $-\sigma^2$.

$$(\ell+1)-\frac{\nu}{2\sigma}\notin -\mathbb{N},$$

these solutions are linearly independent, with Wronskian determinant given by

$$W(f_1,f_2)=f_1f_2'-f_1'f_2=-\frac{\Gamma(2(\ell+1))}{(2\sigma)^{(2\ell+1)}\Gamma((\ell+1)-\frac{\nu}{2\sigma})}.$$

We note that for $(\ell,m)\in\mathcal{I}\setminus\{(0,0)\}$, f_1 is L^2 close to 0, and, according to [1] 13.5.2, f_2 is L^2 close to ∞, but not L^2 close to 0, see [1] 13.5.6, if $(\ell+1)-(\nu/(2\sigma))\notin -\mathbb{N}$. Further for $\ell=m=0$, f_1 is L^2 close to 0 and, according to [1] 13.5.2, f_2 is L^2 close to ∞,

$$\begin{aligned}&u^2\left(\frac{f_1}{u}\right)'\\&=\sigma u^2e^{-\sigma u}\left[-M\left(1-\frac{\nu}{2\sigma},2,2u\sigma\right)+\left(1-\frac{\nu}{2\sigma}\right)M\left(2-\frac{\nu}{2\sigma},3,2u\sigma\right)\right]\to 0,\end{aligned}$$

for $u\to 0$, whereas f_2, see [1] 13.5.7, is L^2 close to 0, if $1-(\nu/(2\sigma))\notin -\mathbb{N}$, but

$$\begin{aligned}&u^2\left(\frac{f_2}{u}\right)'\\&=-\sigma u^2e^{-\sigma u}\left[U\left(1-\frac{\nu}{2\sigma},2,2u\sigma\right)+2\left(1-\frac{\nu}{2\sigma}\right)e^{-u\sigma}\,U\left(2-\frac{\nu}{2\sigma},3,2u\sigma\right)\right]\\&\quad\to -2\sigma\left(1-\frac{\nu}{2\sigma}\right)\frac{1}{\Gamma(2-\frac{\nu}{2\sigma})}=-\frac{2\sigma}{\Gamma(1-\frac{\nu}{2\sigma})},\end{aligned}$$

for $u\to 0$, see [1] 13.5.6 and 13.5.7, if $1-(\nu/(2\sigma))\notin -\mathbb{N}$, i.e., f_1 is in the domain of $\mathcal{U}\hat{H}_{00e}\mathcal{U}^{-1}$ close to 0, but f_2 is not in the domain of $\mathcal{U}\hat{H}_{00e}\mathcal{U}^{-1}$ close to 0, if $1-(\nu/(2\sigma))\notin -\mathbb{N}$.

In a first step, we investigate the regularity or "smoothness" of eigenfunctions, i.e., how "smooth" eigenfunctions are, if existent. For this purpose, we use Theorem 3.4.2 (iv). In addition, we choose $\sigma=(1+i)/\sqrt{2}$ such that $\sigma^2=i$ Then f_1 and f_2 satisfy the assumptions of Theorem 3.4.2 (iv), where

$$D^2_{p,q}=\left(C^2(I,\mathbb{C})\to C(I,\mathbb{C}),\, f\mapsto -f''+\left(-\frac{\nu}{u}+\frac{\Lambda}{u^2}\right)f\right).$$

Hence, the resolvent of the operator $A_{\ell m}$ corresponding to $D^2_{p,q}$ is given by (3.21). If λ is an eigenvalue of $A_{\ell m}$ and f a corresponding eigenvector, then

$$(A_{\ell m}+\sigma^2)f=(\lambda+\sigma^2)f$$

and hence

$$f=(\lambda+\sigma^2)(A_{\ell m}+\sigma^2)^{-1}f\ .$$

Hence, f is continuous. Reiterating this argument, it follows that f is C^∞. This argument can be used for $(\ell, m) \in \mathcal{I}\backslash\{(0,0)\}$. For $\ell = m = 0$, this argument applies, too, since it is easy to show that also in this case $(\hat{A}^*_{00} + \sigma^2)^{-1}$, where $\hat{A}^*_{00}$ is the closure of the extension $\hat{A}_{00}$ of the corresponding A_{00}, with a domain whose elements satisfy (4.9), is given by (3.21), too. Corresponding details are left to the reader.

Exercise 12

Show that $(\hat{A}^*_{00} + \sigma^2)^{-1}$, where $\hat{A}^*_{00}$ is the closure of the extension $\hat{A}_{00}$ of the corresponding A_{00}, with a domain whose elements satisfy (4.9), is given by (3.21).

In the next step, we show that 0 is no eigenvalue. For this purpose, we need to analyze the solutions of

$$f'' + \left(\frac{\nu}{u} - \frac{\Lambda}{u^2}\right) f = 0. \tag{4.14}$$

Using the ansatz

$$f(u) = \sqrt{u}\, g(2\sqrt{\nu u}\,)$$

into (4.2), where g is a twice differentiable function on I, we arrive at the equation

$$\begin{aligned}&(2\sqrt{\nu u}\,)^2 g''(2\sqrt{\nu u}\,) + 2\sqrt{\nu u}\, g'(2\sqrt{\nu u}\,)\\&+ [(2\sqrt{\nu u}\,)^2 - (4\ell^2 + 4\ell + 1)]\, g(2\sqrt{\nu u}\,) = 0,\end{aligned}$$

which is of the type of a Bessel equation. Hence, linearly independent solutions are given by

$$f_3 = \sqrt{u}\, J_{2\ell+1}(2\sqrt{\nu u}\,)\ ,\quad f_4 = \sqrt{u}\, Y_{2\ell+1}(2\sqrt{\nu u}\,)\ .$$

According to [1, 56], these are not square integrable, and hence 0 is no eigenvalue.

For the final step, we return to (4.13). Since, see [1] 13.1.4, except when

$$(\ell + 1) - \frac{\nu}{2\sigma} = 0, -1, -2, \ldots$$

(polynomial cases), for $\mathrm{Re}(2\sigma u) > 0$,

$$f_1(u) \underset{|u|\to\infty}{\sim} (2\sigma)^{-\frac{\nu}{2\sigma}-(\ell+1)} \frac{\Gamma(2(\ell+1))}{\Gamma(\ell + 1 - \frac{\nu}{2\sigma})}\, u^{-\frac{\nu}{2\sigma}} e^{\sigma u} \left[1 + O\left(\frac{1}{2|\sigma|u}\right)\right]\ ,$$

it follows that $-\sigma^2$ is an eigenvalue of $\frac{2m}{\hbar^2\kappa^2}\,\hat{H}^*_{00e}$ and $\frac{2m}{\hbar^2\kappa^2}\,\hat{H}^*_{\ell m}$ for $(\ell, m) \in \mathcal{I}\backslash\{(0,0)\}$, respectively, if and only if

$$(\ell + 1) - \frac{\nu}{2\sigma} = -n,$$

for some $n \in \mathbb{N}$ and hence if and only if

Table 4.1 Table of generalized Laguerre polynomials, where $x > 0$. For fixed $\ell \in \mathbb{N}$, n runs through the natural numbers from $\ell + 1$ to ∞

$L^{(2\ell+1)}_{n-(\ell+1)}(x)$	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$
$n = 1$	1	$2 - x$	$\frac{1}{2}\left(6 - 6x + x^2\right)$	$\frac{1}{6}\left(24 - 36x + 12x^2 - x^3\right)$
$n = 2$	N/A	1	$4 - x$	$\frac{1}{2}\left(20 - 10x + x^2\right)$
$n = 3$	N/A	N/A	1	$6 - x$
$n = 4$	N/A	N/A	N/A	1

$$\sigma = \frac{\nu}{2(n + \ell + 1)}.$$

As a consequence, the set of eigenvalues $\sigma_p(\hat{H}^*_{00e})$ of $\hat{H}^*_{00e}$ and the set of eigenvalues $\sigma_p(\hat{H}^*_{\ell m})$ of $\hat{H}^*_{00e}$ for $(\ell, m) \in \mathcal{I}\backslash\{(0, 0)\}$, respectively, is given by

Eigenvalues of $\hat{H}^*_{00e}$ and $\hat{H}^*_{00e}$ for $(\ell, m) \in \mathcal{I}\backslash\{(0, 0)\}$

$$\sigma_p(\hat{H}^*_{00e}) = -Z^2 \frac{me^4}{2\hbar^2} \cdot \left\{\frac{1}{n^2} : n \in \{1, 2, \dots\}\right\},$$
$$\sigma_p(\hat{H}^*_{\ell m}) = -Z^2 \frac{me^4}{2\hbar^2} \cdot \left\{\frac{1}{n^2} : n \in \{\ell + 1, \ell + 2, \dots\}\right\},$$

for every $(\ell, m) \in \mathcal{I}\backslash\{(0, 0)\}$,

with corresponding eigenfunctions

$$\begin{aligned} f_1(u) &= u^{\ell+1} e^{-\frac{\nu u}{2n}} M\left(\ell + 1 - n\,,\ 2(\ell + 1)\,,\ \frac{\nu u}{n}\right) \\ &= \binom{n + \ell}{2\ell + 1}^{-1} \cdot u^{\ell+1} e^{-\frac{\nu u}{2n}} L^{(2\ell+1)}_{n-(\ell+1)}\left(\frac{\nu u}{n}\right), \end{aligned}$$

and the $L^{(2\ell+1)}_{n-(\ell+1)}$ are generalized Laguerre polynomials, the latter defined according to [1, 56], i.e., consists of infinitely simple eigenvalues, for every $\ell \in \mathbb{N}$ (Table 4.1).

We note that in the case of the hydrogen atom m is the mass of an electron and e the elementary charge. Then[8]

[8] Here c denotes the speed of light in vacuum, and $e^2/(\hbar c)$ is the so called fine structure constant.

$$\boxed{\frac{me^4}{2\hbar^2} = \left(\frac{e^2}{\hbar c}\right)^2 \frac{mc^2}{2} \approx 13.6 \text{ eV}.}$$

As a consequence, we have the following relation between the principal quantum number n and the orbital angular momentum quantum number[9] ℓ as displayed in Table 4.2

Relationship between the Principal Quantum Number n and the Orbital Angular Momentum Quantum Number ℓ.

Table 4.2 Relation between the principal quantum number n and the orbital angular momentum quantum number ℓ. For fixed ℓ, n runs from $\ell + 1$ to ∞

$\ell = 0$	n:	1	2	3	4	$\cdots$
$\ell = 1$	n:		2	3	4	$\cdots$
$\ell = 2$	n:			3	4	$\cdots$
$\ell = 3$	n:				4	$\cdots$

Another way of displaying this relationship is as follows (Table 4.3):

Principal Relationship between the Principal Quantum Number n, the Orbital Angular Momentum Quantum Number ℓ and Magnetic Quantum Number m.

Table 4.3 For every $n \in \mathbb{N}^*$, ℓ runs from 0 to $n - 1$ and for every $\ell \in \mathbb{N}^*$, m runs from $-\ell$ to ℓ. In spectroscopy, the letters $s, p, d, f, g, \ldots$ correspond to $\ell = 0, 1, 2, 3, 4, \ldots$, respectively

	s	p	d
$n = 1$	$\ell = 0$ $m = 0$		
$n = 2$	$\ell = 0$ $m = 0$	$\ell = 1$ $m = -1$ $m = 0$ $m = 1$	
$n = 3$	$\ell = 0$ $m = 0$	$\ell = 1$ $m = -1$ $m = 0$ $m = 1$	$\ell = 2$ $m = -2$ $m = -1$ $m = 0$ $m = 1$ $m = 2$

[9] The quantum number m is called the magnetic quantum number.

Hence for every $n \in \mathbb{N}^*$, the corresponding energy level

$$E_n := -Z^2 \frac{me^4}{2\hbar^2} \cdot \frac{1}{n^2}$$

is degenerate of the order

$$\sum_{\ell=0}^{n-1}(2\ell+1) = 2\sum_{\ell=0}^{n-1}\ell + n = 2\sum_{\ell=1}^{n-1}\ell + n = 2\,\frac{n-1}{2}\,n + n = n^2 \;.$$

In spectroscopy, the corresponding eigenstates are designated by the non-vanishing natural number n, followed by a letter (s, p, d, f, g, ...) indicating the value of ℓ. The quantum number m is not mentioned. Thus the ground state is a 1s state, the first-excited state is four-fold degenerate and contains one 2s state and three 2p states; the second-excited state is nine-fold degenerate and contains one 3s state, three 3p states and five 3d states; and so forth.

4.4.4 Corresponding Normalized Eigenfunctions

Eigenvectors of the Hamiltonian H in the Position Representation

With the help of Lemma 12.9.29, we arrive at the following family of normalized eigenfunctions $(e_{\ell mn})_{(\ell,m,n)\in\mathcal{I}\times\{\ell+1,\ell+2,\dots\}}$ of the Hamiltonian H, where for every $(\ell, m, n) \in \mathcal{I} \times \{\ell+1, \ell+2, \dots\}$, $e_{\ell mn} : \mathbb{R}^3\backslash(\{(0,0)\}\times\mathbb{R}) \to \mathbb{C}$, defined by

$$\begin{aligned}
&e_{\ell mn}(\mathbf{u}) \\
&= \sqrt{\frac{1}{8\pi}\cdot(2\ell+1)\cdot\frac{(\ell-m)!}{(\ell+m)!}\cdot\frac{[n-(\ell+1)]!}{n(n+\ell)!}\left(\frac{\nu}{n}\right)^3} \\
&\quad\cdot\left(\frac{\nu|\mathbf{u}|}{n}\right)^{\ell} e^{-\frac{\nu|\mathbf{u}|}{2n}} L_{n-(\ell+1)}^{(2\ell+1)}\!\left(\frac{\nu|\mathbf{u}|}{n}\right)\cdot P_\ell^m\!\left(\frac{u_3}{|\mathbf{u}|}\right)\cdot\left(\frac{u_1+iu_2}{|u_1+iu_2|}\right)^m,
\end{aligned}$$

for every $\mathbf{u} = (u_1, u_2, u_3) \in \mathbb{R}^3\backslash(\{(0,0)\}\times\mathbb{R})$, where

$$\nu := \frac{2mZe^2}{\hbar^2\kappa},$$

the associated Legendre polynomials of the first kind P_ℓ^m are defined according to Lemma 2.4.2 and the generalized Laguerre polynomials $L_{n-(\ell+1)}^{(2\ell+1)}$ are defined according to [1, 56], is a normalized eigenvector of H corresponding to the eigenvalue

$$E_n := -Z^2\frac{me^4}{2\hbar^2}\cdot\frac{1}{n^2} = -Z^2\left(\frac{e^2}{\hbar c}\right)^2\frac{mc^2}{2}\cdot\frac{1}{n^2}.$$

In the following, we choose the scale κ

$$\kappa := \left(\frac{\hbar^2}{me^2}\right)^{-1}, \tag{4.15}$$

implying that

$$\nu = 2Z.$$

For the case of the hydrogen atom, $Z = 1$, m is the mass of an electron and e the elementary charge. Then[10] κ is the inverse of the so called "Bohr radius" a_0, defined by

$$a_0 := \frac{\hbar^2}{me^2} = \left(\frac{e^2}{\hbar c}\right)^{-1} \frac{\hbar}{mc} \approx 0.53 \cdot 10^{-10}\ \mathrm{m} = 0.53\,\text{Å}.$$

We note that for every $(\ell, m, n) \in \mathcal{I} \times \{\ell+1, \ell+2, \dots\}$,

$$(Ue_{\ell mn})(u, \theta, \varphi) = \sqrt{\left(\frac{\nu}{n}\right)^3 \frac{[n-(\ell+1)]!}{2n(n+\ell)!}} \left(\frac{\nu u}{n}\right)^{\ell} e^{-\frac{\nu u}{2n}} L^{(2\ell+1)}_{n-(\ell+1)}\left(\frac{\nu u}{n}\right) Y_{\ell m}(\theta, \varphi),$$

for all $(u, \theta, \varphi) \in (0, \infty) \times (0, \pi) \times (-\pi, \pi)$.

Further, we note that all eigenvectors are axially symmetric, i.e., rotational symmetric around the u_3-axis. Indeed, this is due to our decomposition and not a physical feature. It is not difficult to give a decomposition that singles out any given axis through the origin and that leads to eigenvectors of H that are axially symmetric around that axis.

Probability Distributions Associated with the Eigenvectors of the Hamiltonian H and Position Measurement

Using the scale (4.15), the probability distribution corresponding to the position measurement of the particle and the state $\mathbb{C}^*.e_{\ell mn}$ is given by

$$\begin{aligned} &|\, e_{\ell mn}(\mathbf{u})|^2 \\ &= \frac{1}{8\pi} \cdot (2\ell+1) \cdot \frac{(\ell-m)!}{(\ell+m)!} \cdot \frac{[n-(\ell+1)]!}{n(n+\ell)!} \left(\frac{2Z}{n}\right)^3 \\ &\quad \cdot \left(\frac{Z|\mathbf{u}|}{2}\right)^{2\ell} e^{-\frac{2Z|\mathbf{u}|}{n}} \left[L^{(2\ell+1)}_{n-(\ell+1)}\left(\frac{2Z|\mathbf{u}|}{n}\right)\right]^2 \cdot \left[P^m_\ell\left(\frac{u_3}{|\mathbf{u}|}\right)\right]^2, \end{aligned}$$

for every $\mathbf{u} = (u_1, u_2, u_3) \in \mathbb{R}^3 \backslash \{(0,0,0)\}$ (Figs. 4.1 and 4.2).

---

[10] If m is the mass of an electron and e the elementary charge, the quantity $a_0 := \frac{\hbar^2}{me^2}$ is called the "Bohr radius" and $\frac{\hbar}{mc}$ is the reduced Compton wavelength of the electron.

To facilitate the interpretation of the graphics of some of the orbitals of the hydrogen atom later on, we give the following reminder. If the particle is in the state $\mathbb{C}^*.e_{\ell mn}$,[11] for some $(\ell, m, n) \in \mathcal{I} \times \{\ell+1, \ell+2, \dots\}$, the probability of finding the position of the particle to belong to the interval $I_1 \times I_2 \times I_3$ in physical space, where

$$I_k = [a_k \kappa^{-1}, b_k \kappa^{-1}],$$

$a_k \in \mathbb{R}$, $b_k \in \mathbb{R}$, $a_k \leqslant b_k$ are dimensionless, for every $k \in \{1, 2, 3\}$, is given by

$$\begin{aligned}&\int_{[a_1,b_1]\times[a_2,b_2]\times[a_3,b_3]} |e_{\ell mn}(\mathbf{u})|^2 \, du_1 du_2 du_3 \\ &= \int_{I_1\times I_2\times I_3} \kappa^3 |e_{\ell mn}(\kappa \mathbf{x})|^2 \, dx_1 dx_2 dx_3,\end{aligned}$$

where $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ are points in physical space. As we already know, in a position representation, the coordinates u_1, u_2, u_3 of points $\mathbf{u} = (u_1, u_2, u_3)$ in the domains of functions belonging to the representation space can be interpreted as numbers whose multiplication by the unit of length κ^{-1} lead to a point $\kappa^{-1}\mathbf{u} = (\kappa^{-1}u_1, \kappa^{-1}u_2, \kappa^{-1}u_3)$ in physical space. In the case of a hydrogen atom, κ^{-1} is given by the Bohr radius a_0.

4.4.5 Continuous Spectrum of $\hat{H}^*_{00e}$ and $\hat{H}^*_{\ell m}$ for $(\ell, m) \in \mathcal{I} \setminus \{(0, 0)\}$

For $\lambda > 0$, we showed in Sect. 4.4.1 the existence of corresponding linearly independent solutions $f \in C^2(I, \mathbb{C})$ and $R \in C^1\big(I, \mathbb{C}^2\big)$ of

$$-f'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2}\right) f - \lambda f = 0$$

such that

$$\begin{aligned}&f = \exp(i\sqrt{\lambda}\, h) \cdot (1 + R_1), \quad f' = \exp(i\sqrt{\lambda}\, h) \cdot (i\sqrt{\lambda} \cdot h' + R_2), \\ &\lim_{u\to\infty} |R(u)| = 0.\end{aligned}$$

We note that, since

$$\lim_{u\to\infty} |R(u)| = 0,$$

there is $u_0 > 1$ such that

$$|f(u)| = |1 + R_1(u)| \geqslant \frac{1}{2},$$

[11] The analogous is true for any other state $\mathbb{C}^*.f$, where $f \in L^2_{\mathbb{C}}(\mathbb{R}^3)$ is such that $\|f\|_2 = 1$.

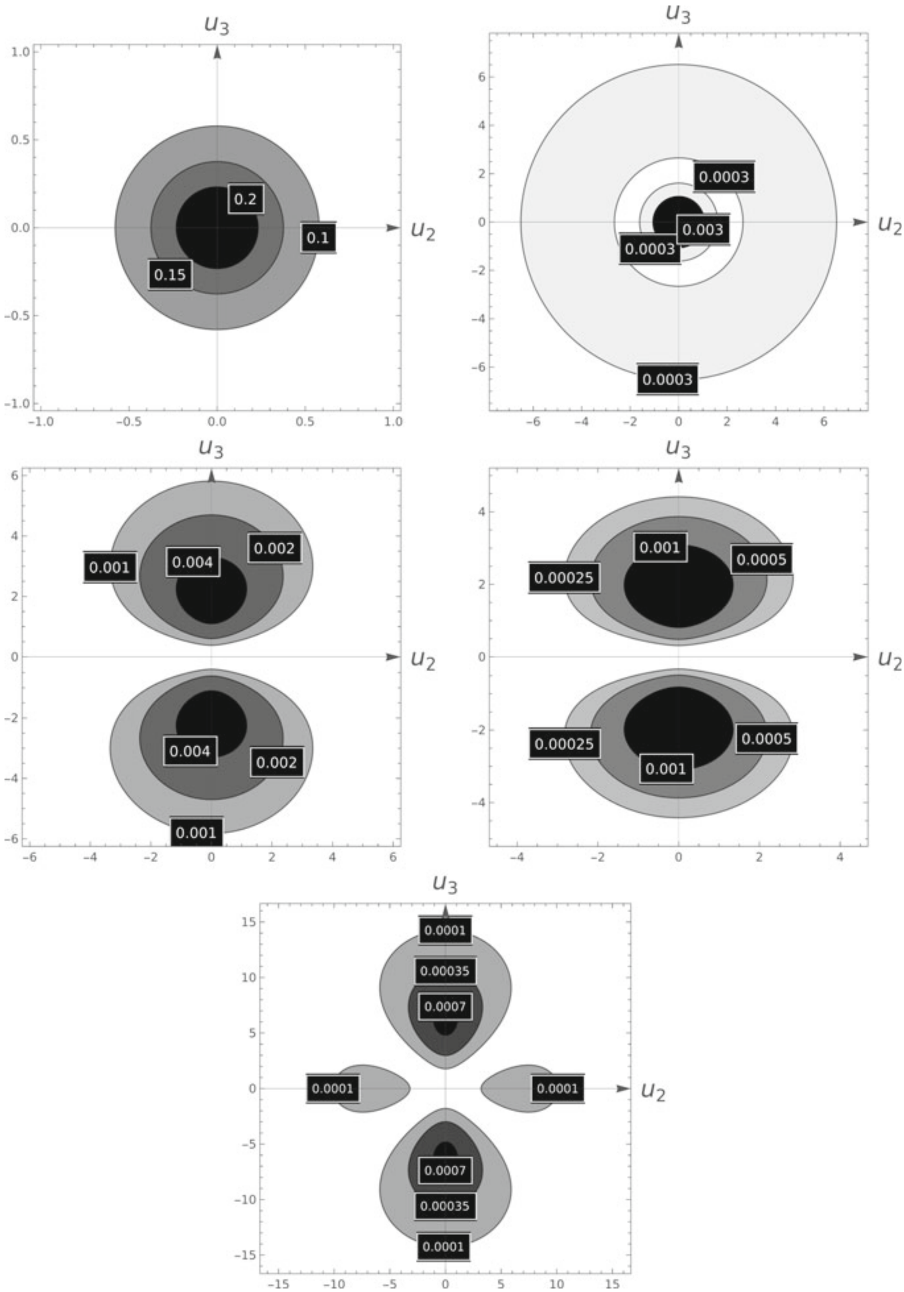


Fig. 4.1 Contour plots of the restrictions to the u_2, u_3-plane of the probability distributions corresponding to $1s$, $2s$, $2p$, $3p$ and $3d$ states. Relatively darker colors indicate relatively higher probabilities. The complete distribution is obtained by rotation around the u_3-axis

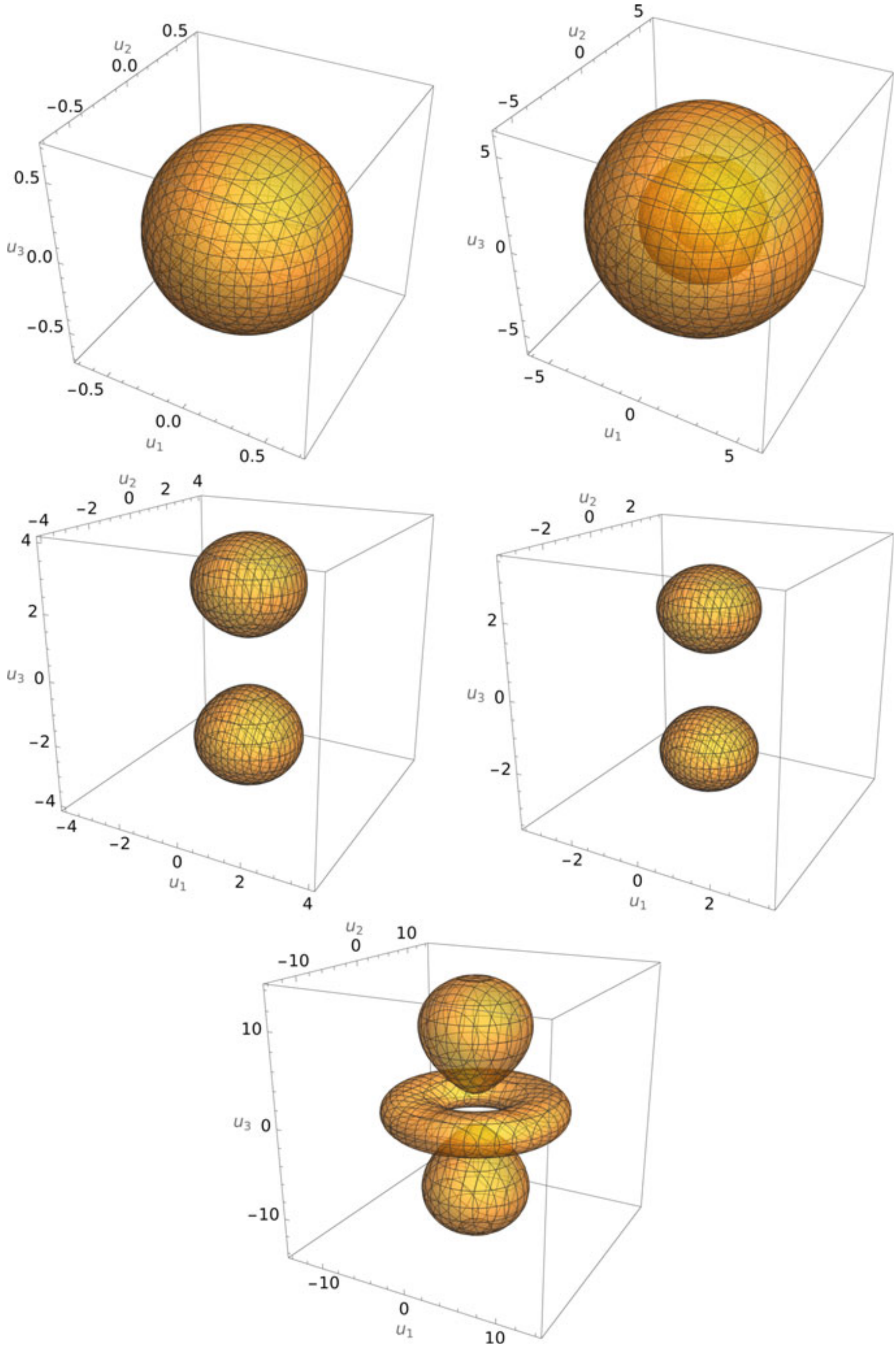


Fig. 4.2 Region plots of the probability distributions corresponding to $1s$, $2s$, $2p$, $3p$ and $3d$ states of the hydrogen atom and probabilities larger than 0.1, 0.0005, 0.003, 0.001 and 0.0001, respectively

for $u \geqslant u_0$. Further, let $\varphi \in C_0^2(I, \mathbb{C})$ be non-trivial and such that

$$\operatorname{supp}(\varphi) \subset [u_0, \infty).$$

We define for $\mu \in \mathbb{N}^*$, $f_\mu \in C_0^2(I, \mathbb{C})$ by

$$f_\mu := \mu^{-1/2}\, \varphi\left(\frac{u}{\mu}\right) \cdot f.$$

Then

$$\begin{aligned}
\|f_\mu\|_2^2 = \mu^{-1} \left\| \varphi\left(\frac{u}{\mu}\right) \cdot f \right\|_2^2 &= \mu^{-1} \int_0^\infty \left|\varphi\left(\frac{u}{\mu}\right)\right|^2 \cdot |f(u)|^2\, du \\
&\leqslant C_f^2\, \mu^{-1} \int_0^\infty \left|\varphi\left(\frac{u}{\mu}\right)\right|^2 du = C_f^2\, \|\varphi\|_2^2,
\end{aligned}$$

where $C_f > 0$ is such that

$$|f(u)| \leqslant C_f.$$

for every $u \geqslant u_0$. We note that

$$\|f_\mu\|_2^2 = \mu^{-1} \int_0^\infty \left|\varphi\left(\frac{u}{\mu}\right)\right|^2 \cdot |f(u)|^2\, du \geqslant (4\mu)^{-1} \int_0^\infty \left|\varphi\left(\frac{u}{\mu}\right)\right|^2 du = \frac{\|\varphi\|^2}{4},$$

and hence that

$$\frac{1}{\|f_\mu\|_2} \leqslant \frac{2}{\|\varphi\|_2},$$

for every $\mu \in \mathbb{N}^*$. In addition, let $C_{f'} > 0$ such that

$$|f'(u)| \leqslant C_{f'}.$$

for every $u \geqslant 1$. We note that such $C_{f'} > 0$ exists, in particular, since

$$h'(u) \leqslant \sqrt{1 + \frac{\nu}{\lambda}},$$

for every $u \geqslant 1$. Hence, it follows that

$$-f_\mu'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2}\right) f_\mu - \lambda f_\mu = -\frac{2}{\mu^{3/2}}\, \varphi'\left(\frac{u}{\mu}\right) f' - \frac{1}{\mu^{5/2}}\, \varphi''\left(\frac{u}{\mu}\right) f$$

and

$$
\begin{aligned}
&\left\| -f_\mu'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2} \right) f_\mu - \lambda f_\mu \right\|_2 \\
&\leqslant \frac{2}{\mu^{3/2}} \left\| \varphi'\left(\frac{u}{\mu}\right) f' \right\|_2 + \frac{1}{\mu^{5/2}} \left\| \varphi''\left(\frac{u}{\mu}\right) f \right\|_2 \\
&= \frac{2}{\mu^{3/2}} \left[\int_0^\infty \left| \varphi'\left(\frac{u}{\mu}\right) \right|^2 |f'|^2 \, du \right]^{1/2} + \frac{1}{\mu^{5/2}} \left[\int_0^\infty \left| \varphi''\left(\frac{u}{\mu}\right) \right|^2 |f|^2 \, du \right]^{1/2} \\
&\leqslant \frac{2C_{f'}}{\mu^{3/2}} \left[\int_0^\infty \left| \varphi'\left(\frac{u}{\mu}\right) \right|^2 du \right]^{1/2} + \frac{C_f}{\mu^{5/2}} \left[\int_0^\infty \left| \varphi''\left(\frac{u}{\mu}\right) \right|^2 du \right]^{1/2} \\
&= \frac{2C_{f'}}{\mu} \|\varphi'\|_2 + \frac{C_f}{\mu^2} \|\varphi''\|_2 .
\end{aligned}
$$

As a consequence,

$$
\lim_{\mu \to \infty} \left\| -f_\mu'' + \left(-\frac{\nu}{u} + \frac{\Lambda}{u^2} \right) f_\mu - \lambda f_\mu \right\|_2 = 0.
$$

Therefore, we conclude from Theorem 12.5.3 that

$$
\sigma(\hat{H}_{00e}^*) \supset (0, \infty), \;\; \sigma(\hat{H}_{\ell m}^*) \supset (0, \infty)
$$

and, since spectra of DSLO are closed subsets of $\mathbb{R}$, that

$$
\boxed{\sigma(\hat{H}_{00e}^*) \supset [0, \infty), \;\; \sigma(\hat{H}_{\ell m}^*) \supset [0, \infty),}
$$

for every $(\ell, m) \in \mathcal{I} \backslash \{(0, 0)\}$.

4.4.6 The Spectrum of $\hat{H}_{00e}^*$ and $\hat{H}_{\ell m}^*$ for $(\ell, m) \in \mathcal{I} \backslash \{(0, 0)\}$

Summarizing our results concerning the spectra of the reduced operators, we have that

$$
\begin{aligned}
\sigma(\hat{H}_{00e}^*) &\supset -Z^2 \frac{me^4}{2\hbar^2} \left\{ 1, \frac{1}{4}, \frac{1}{9}, \ldots \right\} \cup [0, \infty), \\
\sigma(\hat{H}_{\ell m}^*) &\supset -Z^2 \frac{me^4}{2\hbar^2} \left\{ \frac{1}{(\ell+1)^2}, \frac{1}{(\ell+2)^2}, \ldots \right\} \cup [0, \infty).
\end{aligned}
$$

for every $(\ell, m) \in \mathcal{I} \backslash \{(0, 0)\}$. In the following, we are going to show that these sets related by inclusion signs are actually equal.

The Spectra of $\hat{H}^*_{00e}$ and $\hat{H}^*_{\ell m}$ for $(\ell, m) \in \mathcal{I}\backslash\{(0,0)\}$

are given by

$$\sigma(\hat{H}^*_{00e}) = -Z^2 \frac{me^4}{2\hbar^2}\left\{1, \frac{1}{4}, \frac{1}{9}, \dots\right\} \cup [0, \infty), \tag{4.16}$$

$$\sigma(\hat{H}^*_{\ell m}) = -Z^2 \frac{me^4}{2\hbar^2}\left\{\frac{1}{(\ell+1)^2}, \frac{1}{(\ell+2)^2}, \dots\right\} \cup [0, \infty),$$

for every $(\ell, m) \in \mathcal{I}\backslash\{(0,0)\}$.

For this purpose, we go back to the Hamiltonian $\bar{\hat{H}}_1$, see (4.10), from Sect. 4.4.2. It follows from Theorem 12.9.5 in the Apppendix, that the set of eigenvalues $\sigma_p(\bar{\hat{H}}_1)$ of $\bar{\hat{H}}_1$ is given by

$$\sigma_p(\bar{\hat{H}}_1) = \bigcup_{l=0}^{\infty} -Z^2 \frac{me^4}{2\hbar^2}\left\{\frac{1}{(\ell+1)^2}, \frac{1}{(\ell+2)^2}, \dots\right\}.$$

Since $\sigma_p(\bar{\hat{H}}_1)$ is a discrete set, consisting of simple eigenvalues, it follows that the discrete spectrum $\sigma_d(\bar{\hat{H}}_1)$ of $\bar{\hat{H}}_1$ coincides with $\sigma_p(\bar{\hat{H}}_1)$. Since the essential spectrum $\sigma_e(\bar{\hat{H}}_1)$ of $\bar{\hat{H}}_1$ is given by $[0, \infty)$, see (4.11), it follows that the spectrum $\sigma(\bar{\hat{H}}_1)$ of $\bar{\hat{H}}_1$ is given by

The Spectrum $\sigma(\bar{\hat{H}}_1)$ of $\bar{\hat{H}}_1$

is given by

$$\sigma(\bar{\hat{H}}_1) = [0, \infty) \cup \bigcup_{l=0}^{\infty} -Z^2 \frac{me^4}{2\hbar^2}\left\{\frac{1}{(\ell+1)^2}, \frac{1}{(\ell+2)^2}, \dots\right\}. \tag{4.17}$$

Finally, via Theorem 12.9.5, the latter implies (4.16).

Exercise 13

The reduced operators, corresponding to the distance of the particle from the origin coincide with the maximal multiplication operator with the function

$$T = \frac{1}{\kappa}\,\mathrm{id}_I,$$

and the reduced operators, corresponding to the component of the velocity of the particle tangential to concentric circles around the axis $\{0\} \times \{0\} \times \mathbb{R}$, are given by the maximal multiplication operators with the function

$$T_m = m\,\frac{\hbar\kappa}{m}\,\frac{1}{\mathrm{id}_I},$$

where $m \in \mathbb{Z}$. Calculate the expectation values of these operators in the states corresponding to the eigenfunction $e_{\ell mn}$, $(\ell, m, n) \in \mathcal{I} \times \{\ell+1, \ell+2, \dots\}$, and compare the latter to the speed of light.

5 Motion in an Axially-Symmetric Force Field

In a position representation, the minimal Hamiltonian for a particle subject to an axially-symmetric potential $V \circ (\sqrt{u_1^2 + u_2^2}, u_3)$, where for every $k \in \{1, 2, 3\}$ the corresponding u_k denotes the projection of $\mathbb{R}^3$ onto the kth coordinate and $V : (0, \infty) \times \mathbb{R} \to \mathbb{R}$ is a continuous function, is given by

$$\hat{H}_0 = \begin{pmatrix} C_0^2(\mathbb{R}^3, \mathbb{C}) \to L_{\mathbb{C}}^2(\mathbb{R}^3) \\ f \mapsto -\frac{\hbar^2 \kappa^2}{2m} \triangle f + \left[V \circ (\sqrt{u_1^2 + u_2^2}, u_3)\right] \cdot f \end{pmatrix},$$

where we assume that $\left[V \circ (\sqrt{u_1^2 + u_2^2}, u_3)\right] \cdot f \in L_{\mathbb{C}}^2(\mathbb{R}^3)$, for every $f \in C_0^2(\mathbb{R}^3, \mathbb{C})$.

With the help of Lemma 1.2.1, it follows that the operator $\hat{H}_0$ is densely-defined, linear and symmetric. In the following, we are going to use the axial symmetry of the system to define the Hamiltonian as a direct sum of a countable number of densely-defined, linear and symmetric operators. For this, in a first step, we change the representation, using a unitary transformation U induced by cylindrical coordinates.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_5.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_5

5.1 A Change of Representation Induced by Introduction of Cylindrical Coordinates

First, we note the following Lemmas, whose proof is left to the reader.

Lemma 5.11 (Transformation of the Laplace Operator into Cylindrical Coordinates) *For this, let $\Omega \subset \mathbb{R}^3 \setminus (\{0\} \times \{0\} \times \mathbb{R})$ be non-empty and open. In addition, let $\Omega_{cyl} \subset \mathbb{R}^3$ be a non-empty open subset such*

$$g(\Omega_{cyl}) = \Omega \ ,$$

where $g \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ is defined by

$$g(u, \varphi, z) := (u \cos(\varphi), u \sin(\varphi), z)$$

for all $(u, \varphi, z) \in \mathbb{R}^3$. Finally, let $f \in C^2(\Omega, \mathbb{R})$. Then

$$\begin{aligned}(\triangle f)(g(u, \varphi, z)) = {} & \frac{\partial^2 \bar{f}}{\partial u^2}(u, \varphi, z) + \frac{1}{u}\frac{\partial \bar{f}}{\partial u}(u, \varphi, z) + \frac{1}{u^2}\frac{\partial^2 \bar{f}}{\partial \varphi^2}(u, \varphi, z) \\ & + \frac{\partial^2 \bar{f}}{\partial z^2}(u, \varphi, z) \end{aligned} \tag{5.1}$$

for all $(u, \varphi, z) \in \Omega_{cyl}$, where $\bar{f} \in C^2(\Omega_{cyl}, \mathbb{R})$ is defined by

$$\bar{f}(u, \varphi, z) := (f \circ g)(u, \varphi, z) = f(u \cos(\varphi), u \sin(\varphi), z)$$

for all $(u, \varphi, z) \in \Omega_{cyl}$.

Exercise 14

- Prove Lemma 5.11.

Lemma 5.12 (Transformation of $\hat{L}_{30}$ into Cylindrical Coordinates) *For this, let $\Omega \subset \mathbb{R}^3$ be non-empty and open. In addition, let $\Omega_{sph} \subset \mathbb{R}^3$ be a non-empty open subset such*

$$g(\Omega_{sph}) = \Omega \ ,$$

where $g \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ is defined by

$$g(u, \varphi, z) := (u \cos(\varphi), u \sin(\varphi), z) \ ,$$

for all $(u, \varphi, z) \in \Omega_{sph}$. Finally, let $f \in C^1(\Omega, \mathbb{R})$. Then

$$\left(u_1 \frac{\partial f}{\partial u_2} - u_2 \frac{\partial f}{\partial u_1}\right)(g(u, \varphi, z)) = \frac{\partial \bar{f}}{\partial \varphi}(u, \varphi, z) \ , \tag{5.2}$$

for all $(u, \varphi, z) \in \Omega_{sph}$, *where* $\bar{f} \in C^1(\Omega_{sph}, \mathbb{R})$ *is defined by*

$$\bar{f}(u, \varphi, z) := (f \circ g)(u, \varphi, z) = f(u\cos(\varphi), u\sin(\varphi), z) \ ,$$

for all $(u, \varphi, z) \in \Omega_{sph}$.

The map g induces the unitary transformation

$$U : L^2_{\mathbb{C}}(\mathbb{R}^3) \to L^2_{\mathbb{C}}(\Omega, u) \ ,$$

where $\Omega := (0, \infty) \times (-\pi, \pi) \times \mathbb{R}$, defined by

$$Uf := f \circ g|_{\Omega} \ , \tag{5.3}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^3)$. The inverse U^{-1} of U is given by

$$U^{-1}f := f \circ (g|_{\Omega})^{-1} \ ,$$

for every $f \in L^2_{\mathbb{C}}(\Omega, u)$, where $(g|_{\Omega})^{-1} : \mathbb{R}^3 \backslash \mathcal{Z} \to \Omega$ is given by

$$(g|_{\Omega})^{-1}(u) = \begin{cases} (\sqrt{u_1^2 + u_2^2}\,, \arccos(u_1/\sqrt{u_1^2+u_2^2}\,)\,, u_3) & \text{if } u_2 > 0 \\ (\sqrt{u_1^2 + u_2^2}\,, -\arccos(u_1/\sqrt{u_1^2+u_2^2}\,)\,, u_3) & \text{if } u_2 < 0 \end{cases}$$

for all $u = (u_1, u_2, u_3) \in \mathbb{R}^3 \backslash \mathcal{Z}$. Here, $\mathcal{Z} := (-\infty, 0] \times \{0\} \times \mathbb{R}$ is a closed Lebesgue zero set. The proof that U is indeed a unitary linear transformation is mainly an application of Lebesgue's change of variable formula and is left to the reader.

Exercise 15

Show that U is a unitary linear transformation.

As a consequence of Lemma 5.11, it follows that $U\hat{H}_0U^{-1}$ is given by

$$\begin{aligned} U\hat{H}_0U^{-1}f &= -\frac{\hbar^2\kappa^2}{2m}\left(\frac{\partial^2}{\partial u^2} + \frac{1}{u}\frac{\partial}{\partial u} + \frac{1}{u^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2} - \frac{2m}{\hbar^2\kappa^2}V(u,z)\right)f \\ &= -\frac{\hbar^2\kappa^2}{2m}\left(\frac{1}{u}\frac{\partial}{\partial u}u\frac{\partial}{\partial u} + \frac{1}{u^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2} - \frac{2m}{\hbar^2\kappa^2}V(u,z)\right)f \ , \end{aligned}$$

for every $f \in C^2_0(\Omega, \mathbb{C})$, where u, φ, z denote the coordinate projections of $\mathbb{R}^3$ onto the 1st, 2nd and 3rd component, respectively.

5.2 Reduction of $\hat{H}_0$

We decompose $X := L^2_{\mathbb{C}}(\Omega, u)$ into subspaces X_m, $m \in \mathbb{Z}$, using that

$$\left\{ \frac{1}{\sqrt{2\pi}} \cdot e^{im.\mathrm{id}_{(-\pi,\pi)}} : m \in \mathbb{Z} \right\}$$

is a Hilbert basis for $L^2_{\mathbb{C}}(-\pi, \pi)$, see Lemma 2.4.2. For this purpose, we use the following notation:

$$I := (0, \infty) \ , \ \ J := (-\pi, \pi)$$

and for each $f \in L^2_{\mathbb{C}}(I \times \mathbb{R}, u)$, where u denotes the projection of $I \times \mathbb{R}$ onto the 1st component, and each $g \in L^2_{\mathbb{C}}(J)$, the corresponding $f \otimes g \in X$ is defined by

$$(f \otimes g)(u, \varphi, z) := f(u, z) \cdot g(\varphi),$$

for all (u, z) from the domain of f and all φ from the domain of g.

For every $m \in \mathbb{Z}$, the space X_m is then given by the range of the linear isometry $U_m : L^2_{\mathbb{C}}(I \times \mathbb{R}, u) \to X$, defined by

$$U_m f := \frac{1}{\sqrt{2\pi}} f \otimes e^{im.\mathrm{id}_J} \ , \tag{5.4}$$

for all $f \in L^2_{\mathbb{C}}(I \times \mathbb{R}, u)$.

The fact that U_m is isometric is not difficult to prove by using Fubini's theorem. The pairwise orthogonality of the subspaces X_m of X for all $m \in \mathbb{Z}$ follows from the orthogonality of the family

$$\left(\frac{1}{\sqrt{2\pi}} e^{im.\mathrm{id}_J} \right)_{m \in \mathbb{Z}} .$$

Finally, the fact that the span of the union of all X_m, $m \in \mathbb{Z}$, is dense in X is a consequence of the completeness of the previous family in $L^2_{\mathbb{C}}(J)$.

The corresponding sequence of dense subspaces $\mathcal{D}_m$ of X_m, needed for an application of Lemma 2.2.2, is chosen as follows:

$$\mathcal{D}_m := U_m C^2_0(I \times \mathbb{R}, \mathbb{C}) \ ,$$

for every $m \in \mathbb{Z}$. That these spaces are also subspaces of

$$D(U \hat{H}_0 U^{-1}) = U(C^2_0(\mathbb{R}^3, \mathbb{C}))$$

follows from the fact that for every $f \in C^2_0(I \times \mathbb{R}, \mathbb{C})$, we have that

$$\begin{aligned}(U_m f)(u,\varphi,z) &= \frac{1}{\sqrt{2\pi}}\,(f\otimes e^{im.\mathrm{id}_J})(u,\varphi,z)\\ &= \frac{1}{\sqrt{2\pi}}\,f(u,z)\,e^{im\varphi} = \frac{1}{\sqrt{2\pi}}\,f(u,z)\,(e^{i\varphi})^m\\ &= \frac{1}{\sqrt{2\pi}}\,\frac{f(|u\cos(\varphi)+iu\sin(\varphi)|,z)}{|u\cos(\varphi)+iu\sin(\varphi)|^m}\,[u\cos(\varphi)+iu\sin(\varphi)]^m\\ &= h(u\cos(\varphi),u\sin(\varphi),z) = (Uh)(u,\varphi,z)\ ,\end{aligned}$$

for every $(u,\varphi,z)\in\Omega$, where $h:\mathbb{R}^3\to\mathbb{C}$ is defined by

$$h(u_1,u_2,u_3) := \frac{1}{\sqrt{2\pi}}\,\frac{f(|u_1+iu_2|,u_3)}{|u_1+iu_2|^m}\,(u_1+iu_2)^m\ ,$$

for every $u=(u_1,u_2,u_3)\in\mathbb{R}^3$. We note that $h\in C_0^2(\mathbb{R}^3,\mathbb{C})$.

Further, for every $m\in\mathbb{Z}$ and $f\in C_0^2(I\times\mathbb{R},\mathbb{C})$, it follows that

$$\begin{aligned}&U\hat{H}_0U^{-1}(f\otimes e^{im.\mathrm{id}_J})\\ &= -\frac{\hbar^2\kappa^2}{2m}\cdot\left[\left(\frac{1}{u}\frac{\partial}{\partial u}\,u\,\frac{\partial}{\partial u}-\frac{m^2}{u^2}-\frac{2m}{\hbar^2\kappa^2}\,V(u,z)+\frac{\partial^2}{\partial z^2}\right)f\right]\otimes e^{im.\mathrm{id}_J}\ ,\end{aligned}$$

where u and z denote the projection of $I\times\mathbb{R}$ onto the 1st and 2nd component, respectively.

5.3 Motion of a Charged Particle in a Homogeneous Magnetic Field

As an example of the motion of a particle subject to an axisymmetric force field, we consider the motion of a charged particle with charge $q\neq 0$, in a constant magnetic field in the direction of the 3rd coordinate axis, using the notation from Sect. 2.10. In particular, $\Omega=\mathbb{R}^3$, $\rho=0$, $\vec{j}=\vec{0}$, and

$$\phi(x_1,x_2,x_3)=0\ ,\ \ \vec{A}(x_1,x_2,x_3)=\frac{1}{2}\,{}^t(-Bx_2,Bx_1,0)\ ,$$

for every $(x_1,x_2,x_3)\in\mathbb{R}^3$, where $B\neq 0$ has the dimension $(m/l)^{1/2}/t$. Then

$$\vec{\nabla}\cdot\vec{A}=0\ ,\ \ \triangle\vec{A}=\vec{0}\ ,$$

and hence (2.27) and (2.28) are satisfied. Further, from (2.26), it follows that

$$\vec{E} = \vec{0}\ ,\ \ \vec{B} = \vec{\nabla} \times \vec{A} = {}^t(0, 0, B)\ ,$$

i.e., there is no electric field, but only a constant magnetic field in the direction of the 3rd coordinate axis.

In classical physics, the kinetic energy of the particle as well as the component of the velocity of the particle into the direction of the magnetic field are constants of motion. The Lorentz force exerted on the particle by the magnetic field forces the particle into a helical motion around an axis through the point

$$\left(x_1(0) + \frac{mc}{qB}\, v_2(0), x_2(0) - \frac{mc}{qB}\, v_1(0), 0\right)$$

that is parallel to the 3rd coordinate axis. Here $x_1(0)$, $x_2(0)$ and $v_1(0)$, $v_2(0)$ are the components of the position and initial velocity, respectively, of the particle in the direction of the 1st and 2nd coordinate axis. The distance of the motion to this axis is given by

$$\sqrt{v_1^2(0) + v_2^2(0)}\, \frac{mc}{|qB|}\ ,$$

the frequency of the circular motion, given by the projection of the motion into the coordinate plane spanned by the 1st and 2nd coordinate axis, by

$$\omega := \frac{|qB|}{mc}\ , \tag{5.5}$$

and the rotation in this plane is clockwise if $qB > 0$ and counterclockwise if $qB < 0$. Since $\vec{E} = 0$, the energy density ε of the electromagnetic field is constant, given by

$$\varepsilon = \frac{1}{8\pi}\, B^2\ .$$

Hence, the energy content of the electromagnetic field is infinite, which is not physical. On the classical level, this idealization does not create problems, since the motion orthogonal to the magnetic field stays bounded, whereas the motion parallel to the magnetic field is free, i.e., particles never "sense" the infinite extension of the magnetic field. Similar is true for quantum mechanics, since the spectrum of the Hamilton operator corresponding to the system is bounded from below. More precisely, the lowest possible energy is given $\frac{1}{2}\hbar$ times the frequency of the classical circular motion (5.5),

$$\boxed{\frac{1}{2}\,\hbar\omega,}$$

Equation (5.16), signaling absorption of energy from the magnetic field. For an electron subject to a magnetic field of 100 G, the strength of standard magnets that, e.g., are attached to fridges,

$$\frac{1}{2}\,\hbar\omega \approx 0.58 \cdot 10^{-6}\ \mathrm{eV}\ .$$

The situation is different for an electromagnetic field, solely due to constant electric field, that causes unbounded motion, i.e., particles do sense the infinite extension of such a field. Indeed, in this case the spectrum of the Hamilton operator corresponding to the quantum mechanical system is not bounded from below, which is not physical, since opening the possibility of extraction of an infinite amount of energy from the system. For this reason, the associated quantum system is not considered in this book.

In quantum mechanics, a candidate for a minimal Hamiltonian

$$\hat{H}_{00} : C_0^2(\mathbb{R}^3, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^3)\ ,$$

of the physical system is given by

$$\begin{aligned}\hat{H}_{00} f &= \frac{(\hbar\kappa)^2}{2m}\left[-\triangle - \frac{\alpha B}{\kappa^2 q}\cdot\frac{1}{i}\,{}^t(-u_2, u_1, 0)\cdot\vec{\nabla} + \frac{\alpha^2 B^2}{4\kappa^4 q^2}\,(u_1^2 + u_2^2)\right] f \\ &= \frac{(\hbar\kappa)^2}{2m}\left[-\triangle - \frac{\alpha B}{\kappa^2 q}\cdot\frac{1}{\hbar}\,\hat{L}_{30} + \frac{\alpha^2 B^2}{4\kappa^4 q^2}\,(u_1^2 + u_2^2)\right] f\ ,\end{aligned}$$

for every $f \in C_0^2(\mathbb{R}^3, \mathbb{C})$, where

$$\alpha := \frac{q^2}{\hbar c} > 0\ .$$

Then, for every $m \in \mathbb{Z}$ and $f \in C_0^2(I \times \mathbb{R}, \mathbb{C})$, it follows that

$$\begin{aligned}&U\hat{H}_{00}U^{-1}(f \otimes e^{im.\mathrm{id}_J}) \\ &= \frac{\hbar^2\kappa^2}{2m}\cdot\left[\left(-\frac{1}{u}\,\frac{\partial}{\partial u}\,u\,\frac{\partial}{\partial u} + \frac{m^2}{u^2} + \beta^2 u^2 - \frac{\partial^2}{\partial z^2} - 2m\beta\right) f\right] \otimes e^{im.\mathrm{id}_J}\ ,\end{aligned}$$

where

$$\beta := \frac{\alpha B}{2\kappa^2 q} = \frac{1}{4}\,\frac{\frac{qB}{mc}}{\frac{\hbar\kappa^2}{2m}} \neq 0\ ,$$

is dimensionless and u and z denote the projection of $I \times \mathbb{R}$ onto the 1st and 2nd component, respectively.

In the following, we are going to follow a different approach for the definition of the Hamilton operator of the system that uses an orthogonal decomposition of $X := L^2_{\mathbb{C}}(\Omega, u)$.

For this purpose, in a first step, we are going to find a Hilbert basis of eigenfunctions of, (if $m = 0$, an appropriate extension of), the densely-defined, linear and symmetric Sturm–Liouville operator

$$S_m := \begin{pmatrix} C_0^2(I) \to L^2_{\mathbb{C}}(I,u) \\ f \mapsto -\frac{1}{u}(uf')' + \left(\frac{m^2}{u^2} + \beta^2 u^2\right) f \end{pmatrix} ,$$

where u denotes the identical function on I. For this purpose, we use the Hilbert space isomorphism $V : L^2_{\mathbb{C}}(I,u) \to L^2_{\mathbb{C}}(I)$, defined by

$$Vf := u^{1/2} f \ ,$$

for every $f \in L^2_{\mathbb{C}}(I,u)$. The inverse $V^{-1} : L^2_{\mathbb{C}}(I) \to L^2_{\mathbb{C}}(I,u)$ is given by

$$V^{-1} f := u^{-1/2} f \ ,$$

for every $f \in L^2_{\mathbb{C}}(I)$. Then $\mathcal{S}_m := V S_m V^{-1} : C_0^2(I,\mathbb{C}) \to L^2_{\mathbb{C}}(I)$ is given by

$$\mathcal{S}_m f = -f'' + \left(\frac{m^2 - \frac{1}{4}}{u^2} + \beta^2 u^2\right) f \ ,$$

for every $f \in C_0^2(I,\mathbb{C})$ (Fig. 5.1).

5.3.1 Construction of a Hilbert Basis of $\mathbf{L^2_{\mathbb{C}}(0,\infty)}$

For the construction of the Hilbert basis $(e_{mn})_{n\in\mathbb{N}}$ of $L^2_{\mathbb{C}}(I)$, we note that $\mathcal{S}_m$ is induced by the linear differential operator

$$D^2_{1_{\mathbb{R}},\left(m^2-\frac{1}{4}\right)u^{-2}+\beta^2u^2} := \left(C^2(I,\mathbb{C}) \to C(I,\mathbb{C}),\, f \mapsto -f'' + \left(\frac{m^2-\frac{1}{4}}{u^2} + \beta^2 u^2\right)\cdot f\right) \ ,$$

where 1_I denotes the constant function of value 1 on I and u denotes the identical function on I.

In the following, we consider the solutions of the ordinary differential equation

$$\left(D^2_{1_{\mathbb{R}},\left(m^2-\frac{1}{4}\right)u^{-2}+\beta^2u^2} - \lambda\right) f = 0 \ , \tag{5.6}$$

where $\lambda \in \mathbb{C}$. For this purpose, we note that if $g \in C^2(I,\mathbb{C})$ is a solution of the confluent hypergeometric differential equation

$$vg''(v) + (|m| + 1 - v)\, g'(v) - \left(\frac{|m|+1}{2} - \frac{\lambda}{4|\beta|}\right) g(v) = 0 \ , \tag{5.7}$$

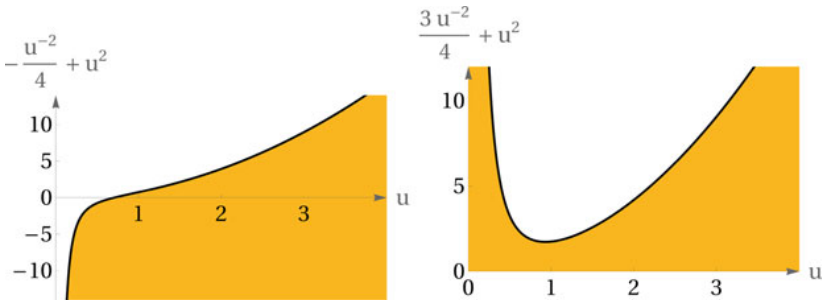


Fig. 5.1 Graphs of the potentials of $\mathcal{S}_m$ for $m=0$ and $m=1$. In both cases $\beta=1$

for every $v \in \mathbb{R}$, then $f \in C^2(I, \mathbb{C})$, defined by

$$f(u) := u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} g(|\beta|u^2) \ ,$$

for every $u \in I$, is a solution of (5.6).

Hence for $\lambda = 2(|m|+1)|\beta|$, such that

$$\frac{|m|+1}{2} - \frac{\lambda}{4|\beta|} = 0 \ ,$$

two linearly independent solutions of (5.7) are given by $g_1, g_2 : I \to \mathbb{R}$, defined by

$$g_1(v) := 1 \ , \ g_2(v) := \int_1^v \frac{e^v}{v^{|m|+1}} \, dv \ ,$$

for every $v \in I$, and hence two linearly independent solutions of (5.6) are given by $f_1, f_2 : I \to \mathbb{R}$, defined by

$$f_1(u) := u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} \ , \ f_2(u) := f_1(u) \int_1^{|\beta|u^2} \frac{e^v}{v^{|m|+1}} \, dv \ ,$$

for every $u \in I$. We note for $|u| \geqslant 1/\sqrt{|\beta|}$ that

$$\left| \int_1^{|\beta|u^2} \frac{e^v}{v^{|m|+1}} \, dv \right| = \int_1^{|\beta|u^2} \frac{e^v}{v^{|m|+1}} \, dv \geqslant \frac{1}{(|\beta|u^2)^{|m|+1}} \int_1^{|\beta|u^2} e^v \, dv = \frac{e^{|\beta|u^2} - e}{(|\beta|u^2)^{|m|+1}}$$

and hence that

$$|f_2(u)| \geqslant u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} \frac{e^{|\beta|u^2} - e}{(|\beta|u^2)^{|m|+1}} = \frac{1}{|\beta|^{|m|+1}} u^{-(|m|+\frac{3}{2})} (e^{\frac{|\beta|u^2}{2}} - e^{1-\frac{|\beta|u^2}{2}}) \ .$$

Therefore, f_1 is L^2 at ∞, whereas f_2 is not L^2 at ∞. Hence, we arrive at the following result.

> The differential operator $D^2_{1_{\mathbb{R}},\left(m^2-\frac{1}{4}\right)u^{-2}+\beta^2u^2}$ is of limit point type at ∞.

Further, we note for $m \neq 0$ and $|u| \leqslant 1/\sqrt{|\beta|}$ that

$$\left|\int_1^{|\beta|u^2} \frac{e^v}{v^{|m|+1}}\,dv\right| = \int_{|\beta|u^2}^1 \frac{e^v}{v^{|m|+1}}\,dv \geqslant \int_{|\beta|u^2}^1 \frac{dv}{v^{|m|+1}} = \frac{1}{|m|}\left[(|\beta|u^2)^{-|m|} - 1\right]$$

and hence that

$$\begin{aligned}|f_2(u)| &\geqslant u^{|m|+\frac{1}{2}}e^{-\frac{|\beta|u^2}{2}}\frac{1}{|m|}\left[(|\beta|u^2)^{-|m|} - 1\right] \\ &= \frac{1}{|m||\beta|^{|m|}}\left(u^{\frac{1}{2}-|m|} - |\beta|^{|m|}u^{|m|+\frac{1}{2}}\right)e^{-\frac{|\beta|u^2}{2}} \;.\end{aligned}$$

Therefore, f_1 is L^2 at 0, whereas f_2 is not L^2 at 0. As a consequence, the following is true.

> If $m \neq 0$, then $D^2_{1_{\mathbb{R}},\left(m^2-\frac{1}{4}\right)u^{-2}+\beta^2u^2}$ is of limit point type at 0.

Even further, we note for $m = 0$ and $|u| \leqslant 1/\sqrt{|\beta|}$ that

$$\left|\int_1^{|\beta|u^2} \frac{e^v}{v}\,dv\right| = \int_{|\beta|u^2}^1 \frac{e^v}{v}\,dv \leqslant e\cdot\int_{|\beta|u^2}^1 \frac{dv}{v} = e\,|\ln(|\beta|u^2)|$$

and hence that

$$|f_2(u)| \leqslant e\,u^{\frac{1}{2}}\,|\ln(|\beta|u^2)|\,e^{-\frac{|\beta|u^2}{2}} \;.$$

Therefore, f_1 and f_2 are both L^2 at 0. Hence, we arrive at the following result.

> If $m = 0$, then $D^2_{1_{\mathbb{R}},\left(m^2-\frac{1}{4}\right)u^{-2}+\beta^2u^2}$ is of limit circle type at 0.

Summarizing the previous, we conclude that the following is true.

The ordinary differential operator

$$D^2_{1_{\mathbb{R}},\left(m^2-\frac{1}{4}\right)u^{-2}+\beta^2u^2}$$

is of limit circle type at 0, if $m = 0$, is of limit point type at 0, if $m \neq 0$, and is of limit point type at ∞. As a consequence, $\mathcal{S}_m$ is essentially self-adjoint for $m \neq 0$, whereas the deficiency indices of $\mathcal{S}_0$ are equal to 1.

In particular, since $\mathcal{S}_m$ is essentially self-adjoint if $m \neq 0$, the corresponding self-adjoint extension is given by its adjoint $\mathcal{S}_m^*$. from the general theory for Sturm–Liouville operators (see, e.g., [80]), it follows that the following is true.

A Larger Core for $\mathcal{S}_m$ if $m \neq 0$

The subspace

$$D_m := \left\{ f \in C^2(I,\mathbb{C}) \cap L^2_{\mathbb{C}}(I) : -f'' + \left(\frac{m^2-\frac{1}{4}}{u^2} + \beta^2u^2\right)\cdot f \in L^2_{\mathbb{C}}(I) \right\}$$

of $L^2_{\mathbb{C}}(I)$ is a core for $\bar{\mathcal{S}}_m$. For every $f \in D_m$,

$$\bar{\mathcal{S}}_m f = -f'' + \left(\frac{m^2-\frac{1}{4}}{u^2} + \beta^2u^2\right)\cdot f \ .$$

Later, we are going to show that the eigenvectors of $\bar{\mathcal{S}}_m$, $m \neq 0$, are elements of $D_{\ell m}$.

In the following, we are going to construct the self-adjoint extensions of $\mathcal{S}_0$, by using the method described in Sect. 4.4.2. For the application of this method, we let π denote the canonical projection of $D(\mathcal{S}_0^*)$ onto the quotient space $D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0)$ and define $\langle\ ,\ \rangle : (D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0))^2 \to \mathbb{C}$ by

$$\langle f + D(\bar{\mathcal{S}}_0), g + D(\bar{\mathcal{S}}_0)\rangle := i\left(\langle \mathcal{S}_0^* f|g\rangle_2 - \langle f|\mathcal{S}_0^* g\rangle_2\right) \ ,$$

for all $f, g \in D(\mathcal{S}_0^*)$, where $\langle\ |\ \rangle_2$ denotes the scalar product of $L^2_{\mathbb{C}}(J)$. Since both deficiency indices of $\mathcal{S}_0$ are equal to 1, $D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0)$ is a 2-dimensional complex vector space and $\langle\ ,\ \rangle$ defines an inner product (i.e., a nondegenerate symmetric sesquilinear form) of signature $(1, 1)$ on $D(\mathcal{S}_0^*)/D(\mathcal{S}_0)$. A subspace D of $D(\mathcal{S}_0^*)$ "is" the domain of a linear self-adjoint extension of $\mathcal{S}_0$ if and only if $\pi(D)$ is a maximal null space of $(D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0), \langle , \rangle)$, i.e., iff the equality

$$\pi(D) = \{f + D(\bar{\mathcal{S}}_0) \in D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0) : \langle f + D(\bar{\mathcal{S}}_0), g + D(\bar{\mathcal{S}}_0)\rangle = 0, \\ \text{for all } g \in D\}$$

is valid. Hence, given an orthonormal basis $f_1 + D(\bar{\mathcal{S}}_0)$, $f_2 + D(\bar{\mathcal{S}}_0)$ of $(D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0), \langle\, , \rangle)$, i.e.,

$$\langle f_j + D(\bar{\mathcal{S}}_0), f_k + D(\bar{\mathcal{S}}_0)\rangle = \eta_{jk} \ ,$$

for $j, k \in \{1, 2\}$, where:

$$\eta_{11} = 1 \, , \ \eta_{22} = -1 \, , \ \eta_{12} = \eta_{21} = 0 \ ,$$

constructed below, the domains of linear self-adjoint extensions of $\mathcal{S}_0$ can be seen to be given by the sequence $(\mathcal{D}_\gamma)_{\gamma\in[0,\pi)}$ of pairwise different subspaces of $D(\mathcal{S}_0^*)$, where

$$\mathcal{D}_\gamma := \{f \in D(\mathcal{S}_0^*) : i\,(\left\langle \mathcal{S}_0^*(f_1 + e^{2i\gamma} f_2)|f \right\rangle_2 - \left\langle f_1 + e^{2i\gamma} f_2 | \mathcal{S}_0^* f \right\rangle_2) = 0\} \ ,$$

for $\gamma \in [0, \pi)$. By the general theory for Sturm–Liouville operators (see, e.g., [80]),

$$D_0 := \{f : f \in C^2(I, \mathbb{C}) \cap L^2_{\mathbb{C}}(I) \text{ and } -f'' + \left(-\frac{1}{4u^2} + \beta^2 u^2\right) f \in L^2_{\mathbb{C}}(I)\}$$

defines a core for $\mathcal{S}_0^*$, and for $f \in D_0$ the corresponding $\mathcal{S}_0^* f$ is given by

$$\mathcal{S}_0^* f = -f'' + \left(-\frac{1}{4u^2} + \beta^2 u^2\right) f \ .$$

Hence for $f, g \in D_0$,

$$\begin{aligned}\langle f + D(\bar{\mathcal{S}}_0), g + D(\bar{\mathcal{S}}_0)\rangle &:= i\,(\langle \mathcal{S}_0^* f|g\rangle_2 - \langle f|\mathcal{S}_0^* g\rangle_2) \\ &= i \int_0^\infty \left(f^* g' - f'^* g\right)' du \ .\end{aligned}$$

We note that

$$g_1 := -h u^{1/2} \ln(u) \ , \ \ g_2 := h u^{1/2} \ ,$$

where $h \in C^\infty(I, \mathbb{R})$ is an otherwise arbitrary auxiliary function which is equal to 1 on $(0, 1/4]$ and is equal to 0 on $[3/4, \infty)$ (such a function is of course easy to construct), are linearly independent elements of D_0 satisfying

$$\langle g_1 + D(\bar{\mathcal{S}}_0), g_1 + D(\bar{\mathcal{S}}_0)\rangle = \langle g_2 + D(\bar{\mathcal{S}}_0), g_2 + D(\bar{\mathcal{S}}_0)\rangle = 0 \ ,$$
$$\langle g_1 + D(\bar{\mathcal{S}}_0), g_2 + D(\bar{\mathcal{S}}_0)\rangle = -i \ , \ \ \langle g_2 + D(\bar{\mathcal{S}}_0), g_1 + D(\bar{\mathcal{S}}_0)\rangle = i \ .$$

As a consequence, defining

$$f_1 := \frac{\sqrt{2}}{2}\,(g_1 + i g_2)\ ,\ \ f_2 := \frac{\sqrt{2}}{2}\,(g_1 - i g_2) = f_1^*\ ,$$

we obtain

$$\begin{aligned}&\langle f_1 + D(\bar{\mathcal{S}}_0), f_1 + D(\bar{\mathcal{S}}_0)\rangle = 1\ ,\ \langle f_2 + D(\bar{\mathcal{S}}_0), f_2 + D(\bar{\mathcal{S}}_0)\rangle = -1\ ,\\ &\langle f_1 + D(\bar{\mathcal{S}}_0), f_2 + D(\bar{\mathcal{S}}_0)\rangle = \langle f_2 + D(\bar{\mathcal{S}}_0), f_1 + D(\bar{\mathcal{S}}_0)\rangle = 0\ ,\end{aligned}$$

i.e., $f_1 + D\left(\bar{\mathcal{S}}_0\right), f_2 + D\left(\bar{\mathcal{S}}_0\right)$ is an orthonormal basis of $(D(\mathcal{S}_0^*)/D(\bar{\mathcal{S}}_0), \langle\ ,\ \rangle)$. (In particular, it follows that both f_1 and f_2 are not contained in the domain of $\bar{\mathcal{S}}_0$.) Hence by $(\mathcal{S}_0^*|_{\mathcal{D}_\gamma})_{\gamma\in[0,\pi)}$ it is given a sequence of pairwise different linear self-adjoint extensions of $\mathcal{S}_0^*$ which includes all linear self-adjoint extension of $\mathcal{S}_0$. Furthermore, for any $\gamma \in [0, \pi)$ the subspace $\mathcal{D}_\gamma \cap D_0$ and $\mathcal{D}'_\gamma$ defined below are cores for $\mathcal{S}_0^*|_{\mathcal{D}_\gamma}$. We note that

$$\begin{aligned}&\mathcal{D}_\gamma \cap D_0\\ &= \Bigg\{ f \in C^2(I,\mathbb{C}) \cap L^2_{\mathbb{C}}(I) : -f'' + \left(-\frac{1}{4u^2} + \beta^2 u^2\right) f \in L^2_{\mathbb{C}}(I)\\ &\qquad \text{and } \lim_{u\to 0}\left\{[\cos(\gamma)g_1 + \sin(\gamma)g_2]^2\left[\frac{f}{\cos(\gamma)g_1 + \sin(\gamma)g_2}\right]'\right\}(u) = 0\Bigg\}\ ,\end{aligned}$$

for $\gamma \in [0, \pi)$. and $\mathcal{D}'_\gamma\ \big(\subset \mathcal{D}_\gamma \cap D_0\big)$ is given by

$$\mathcal{D}'_\gamma := C^2_0(J,\mathbb{C}) + \mathbb{C}\,[\cos(\gamma)g_1 + \sin(\gamma)g_2]\,. \tag{5.8}$$

We note that for $\gamma = \pi/2$ that

$$\cos(\gamma)g_1 + \sin(\gamma)g_2 = hu^{1/2}\ .$$

As a consequence,

$$\begin{aligned}&\mathcal{D}_{\pi/2} \cap D_0 =\\ &\Bigg\{ f \in C^2(I,\mathbb{C}) \cap L^2_{\mathbb{C}}(I) : -f'' + \left(-\frac{1}{4u^2} + \beta^2 u^2\right) f \in L^2_{\mathbb{C}}(I)\\ &\quad \wedge \lim_{u\to 0} u\cdot(u^{-1/2}f)'(u) = 0\Bigg\}\ ,\\ &\mathcal{D}'_{\pi/2} = C^2_0(J,\mathbb{C}) + \mathbb{C}.hu^{1/2}\ .\end{aligned}$$

The Appropriate Essentially Self-Adjoint Extension of $\mathcal{S}_0$

The extension $\mathcal{S}_{0e}$ of $\mathcal{S}_0$, given by

$$\mathcal{S}_{0e} f := -f'' + \left(-\frac{1}{4u^2} + \beta^2 u^2\right) f \ ,$$

for every $f \in C^2(I, \mathbb{C}) \cap L^2_{\mathbb{C}}(I)$ such that

$$-f'' + \left(-\frac{1}{4u^2} + \beta^2 u^2\right) f \in L^2_{\mathbb{C}}(I)$$
$$\text{and } \lim_{u \to 0} u \cdot (u^{-1/2} f)'(u) = 0 \ , \tag{5.9}$$

is essentially self-adjoint.

For later use, we note the following.

The Corresponding Extension of S_0

The corresponding extension S_{0e} of S_0 is given by

$$S_{0e} f := -\frac{1}{u}\,(uf')' + \beta^2 u^2 f \ ,$$

for every $f \in C^2(I, \mathbb{C}) \cap L^2_{\mathbb{C}}(I, u)$ such that

$$-\frac{1}{u}\,(uf')' + \beta^2 u^2 f \in L^2_{\mathbb{C}}(I, u) \text{ and } \lim_{u \to 0} uf'(u) = 0 \ . \tag{5.10}$$

In the following, we study the regularity or smoothness of the eigenfunctions of $\bar{\mathcal{S}}_m$ for $m \neq 0$ and $\bar{\mathcal{S}}_{0e}$. For this purpose, we consider the case that $\lambda = -2(|m| + 1)|\beta|$, such that

$$\frac{|m| + 1}{2} - \frac{\lambda}{4|\beta|} = |m| + 1 \ .$$

Then, two linearly independent solutions $g_1, g_2 \in C^2(I, \mathbb{C})$ of (5.7) are given by

$$g_1(v) = e^v \ , \ g_2(v) = e^v \cdot \int_v^\infty w^{-(|m|+1)} e^{-w} \, dw \ ,$$

for every $v \in \mathbb{R}$. Hence two linearly independent solutions of (5.6) are given by $f_1, f_2 : I \to \mathbb{R}$, defined by

$$f_1(u) := u^{|m|+\frac{1}{2}} e^{\frac{|\beta|u^2}{2}} \ , \ f_2(u) := -\frac{|\beta|^{|m|}}{2}\, u^{|m|+\frac{1}{2}} e^{\frac{|\beta|u^2}{2}} \int_{|\beta|u^2}^{\infty} v^{-(|m|+1)} e^{-v}\, dv \ ,$$

for every $u \in I$. We note that

$$\begin{aligned}
|f_2(u)| &= \frac{|\beta|^{|m|}}{2}\, u^{|m|+\frac{1}{2}} e^{\frac{|\beta|u^2}{2}} \int_{|\beta|u^2}^{\infty} v^{-(|m|+1)} e^{-v}\, dv \\
&\leqslant \frac{|\beta|^{|m|}}{2}\, u^{|m|+\frac{1}{2}} e^{\frac{|\beta|u^2}{2}} (|\beta|u^2)^{-(|m|+1)} \int_{|\beta|u^2}^{\infty} e^{-v}\, dv \\
&= \frac{|\beta|^{|m|}}{2}\, u^{|m|+\frac{1}{2}} e^{\frac{|\beta|u^2}{2}} (|\beta|u^2)^{-(|m|+1)} e^{-|\beta|u^2} \\
&= \frac{|\beta|^{|m|}}{2}\, |\beta|^{-(|m|+1)} u^{-(|m|+\frac{3}{2})} e^{-\frac{|\beta|u^2}{2}} = \frac{1}{2|\beta|}\, u^{-(|m|+\frac{3}{2})} e^{-\frac{|\beta|u^2}{2}} \ ,
\end{aligned}$$

for every $u \in I$. Hence, f_1 is L^2 at 0 and f_2 is L^2 at ∞. In addition, the Wronski determinant $W(f_1, f_2)$ of f_1 and f_2 is constant of value 1:

$$W(f_1, f_2) = f_1 f_2' - f_1' f_2 = 1 \ .$$

We define for every $h \in C_0(I, \mathbb{C})$ a corresponding function $\mathrm{Kh} : I \to \mathbb{C}$ by

$$\begin{aligned}
\mathrm{Kh}(u) &:= -\left[f_2(u) \int_0^u f_1(v) h(v) dv + f_1(u) \int_u^{\infty} f_2(v) h(v) dv \right] \\
&= \int_I G_m(u, v) h(v) dv \ ,
\end{aligned} \tag{5.11}$$

for every $u \in I$, where

$$G_m(u, v) := \begin{cases} -f_2(u) f_1(v) & 0 < v < u \\ -f_1(u) f_2(v) & u < v \end{cases} \ ,$$

for almost all $(u, v) \in I^2$. We note that $\mathrm{Kh} \in C^2(I, \mathbb{C})$ such that

$$\left(D^2_{1_{\mathbb{R}}, \left(m^2 - \frac{1}{4}\right) u^{-2} + \beta^2 u^2} - \lambda \right) \mathrm{Kh} = h$$

and that

$$\mathrm{Kh}(u) = \begin{cases} -f_1(u) \int_0^{\infty} f_2(v) h(v) dv & \text{for sufficiently small } u \in I \\ -f_2(u) \int_0^{\infty} f_1(v) h(v) dv & \text{for sufficiently large } u \in I \end{cases} \ .$$

In particular, $\mathrm{Kh} \in L^2_{\mathbb{C}}(I)$ and if $m = 0$, then

$$\lim_{u \to 0} u \cdot (u^{-1/2}\mathrm{Kh})' = 0 \ ,$$

since

$$\lim_{u \to 0} u \cdot (u^{-1/2} f_1)' = \lim_{u \to 0} u \cdot (e^{\frac{|\beta| u^2}{2}})' = |\beta| \lim_{u \to 0} u^2 e^{\frac{|\beta| u^2}{2}} = 0 \ ,$$

i.e., Kh is in the domain of S_{0e}. Further, if

$$h = \left(D^2_{1_{\mathbb{R}}, \left(m^2 - \frac{1}{4}\right) u^{-2} + \beta^2 u^2} - \lambda \right) f \ ,$$

where $f \in C_0^2(I, \mathbb{C})$, then it follows from partial integration that Kh has a compact support. Hence, $\mathrm{Kh} - f \in C_0^2(I, \mathbb{C})$. Since,

$$\left(D^2_{1_{\mathbb{R}}, \left(m^2 - \frac{1}{4}\right) u^{-2} + \beta^2 u^2} - \lambda \right) (\mathrm{Kh} - f) = 0 \ ,$$

it follows that $\mathrm{Kh} = f$. Continuing, we note that for $u, v \in I$ satisfying $0 < v < u$

$$|G_m(u, v)| = |f_2(u)| \cdot |f_1(v)| \leqslant \frac{1}{2|\beta|} \, u^{-(|m| + \frac{3}{2})} v^{|m| + \frac{1}{2}} e^{-\frac{|\beta| u^2}{2}} e^{\frac{|\beta| v^2}{2}} \ ,$$

and for $u, v \in I$ satisfying $u < v$ that

$$|G_m(u, v)| = |f_1(u)| \cdot |f_2(v)| \leqslant \frac{1}{2|\beta|} \, u^{|m| + \frac{1}{2}} v^{-(|m| + \frac{3}{2})} e^{\frac{|\beta| u^2}{2}} e^{-\frac{|\beta| v^2}{2}} \ .$$

Hence it follows for $u \in I$ that

$$\begin{aligned}
&\int_0^\infty |G_m(u, v)| \, dv = \int_0^u |G_m(u, v)| \, dv + \int_u^\infty |G_m(u, v)| \, dv \\
&\leqslant \frac{1}{2|\beta|} \, u^{-(|m| + \frac{3}{2})} e^{-\frac{|\beta| u^2}{2}} \int_0^u v^{|m| + \frac{1}{2}} e^{\frac{|\beta| v^2}{2}} \, dv \\
&\quad + \frac{1}{2|\beta|} \, u^{|m| + \frac{1}{2}} e^{\frac{|\beta| u^2}{2}} \int_u^\infty v^{-(|m| + \frac{3}{2})} e^{-\frac{|\beta| v^2}{2}} \, dv \\
&\leqslant \frac{1}{2|\beta|} \, u^{-(|m| + \frac{3}{2})} \int_0^u v^{|m| + \frac{1}{2}} \, dv + \frac{1}{2|\beta|} \, u^{|m| + \frac{1}{2}} \int_u^\infty v^{-(|m| + \frac{3}{2})} \, dv \\
&= \frac{1}{2|\beta|} \left(\frac{1}{|m| + \frac{1}{2}} + \frac{1}{|m| + \frac{3}{2}} \right)
\end{aligned}$$

and for $v \in I$ that

$$
\begin{aligned}
\int_0^\infty |G_m(u,v)|\,du &= \int_0^v |G_m(u,v)|\,du + \int_v^\infty |G_m(u,v)|\,du \\
&\leqslant \frac{1}{2|\beta|}\, v^{-(|m|+\frac{3}{2})} e^{-\frac{|\beta|v^2}{2}} \int_0^v u^{|m|+\frac{1}{2}} e^{\frac{|\beta|u^2}{2}}\,du \\
&\quad + \frac{1}{2|\beta|}\, v^{|m|+\frac{1}{2}} e^{\frac{|\beta|v^2}{2}} \int_v^\infty u^{-(|m|+\frac{3}{2})} e^{-\frac{|\beta|u^2}{2}}\,du \\
&\leqslant \frac{1}{2|\beta|}\, v^{-(|m|+\frac{3}{2})} \int_0^v u^{|m|+\frac{1}{2}}\,du + \frac{1}{2|\beta|}\, v^{|m|+\frac{1}{2}} \int_v^\infty u^{-(|m|+\frac{3}{2})}\,du \\
&= \frac{1}{2|\beta|}\left(\frac{1}{|m|+\frac{1}{2}} + \frac{1}{|m|+\frac{3}{2}}\right) .
\end{aligned}
$$

Hence the function G_m induces a bounded linear integral operator $\mathrm{Int}(G_m)$ on $L^2_C(I)$, with kernel function G_m. In particular, the operator norm $\|\mathrm{Int}(G_m)\|$ satisfies

$$
\|\mathrm{Int}(G_m)\| \leqslant \frac{1}{2|\beta|}\left(\frac{1}{|m|+\frac{1}{2}} + \frac{1}{|m|+\frac{3}{2}}\right) .
$$

From the previous, it follows in particular that

$$
\begin{cases}
(\bar{\mathcal{S}}_m - \lambda)\,\mathrm{Int}(G_m)\,h = h & \text{if } m \neq 0 \\
(\bar{\mathcal{S}}_{0e} - \lambda)\,\mathrm{Int}(G_0)\,h = h &
\end{cases} , \tag{5.12}
$$

for every $h \in C_0(I,\mathbb{C})$. Since $C_0(I,\mathbb{C})$ is dense in $L^2_C(I)$, $\mathrm{Int}(G_m)$ is a bounded linear operator on $L^2_C(I)$, and $\bar{\mathcal{S}}_m - \lambda$ for $m \neq 0$ as well as $\bar{\mathcal{S}}_{0e} - \lambda$ are closed, the latter implies that (5.12) is true for every $h \in L^2_C(I)$. Hence, $\bar{\mathcal{S}}_m - \lambda$ for $m \neq 0$ and $\bar{\mathcal{S}}_{0e} - \lambda$ are surjective. According to Theorem 12.4.7, the latter implies that $\bar{\mathcal{S}}_m - \lambda$ for $m \neq 0$ and $\bar{\mathcal{S}}_{0e} - \lambda$ are injective and hence as whole bijective. Summarizing, we have the following result.

Inverses of $\bar{\mathcal{S}}_m - \lambda$ for $m \neq 0$ and $\bar{\mathcal{S}}_{0e} - \lambda$

The value $\lambda = -2(|m|+1)|\beta|$ for $m \neq 0$ and $\lambda = -2|\beta|$ is contained in the resolvent set of $\bar{\mathcal{S}}_m$ if $m \neq 0$ and $\bar{\mathcal{S}}_{0e}$, respectively. In particular,

$$
(\bar{\mathcal{S}}_m - \lambda)^{-1} = \mathrm{Int}(G_m) ,
$$

for $m \neq 0$, and

$$
(\bar{\mathcal{S}}_{0e} - \lambda)^{-1} = \mathrm{Int}(G_0) .
$$

As a consequence, if $\mathcal{S} = \bar{\mathcal{S}}_m$ for $m \neq 0$ or $\mathcal{S} = \bar{\mathcal{S}}_{0e}$, then the domain $D(\mathcal{S})$ of $\mathcal{S}$ is given by

$$D(\mathcal{S}) = \mathrm{Ran}(\mathcal{S} - \lambda) \subset C(I, \mathbb{C}) \cap L^2_{\mathbb{C}}(I) \ .$$

Hence, if $\mu \in \mathbb{R}$ is an eigenvalue of $\mathcal{S}$ and f a corresponding eigenfunction, then $f \in C^2(I, \mathbb{C})$, since f satisfies the "integral equation"

$$f = (\mu - \lambda)(\mathcal{S} - \lambda)^{-1} f \ .$$

Regularity of the eigenfunctions of $\bar{\mathcal{S}}_m$ for $m \neq 0$ and $\bar{\mathcal{S}}_{0e}$

If $\lambda \in \mathbb{R}$ is an eigenvalue of $\bar{\mathcal{S}}_m$ for $m \neq 0$ or $\bar{\mathcal{S}}_{0e}$ and f a corresponding eigenfunction, then $f \in C^2(I, \mathbb{C}) \cap L^2_{\mathbb{C}}(I)$.

A solution of (5.6) that is regular at the origin is given by

$$f_1(u) := u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} M\left(\frac{|m|+1}{2} - \frac{\lambda}{4|\beta|}, |m|+1, |\beta|u^2\right) \ ,$$

for every $u \in I$. In particular for $m = 0$,

$$u^{-1/2} f_1(u) = e^{-\frac{|\beta|u^2}{2}} M\left(\frac{1}{2} - \frac{\lambda}{4|\beta|}, 1, |\beta|u^2\right) \ ,$$

for every $u \in I$, and hence

$$\lim_{u \to 0} u \cdot (u^{-1/2} f_1)'(u) = 0 \ .$$

If

$$\frac{|m|+1}{2} - \frac{\lambda}{4|\beta|} \notin -\mathbb{N} \ ,$$

a condition that is equivalent to the condition that

$$\lambda \notin [2(|m|+1) + 4\mathbb{N}]\,|\beta| \ ,$$

it follows from (13.1.4) of [1] that

$$f_1(u) = |\beta|^{-\left(\frac{|m|+1}{2}+\frac{\lambda}{4|\beta|}\right)} \frac{\Gamma(|m|+1)}{\Gamma(\frac{|m|+1}{2} - \frac{\lambda}{4|\beta|})} \, u^{-\frac{1}{2}\left(1+\frac{\lambda}{|\beta|}\right)} \, e^{\frac{|\beta|u^2}{2}} \left[1 + O((|\beta|u^2)^{-1})\right]$$

for $u \to \infty$. We conclude that $f_1 \in D(\bar{\mathcal{S}}_m)$ for $m \neq 0$ or $f_1 \in D(\bar{\mathcal{S}}_{0e})$ if and only if

$$\lambda \in [2(|m|+1) + 4\mathbb{N}]\,|\beta| \ .$$

Further, if

$$\lambda_n = [2(|m|+1) + 4n]\,|\beta| \ ,$$

Table 5.1 Table of generalized Laguerre polynomials, where $x > 0$

$L_n^{\|m\|}(x)$	$n = 0$	$n = 1$	$n = 2$	$n = 3$
$\|m\| = 0$	1	$1 - x$	$\frac{1}{2}\left(2 - 4x + x^2\right)$	$\frac{1}{6}\left(6 - 18x + 9x^2 - x^3\right)$
$\|m\| = 1$	1	$2 - x$	$\frac{1}{2}\left(6 - 6x + x^2\right)$	$\frac{1}{6}\left(24 - 36x + 12x^2 - x^3\right)$
$\|m\| = 2$	1	$3 - x$	$\frac{1}{2}\left(12 - 8x + x^2\right)$	$\frac{1}{6}\left(60 - 60x + 15x^2 - x^3\right)$
$\|m\| = 3$	1	$4 - x$	$\frac{1}{2}\left(20 - 10x + x^2\right)$	$\frac{1}{6}\left(120 - 90x + 18x^2 - x^3\right)$

for some $n \in \mathbb{N}$, then λ_n is an eigenvalue of $\bar{S}_m$ for $m \neq 0$ or $\bar{S}_{0e}$ and f_1 is a corresponding eigenfunction. We note that in this case

$$f_1(u) = \frac{n!}{(|m|+1)_n}\, u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} L_n^{|m|}(|\beta|u^2)$$

for every $u \in I$, where the generalized Laguerre polynomials

$$(L_n^{|m|})_{(|m|,n)\in\mathbb{N}^2}$$

are defined according to [1] 22.5.54. Indeed, for every $m \in \mathbb{Z}$, the corresponding family of functions

$$\left(u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} L_n^{|m|}(|\beta|u^2)\right)_{n\in\mathbb{N}} \tag{5.13}$$

is dense in $L^2_{\mathbb{C}}(I)$. This follows from Theorem 5.7.1 in [75]. The details of the proof are left to the reader.

Exercise 16

Using Theorem 5.7.1 in [75], show that the family (5.13) is dense in $L^2_{\mathbb{C}}(I)$.

Hence, we arrive at the following result (Table 5.1).

For every m, a Hilbert basis of eigenfunctions $(e_{mn})_{n\in\mathbb{N}}$ of $\bar{S}_m$ for $m \neq 0$ and $\bar{S}_{0e}$ is given by

$$e_{mn}(u) = \left[\frac{2n!}{\Gamma(|m|+n+1)}\,|\beta|^{|m|+1}\right]^{1/2} u^{|m|+\frac{1}{2}} e^{-\frac{|\beta|u^2}{2}} L_n^{|m|}(|\beta|u^2)\ ,$$

for every $u \in I$, satisfying

$$\mathcal{S} e_{mn} = [2(|m|+1)+4n]\,|\beta|\, e_{mn} \ ,$$

and

$$(V^{-1}e_{mn})(u) = \left[\frac{2n!}{\Gamma(|m|+n+1)}\,|\beta|^{|m|+1}\right]^{1/2} u^{|m|} e^{-\frac{|\beta|u^2}{2}} L_n^{|m|}(|\beta|u^2) \ .$$

for every $u \in I$.

Here, [1] 22.2.12 is used for normalization. As a consequence, the spectrum $\sigma(\mathcal{S})$ of $\mathcal{S} = \bar{\mathcal{S}}_m$ for $m \neq 0$ or $\mathcal{S} = \bar{\mathcal{S}}_{0e}$ is purely discrete and given by (Figs. 5.2, 5.3, 5.4, 5.5, 5.6 and Table 5.2)

$$\boxed{\sigma(\mathcal{S}) = \{[2(|m|+1)+4n]\,|\beta| : n \in \mathbb{N}\}\ .}$$

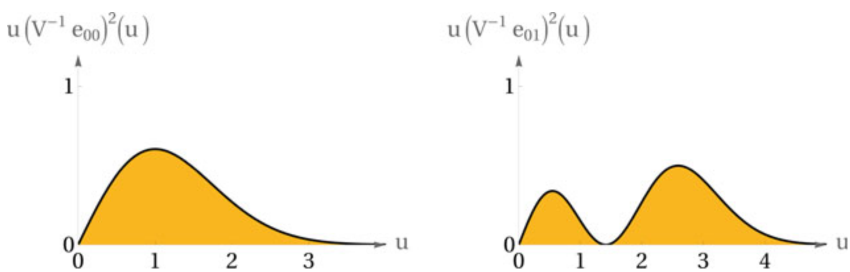


Fig. 5.2 Graphs of $u\,|V^{-1}e_{mn}|^2(u)$ for $(m,n) = (0,0)$ and $(m,n) = (0,1)$, where $\beta = \frac{1}{2}$.

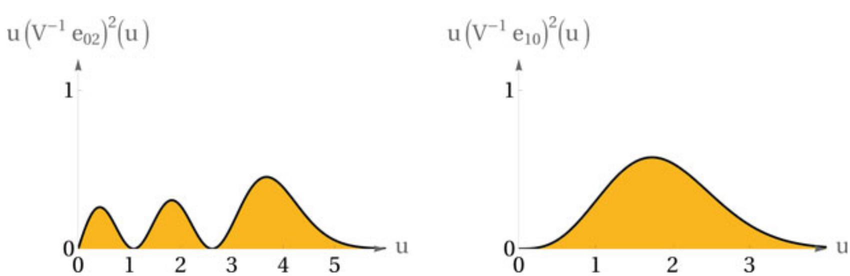


Fig. 5.3 Graphs of $u\,|V^{-1}e_{mn}|^2(u)$ for $(m,n) = (0,2)$ and $(m,n) = (1,0)$, where $\beta = \frac{1}{2}$

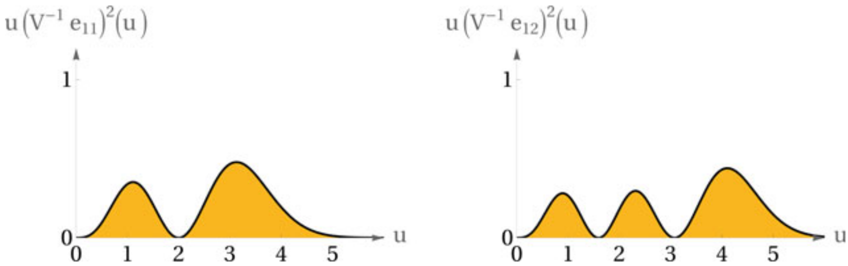


Fig. 5.4 Graphs of $u\,|V^{-1}e_{mn}|^2(u)$ for $(m,n)=(1,1)$ and $(m,n)=(1,2)$, where $\beta=\frac{1}{2}$

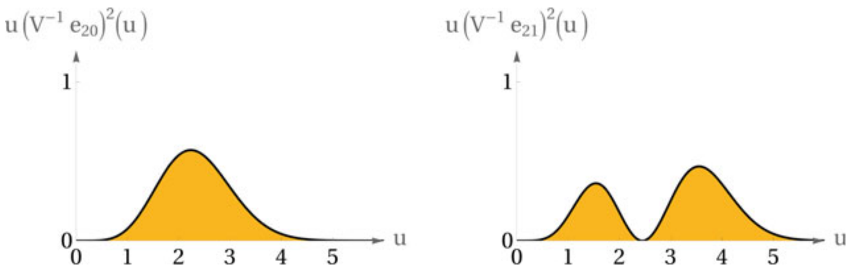


Fig. 5.5 Graphs of $u\,|V^{-1}e_{mn}|^2(u)$ for $(m,n)=(2,0)$ and $(m,n)=(2,1)$, where $\beta=\frac{1}{2}$

Fig. 5.6 Graph of $u\,|V^{-1}e_{mn}|^2(u)$ for $(m,n)=(2,2)$, where $\beta=\frac{1}{2}$

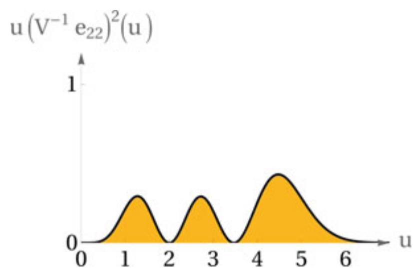


Table 5.2 Table of the functions $u\,|V^{-1}e_{mn}|^2(u)\cdot e^{\frac{u^2}{2}}$ for m and n from 0 to 2, where $\beta=\frac{1}{2}$

$u\,\lvert V^{-1}e_{mn}\rvert^2(u)\cdot e^{\frac{u^2}{2}}$	$n=0$	$n=1$	$n=2$
$m=0$	u	$\frac{u}{4}\left(u^2-2\right)^2$	$\frac{u}{64}\left(u^4-8u^2+8\right)^2$
$m=1$	$\frac{u^3}{2}$	$\frac{u^3}{16}\left(u^2-4\right)^2$	$\frac{u^3}{384}\left(u^4-12u^2+24\right)^2$
$m=2$	$\frac{u^5}{8}$	$\frac{u^5}{96}\left(u^2-6\right)^2$	$\frac{u^5}{3072}\left(u^4-16u^2+48\right)^2$

5.3.2 Synthesis and Properties of the Hamilton Operator $\hat{H}$ of the System

As a result of Sect. 5.3.1, it follows that the family

$$\boxed{\left(e_{mn} \otimes \frac{1}{\sqrt{2\pi}}\, e^{im.\mathrm{id}_J}\right)_{(m,n)\in\mathbb{Z}\times\mathbb{N}}} \tag{5.14}$$

is a Hilbert basis of $L^2(I \times J)$. We decompose $X = L^2_{\mathbb{C}}(\Omega, u)$ into subspaces X_{mn}, $(m, n) \in \mathbb{Z} \times \mathbb{N}$. For every $(m, n) \in \mathbb{Z} \times \mathbb{N}$, the space X_{mn} is then given by the range of the linear isometry $U_{mn} : L^2_{\mathbb{C}}(\mathbb{R}) \to X$, defined by

$$U_{mn} f := (V^{-1}e_{mn}) \otimes \frac{1}{\sqrt{2\pi}}\, e^{im.\mathrm{id}_J} \otimes f \ , \tag{5.15}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R})$. The fact that U_{mn} is isometric is not difficult to prove by using Fubini's theorem. The pairwise orthogonality of the subspaces X_{mn} of X for all $(m, n) \in \mathbb{Z} \times \mathbb{N}$ follows from the orthogonality of the family (5.14). Finally, the fact that the span of the union of all X_{mn}, $(m, n) \in \mathbb{Z} \times \mathbb{N}$, is dense in X is a consequence of the completeness of the family in (5.14). We note that the functions e_{mn}, $(m, n) \in \mathbb{Z} \times \mathbb{N}$, do not have a compact support. The corresponding sequence of dense subspaces $\mathcal{D}_{mn}$ of X_{mn}, needed for an application of Lemma 2.2.5, is chosen as follows:

$$\mathcal{D}_{mn} := U_{mn} C^2_0(\mathbb{R}, \mathbb{C}) \ ,$$

for every $m \in \mathbb{Z}$. Taking into account that for every $(m, n) \in \mathbb{Z} \times \mathbb{N}$

$$\begin{aligned}
&\left(-\frac{1}{u}\frac{\partial}{\partial u}\, u\, \frac{\partial}{\partial u} - \frac{1}{u^2}\frac{\partial^2}{\partial \varphi^2} + \beta^2 u^2 - \frac{\partial^2}{\partial z^2} - \frac{2\beta}{i}\frac{\partial}{\partial \varphi}\right)(V^{-1}e_{mn}) \otimes \frac{e^{im.\mathrm{id}_J}}{\sqrt{2\pi}} \otimes f \\
&= (V^{-1}e_{mn}) \otimes \frac{e^{im.\mathrm{id}_J}}{\sqrt{2\pi}} \otimes \left\{-f'' + [2\,(|m| \mp m + 1) + 4n]\,|\beta| f\right\} \ ,
\end{aligned}$$

for every $f \in C^2_0(\mathbb{R}, \mathbb{C})$, where the minus sign in $\mp m$ applies if $\beta > 0$ and the plus sign applies if $\beta < 0$, we define the densely-defined, linear, symmetric and essentially self-adjoint operator $A_{mn} : \mathcal{D}_{mn} \to X_{mn}$ in X_{mn} by

$$\begin{aligned}
A_{mn}\, U_{mn} f &= A_{mn}\, (V^{-1}e_{mn}) \otimes \frac{1}{\sqrt{2\pi}}\, e^{im.\mathrm{id}_J} \otimes f \\
&:= (V^{-1}e_{mn}) \otimes \frac{e^{im.\mathrm{id}_J}}{\sqrt{2\pi}} \otimes \left\{-f'' + [2\,(|m| \mp m + 1) + 4n]\,|\beta| f\right\} \ ,
\end{aligned}$$

for every $f \in C^2_0(\mathbb{R}, \mathbb{C})$. Finally, we define the subspace $\mathcal{D} \leqslant X$ by

$$\mathcal{D} := \left\{ \sum_{j=0}^{n} f_j : \; n \in \mathbb{N} \text{ and } f_j \in \mathcal{D}_{\mu(j)}, \; \text{for every } j \in \{1, \dots, n\} \right\} ,$$

where $\mu : \mathbb{N} \to \mathbb{Z} \times \mathbb{N}$ is a bijection, and $A : \mathcal{D} \to X$ by

$$A \sum_{j=0}^{n} f_j := \sum_{j=0}^{n} A_{\mu(j)} f_j \; ,$$

where $n \in \mathbb{N}$ and $f_j \in \mathcal{D}_j$, for every $j \in \{0, \dots, n\}$. Then, it follows from Lemma 2.2.5 that A is a densely-defined, linear, symmetric and essentially self-adjoint operator in X and that every X_{mn}, $(m, n) \in \mathbb{Z} \times \mathbb{N}$, is as closed invariant subspace of the closure $\bar{A}$ of A. Finally, we define the Hamilton operator $\hat{H}$ of the system by

$$\boxed{\hat{H} := \frac{\hbar^2 \kappa^2}{2m} \, U^{-1} \bar{A} \, U}$$

and note that it follows from Theorem 2.2.4 that the spectrum $\sigma(\hat{H})$ of $\hat{H}$ is given by closure of

$$\frac{\hbar^2 \kappa^2}{2m} \bigcup_{(m,n) \in \mathbb{Z} \times \mathbb{N}} [\, [2\,(|m| \mp m + 1) + 4n]\, |\beta|, \infty) \; .$$

Since

$$[\, [2\,(|m| \mp m + 1) + 4n]\, |\beta|, \infty) \subset [2\, |\beta|, \infty) \; ,$$

for every $(m, n) \in \mathbb{Z} \times \mathbb{N}$, this implies that

$$\boxed{\sigma(\hat{H}) = \left[\frac{1}{2} \, \hbar\omega, \infty \right) .} \tag{5.16}$$

5.3.3 Calculation of the Time Evolution Generated by $\hat{H}$

The time evolution generated by $\hat{H}$ is given as follows. It follows from Lemma 2.2.1 for every $(m, n) \in \mathbb{Z} \times \mathbb{N}$, $t \in \mathbb{R}$ and $f \in L^2_{\mathbb{C}}(\mathbb{R})$ that

$$
\begin{aligned}
&U \exp\!\left(-i\,\frac{t}{\hbar}\,\hat{H}\right) U^{-1} U_{mn} f = \exp\!\left(-i\,\frac{\hbar\kappa^2}{2m}\,t\bar{A}\right) U_{mn} f \\
&= \exp\!\left(-i\,\frac{\hbar\kappa^2}{2m}\,t\bar{A}_{mn}\right)(V^{-1}e_{mn}) \otimes \frac{1}{\sqrt{2\pi}}\,e^{im.\mathrm{id}_J} \otimes f \\
&= \frac{1}{\sqrt{2\pi}}\,\exp\!\left(-i\,[2\,(|m| \mp m + 1) + 4n]\,|\beta|\,\frac{\hbar\kappa^2}{2m}\,t\right) \\
&\quad [(V^{-1}e_{mn}) \circ (p_1^2 + p_2^2)^{1/2}] \cdot \left(\frac{p_1 + ip_2}{\sqrt{p_1^2 + p_2^2}}\right)^m \otimes \left[\exp\!\left(-it\,\frac{\hbar\kappa^2}{2m}\,\overline{(-\triangle_1)}\right) f\right] \\
&= \frac{1}{\sqrt{2\pi}}\,\exp\!\left(-\frac{i}{2}\,(|m| \mp m + 1 + 2n)\,\omega t\right) \\
&\quad [(V^{-1}e_{mn}) \circ (p_1^2 + p_2^2)^{1/2}] \cdot \left(\frac{p_1 + ip_2}{\sqrt{p_1^2 + p_2^2}}\right)^m \otimes \left[\exp\!\left(-\frac{i}{2}\,\omega t\;\overline{(-\triangle_1)}\right) f\right] ,
\end{aligned}
$$

where p_1 and p_2 denote the coordinate pojections of $\mathbb{R}^2$ onto the first and second coordinate, respectively, and $\overline{(-\triangle_1)}$ denotes the closure of the negative of the Laplace operator in 1-space dimension, see (1.29), and we choose the length scale

$$
\boxed{\kappa := \sqrt{\frac{|qB|}{\hbar c}}.}
$$

The latter leads to

$$
\boxed{\frac{\hbar\kappa^2}{2m} = \frac{\omega}{2}\ ,\ \ |\beta| = \frac{1}{2}.}
$$

For an electron subject to a magnetic field of 100 G, we have

$$
\frac{\hbar\kappa^2}{2m} = \frac{\omega}{2} \approx 0.88 \cdot 10^9\,\mathrm{s}^{-1}\ ,\ \ \kappa^{-1} \approx 2.57 \cdot 10^{-5}\,\mathrm{cm}\ .
$$

As we already know, in a position representation, the coordinates u_1, u_2, u_3 of points $\mathbf{u} = (u_1, u_2, u_3)$ in the domains of functions belonging to the representation space can be interpreted as numbers whose multiplication by the unit of length κ^{-1} lead to a point $\kappa^{-1}\mathbf{u} = (\kappa^{-1}u_1, \kappa^{-1}u_2, \kappa^{-1}u_3)$ in physical space.

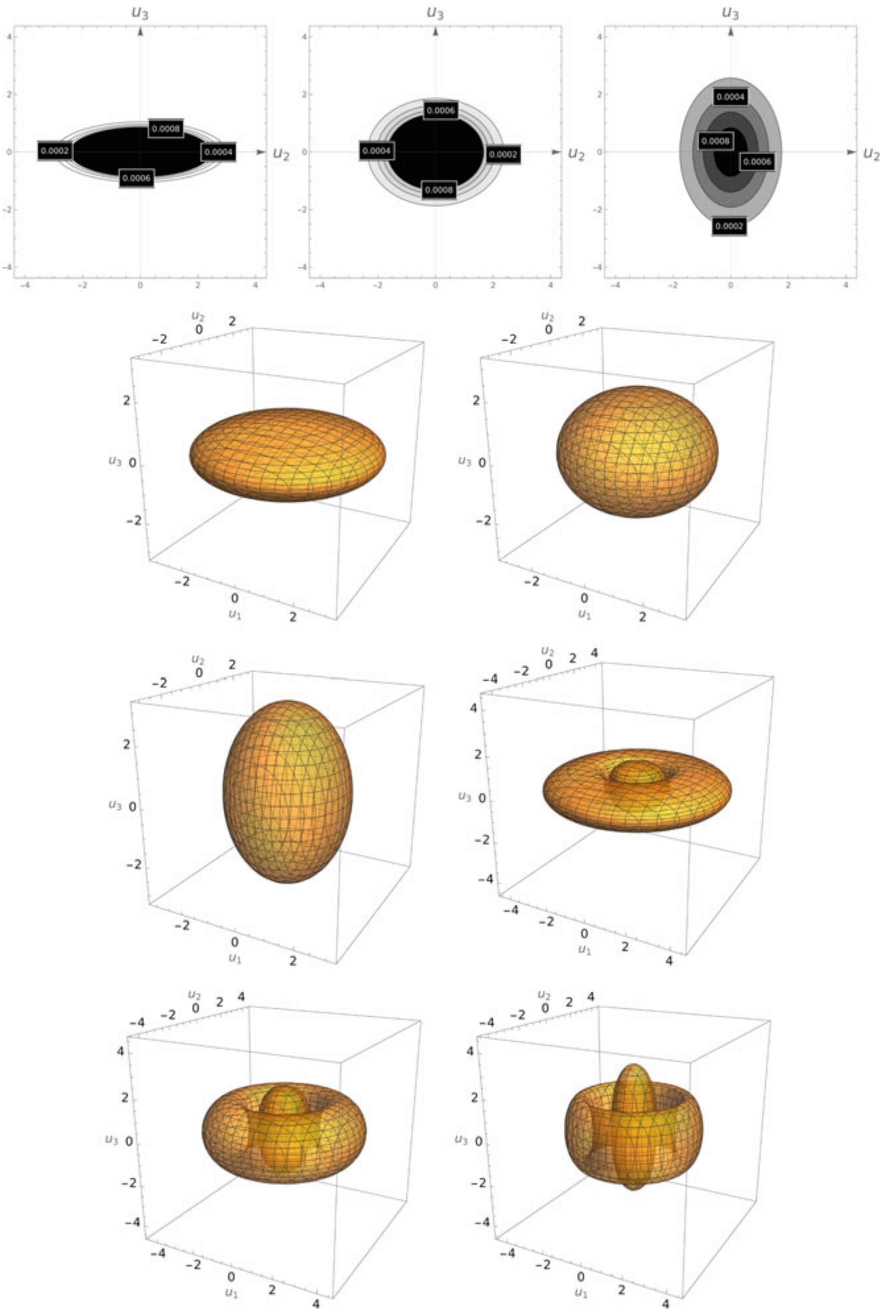


Fig. 5.7 Contour plots of the restrictions to the u_2, u_3-plane and region plots of the regions corresponding to probabilities larger than 0.0001, of the probability distribution $|U \exp(-i\,(t/\hbar)\,\hat{H})U^{-1}[(V^{-1}e_{mn}) \otimes (2\pi)^{-1/2}\,e^{im.\mathrm{id}_J} \otimes (2\sigma/\pi)^{1/4}\exp(-\sigma|\mathrm{id}_{\mathbb{R}} - u_{30}|^2)]|^2$, for $m = n = 0, \sigma = 1, u_{30} = 0, \omega t = 0$, 1 and 2 as well as for $m = 0, n = 1, \sigma = 1, u_{30} = 0, \omega t = 0$, 1 and 2

Hence, it follows for every $(m, n) \in \mathbb{Z} \times \mathbb{N}$, $t \in \mathbb{R}$ and $f \in L^2_{\mathbb{C}}(\mathbb{R})$ that

$$\left[U \exp\left(-i\,\frac{t}{\hbar}\,\hat{H}\right) U^{-1}\right] (V^{-1} e_{mn}) \otimes \frac{1}{\sqrt{2\pi}}\, e^{im.\mathrm{id}_J} \otimes f$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{i}{2}\,(|m| \mp m + 1 + 2n)\,\omega t\right) \cdot \left\{ \left(\frac{p_1 + i p_2}{\sqrt{p_1^2 + p_2^2}} \right)^m \right.$$

$$\left. [(V^{-1} e_{mn}) \circ (p_1^2 + p_2^2)^{1/2}] \right\} \otimes \left[\exp\left(-\frac{i}{2}\,\omega t\, \overline{(-\triangle_1)}\right) f\right]$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{i}{2}\,(|m| \mp m + 2n + 1)\,\omega t\right) \cdot \left\{ \left(\frac{p_1 + i p_2}{\sqrt{p_1^2 + p_2^2}} \right)^m \right.$$

$$\left. [(V^{-1} e_{mn}) \circ (p_1^2 + p_2^2)^{1/2}] \right\} \otimes [F_2^{-1} T_{\exp\left(-\frac{i}{2}\,\omega t\,|\;|^2\right)} F_2 f] \,,$$

where $\overline{(-\triangle_1)}$ denotes the closure of the negative of the Laplace operator in 1-space dimension, see (1.29), and $F_2 : L^2_{\mathbb{C}}(\mathbb{R}) \to L^2_{\mathbb{C}}(\mathbb{R})$ is the Fourier transformation in 1-space dimension.

From (1.24), it follows that

$$\left| e^{-\frac{i}{2}\,\omega t\,\overline{(-\triangle_1)}} \left(\frac{2\sigma}{\pi}\right)^{1/4} \exp(-\sigma|\mathrm{id}_{\mathbb{R}} - u_{30}|^2) \right|^2$$

$$= \left[\frac{1}{\pi}\,\frac{2\sigma}{1 + (2\sigma\omega t)^2}\right]^{1/2} \exp\left[-\frac{2\sigma}{1 + (2\sigma\omega t)^2}\,|\mathrm{id}_{\mathbb{R}} - u_{30}|^2\right] \,,$$

for every $t \in \mathbb{R}$, $\sigma > 0$ and $u_{30} \in \mathbb{R}$. Hence, for every $(m, n) \in \mathbb{Z} \times \mathbb{N}$, $t \in \mathbb{R}$, $\sigma > 0$ and $u_{30} \in \mathbb{R}$ (Fig. 5.7)

$$\left| \left[U \exp\left(-i\,\frac{t}{\hbar}\,\hat{H}\right) U^{-1}\right] (V^{-1} e_{mn}) \otimes \frac{1}{\sqrt{2\pi}}\, e^{im.\mathrm{id}_J} \right.$$

$$\left. \otimes \left(\frac{2\sigma}{\pi}\right)^{1/4} \exp(-\sigma|\mathrm{id}_{\mathbb{R}} - u_{30}|^2) \right|^2$$

$$= \frac{1}{2\pi} \left[\frac{1}{\pi}\,\frac{2\sigma}{1 + (2\sigma\omega t)^2}\right]^{1/2}$$

$$|[(V^{-1} e_{mn}) \circ (p_1^2 + p_2^2)^{1/2}]|^2 \otimes \exp\left[-\frac{2\sigma}{1 + (2\sigma\omega t)^2}\,|\mathrm{id}_{\mathbb{R}} - u_{03}|^2\right] \,.$$

6 The Path Integral Approach to Quantum Mechanics

The following Trotter product formulas, for the proofs see Corollaries 12.9.18, 12.9.20 in the Appendix, can be considered as providing a mathematical basis for Feynman's path integral approach to quantum mechanics, see [29, 30].

Theorem 6.0.1 (Trotter Product Formula for Self-Adjoint Operators) *Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, A and B densely-defined, linear and self-adjoint operators in X such that $A + B$ is densely-defined, linear and self-adjoint. Then*

$$\lim_{k\to\infty} [\, e^{-i\,(\tau/k)\,B} e^{-i\,(\tau/k)\,A}\,]^k f = e^{-i\tau\,(A+B)} f \ ,$$

for every $f \in X$ and $\tau \in \mathbb{R}$.

As part of a typical application in quantum mechanics, the operator A would be the multiple $\varepsilon_0^{-1}\,\hat{H}$ of the Hamilton operator of an "unperturbed" system and $\varepsilon_0 > 0$ has the dimension of an energy, B a perturbation of that system by a multiplication operator, given by the multiple $\varepsilon_0^{-1}\,V(\kappa^{-1}\cdot \mathrm{id}_{\mathbb{R}^n})$ of the perturbing potential V, and $\tau = \varepsilon_0 t/\hbar$. If the system is in the state $f \in X$ at the "time" $\tau = 0$, then the system reaches the kth approximation, $k \in \mathbb{N}^*$, to the state $e^{-i\tau(A+B)} f$ at time τ, by free propagation of the state f for the time τ/k, in this way the system arrives at the state $e^{-i\,(\tau/k)A} f$, subsequent propagation of $e^{-i\,(\tau/k)A} f$ for the time τ/k under the perturbation, in this way the system arrives at the state $e^{-i\,(\tau/k)B} e^{-i\,(\tau/k)A} f$, subsequent free propagation of $e^{-i\,(\tau/k)B} e^{i\,(\tau/k)A} f$ for the time

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_6.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_6

τ/k, in this way the system arrives at the state $e^{-i\,(\tau/k)A}e^{-i\,(\tau/k)B}e^{-i\,(\tau/k)A}f$, and so on, until reaching the state $[\,e^{-i\,(\tau/k)B}e^{-i\,(\tau/k)A}\,]^k f$. We also note that the k-th approximation is given by an unitary linear operator. For $k \to \infty$, we arrive at the state, $e^{-i\tau(A+B)}f$, of the system at time τ. This leads to a quite modern view of the scattering process in quantum theory, applying in particular to quantum field theory.

This process reminds Brownian motion of particles immersed in a fluid and in this way colliding randomly with the fluid particles. Between the collisions there is free motion. The "collision" process is described by the perturbing potential. Indeed, such a connection can be made, through analytic continuation in the time variable t. Before making this connection, we give Trotter product formulas which we are going to use for the derivation of Feynman path integrals.

Theorem 6.0.2 (Trotter Product Formulas for Semibounded Self-Adjoint Operators) *Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, A and B semibounded densely-defined, linear and self-adjoint operators in X, with lower bound $\gamma_1 \in \mathbb{R}$ and lower bound $\gamma_2 \in \mathbb{R}$, respectively, and such that $A + B$ is densely-defined, linear and self-adjoint. Further, let $z \in \mathbb{R} \times (-\infty, 0]$. Then*

$$\lim_{k\to\infty} [\,e^{-i\,(\tau/k)\,zB}e^{-i\,(\tau/k)\,zA}\,]^k f = e^{-i\tau z\,(A+B)} f \ ,$$

for every $f \in X$ and $\tau \in \mathbb{R}$.

We note that according to Corollary 12.7.2 for every $t > 0$, $z \in \mathbb{R} \times (-\infty, 0)$

$$\begin{aligned} e^{-i\,(t/\hbar)\,z\hat{H}} f &= \left(\pi i\, 4\, \frac{\varepsilon_0 t}{\hbar}\, z\right)^{-n/2} e^{i\,|\;|^2/\left(4\,\frac{\varepsilon_0 t}{\hbar}\,z\right)} * f \\ &= (\pi i\, 4\,\tau\, z)^{-n/2}\, e^{i\,|\;|^2/(4\,\tau\, z)} * f \ , \end{aligned} \tag{6.1}$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $\hat{H}$ is the free Hamiltonian from Sect. 1.4 and

$$\tau := \frac{\varepsilon_0 t}{\hbar} \ , \ \varepsilon_0 := \frac{\hbar^2 \kappa^2}{2m} \ .$$

In addition, we assume that the perturbing potential V is a.e. everywhere defined and bounded on $\mathbb{R}^n$. According to the Rellich-Kato theorem 1.6.1, $\hat{H} + T_{\mathcal{V}}$, where $T_{\mathcal{V}}$ denotes the maximal multiplication operator on $L^2_{\mathbb{C}}(\mathbb{R}^n$ with $\mathcal{V} := V(\kappa^{-1} \cdot \mathrm{id}_{\mathbb{R}^n})$, is a densely-defined linear and self-adjoint operator in $L^2_{\mathbb{C}}(\mathbb{R}^n)$ that is semibounded from below and whose domain coincides with the domain $D(\hat{H})$ of $\hat{H}$.[1] Further, according to the functional calculus for maximal multiplication operators, see Corollary 12.6.9, we have that

[1] We note that $\hat{H}$ is positive and $T_{\mathcal{V}}$ is bounded from below. Hence, the assumptions of Theorem 6.0.2 are satisfied.

$$e^{-i\,(t/\hbar)\,z\,T_{\mathcal{V}}} f = e^{-i\,\tau z\,\mathcal{V}/\varepsilon_0} f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. As a consequence, we obtain

$$\begin{aligned} e^{-i\,[(t/k)/\hbar]\,zT_{\mathcal{V}}} e^{-i\,[(t/k)/\hbar]\,z\hat{H}} f &= e^{-i\,(\tau/k)\,z\,T_{\mathcal{V}/\varepsilon_0}}\, e^{-i\,(\tau/k)\,z\,\varepsilon_0^{-1}\hat{H}} f \\ &= g_B \cdot (g_A * f) \ , \end{aligned}$$

for $k \in \mathbb{N}^*$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $x := \mathrm{Re}(z)$, $y := \mathrm{Im}(z) < 0$ and

$$\begin{aligned} g_A &:= (\pi i\, 4z\tau/k)^{-n/2}\ e^{ik\,|\ |^2/(4z\tau)} \\ &= (\pi i\, 4z\tau/k)^{-n/2}\ e^{ikx\,|\ |^2/\left(4\,|z|^2\tau\right)} e^{-k\,|y|\,|\ |^2/\left(4|z|^2\tau\right)} \in L^1_{\mathbb{C}}(\mathbb{R}^n) \ , \\ g_B &:= e^{-i\,(\mathcal{V}/\varepsilon_0)\,z\tau/k} = e^{ix\,(\mathcal{V}/\varepsilon_0)\,\tau/k} e^{-|y|\,(\tau/k)\,(\mathcal{V}/\varepsilon_0)} \in L^\infty_{\mathbb{C}}(\mathbb{R}^n) \ . \end{aligned}$$

Using that the Banach space $L^1_{\mathbb{C}}(\mathbb{R}^n)$, equipped with the convolution as a multiplication, is a commutative Banach algebra and using Fubini's theorem, it follows for $f \in L^2_{\mathbb{C}}(\mathbb{R}^n) \cap L^1_{\mathbb{C}}(\mathbb{R}^n)$ and $k \geqslant 2$ that

$$\begin{aligned} &\left\{\left[e^{-i\,(\tau/k)\,z\,T_{\mathcal{V}/\varepsilon_0}}\, e^{-i\,(\tau/k)\,z\,\varepsilon_0^{-1}\hat{H}} f\right]^k f\right\}(u_{k+1}) \\ &= \left\{\left[e^{-i\,[(t/k)/\hbar]\,zT_{\mathcal{V}}} e^{-i\,[(t/k)/\hbar]\,z\hat{H}}\right]^k f\right\}(u_{k+1}) \\ &= g_B(u_{k+1}) \int_{(\mathbb{R}^n)^k} g_B(u_{k+1}-u_k)\cdots g_B(u_{k+1}-u_k-u_{k-1}-\cdots-u_2) \\ &\qquad\qquad f(u_{k+1}-u_k\cdots-u_1)\, g_A(u_1)\ldots g_A(u_k)\, du_1\ldots du_k \\ &= g_B(u_{k+1}) \int_{(\mathbb{R}^n)^k} g_A(u_{k+1}-u_k)\cdots g_A(u_2-u_1) \\ &\qquad\qquad f(u_1)\, g_B(u_2)\cdots g_B(u_k)\, du_1\cdots du_k \\ &= (\pi i\, 4z\tau/k)^{-kn/2}\ e^{-i\,[\mathcal{V}(u_{k+1})/\varepsilon_0]\,z\tau/k} \\ &\quad \cdot \int_{(\mathbb{R}^n)^k} e^{ik\,|u_{k+1}-u_k|^2/(4z\tau)}\ldots e^{ik\,|u_2-u_1|^2/(4z\tau)} \\ &\qquad\qquad f(u_1)\, e^{-i\,[\mathcal{V}(u_2)/\varepsilon_0]\,z\tau/k}\ldots e^{-i\,[\mathcal{V}(u_k)/\varepsilon_0]\,z\tau/k}\, du_1\cdots du_k \\ &= \left(\pi i\,\frac{4z\tau}{k}\right)^{-kn/2} \cdot \int_{(\mathbb{R}^n)^k} e^{i\sum_{l=1}^k \frac{z\tau}{k}\left[\frac{(u_{l+1}-u_l)^2}{(2z\tau/k)^2} - \frac{\mathcal{V}(u_{l+1})}{\varepsilon_0}\right]} f(u_1)\, du_1\cdots du_k \\ &= \left[z\,\frac{2\pi i\hbar\,(t/k)}{m}\right]^{-kn/2} \\ &\quad \cdot \int_{(\mathbb{R}^n)^k} e^{\frac{i}{\hbar}\left\{\frac{1}{z}\sum_{l=1}^k \frac{m}{2}\,\frac{[(u_{l+1}/\kappa)-(u_l/\kappa)]^2}{t/k} - z\,\frac{t}{k}\sum_{l=1}^k V(u_{l+1}/\kappa)\right\}} \\ &\qquad\qquad \cdot f(u_1)\left(\kappa^{-n}\right)^k du_1\cdots du_k \ , \end{aligned}$$

for every $u_{k+1} \in \mathbb{R}^n$.

Regularized Feynman path integrals

Hence, it follows for every $z \in \mathbb{R} \times (-\infty, 0)$, $t > 0$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n) \cap L^1_{\mathbb{C}}(\mathbb{R}^n)$ that

$$
\begin{aligned}
&\left\{\left[e^{-i\,[(t/k)/\hbar]\,zT_{\mathcal{V}}}\, e^{-i\,[(t/k)/\hbar]\,z\hat{H}}\right]^k f\right\}(u_{k+1}) \\
&= \left[z\,\frac{2\pi i\hbar\,(t/k)}{m}\right]^{-kn/2} \\
&\quad \cdot \int_{(\mathbb{R}^n)^k} e^{\frac{i}{\hbar}\left\{\frac{1}{z}\sum_{l=1}^{k}\frac{m}{2}\frac{[(u_{l+1}/\kappa)-(u_l/\kappa)]^2}{t/k} - z\,\frac{t}{k}\sum_{l=1}^{k} V(u_{l+1}/\kappa)\right\}} \\
&\qquad \cdot f(u_1)\left(\kappa^{-n}\right)^k du_1 \cdots du_k\ ,
\end{aligned}
\tag{6.2}
$$

for every $u_{k+1} \in \mathbb{R}^n$ and from Theorem 6.0.2 that

$$
\begin{aligned}
&\lim_{k\to\infty}\left\{\left[e^{-i\,[(t/k)/\hbar]\,zT_{\mathcal{V}}}\, e^{-i\,[(t/k)/\hbar]\,z\hat{H}}\right]^k f\right\}(u_{k+1}) \\
&= [e^{-i\,(t/\hbar)\,z\,(\hat{H}+T_{\mathcal{V}})} f](u_{k+1})\ ,
\end{aligned}
\tag{6.3}
$$

for almost all $u_{k+1} \in \mathbb{R}^n$.

We note that

$$
\frac{m}{2}\,\frac{[(u_{l+1}/\kappa) - (u_l/\kappa)]^2}{t/k}
$$

is the least (or extremal) action needed for a free classical particle of mass m to move from the point u_l/κ to the point $u_{(l+1)}/\kappa$ within time t/k. The term

$$
-\,\frac{t}{k}\,V(u_{l+1}/\kappa)
$$

is a correction term that takes into account the presence of the potential V so that

$$
\frac{m}{2}\,\frac{[(u_{l+1}/\kappa) - (u_l/\kappa)]^2}{t/k} - \frac{t}{k}\,V(u_{l+1}/\kappa)
$$

is an approximation to the least action needed for a classical particle of mass m under the influence of the potential V to move from the point u_l/κ to the point $u_{(l+1)}/\kappa$ within time t/k. The latter approximation becomes increasingly accurate for $k \to \infty$.

Formulas 6.2, 6.3 provide a basis for Feynman's path integral approach to quantum mechanics. Formally, the substitution $z = 1$ into these formulas lead to Feynman's representation from [29]. Starting from the principle of least action of classical mechanics, he arrived at the latter formulas. In this, the factor in front of the integral had to be adjusted to achieve compatibility with Schrödinger's equation so that the approach is not completely independent of the standard approach to quantum mechanics.

It is a consequence of the spectral theorem, Theorem 12.6.4, that

$$\lim_{z\to 1, z\in\mathbb{R}\times(-\infty,0)} \left[e^{-i\,[(t/k)/\hbar]\,zT_{\mathcal{V}}}e^{-i\,[(t/k)/\hbar]\,z\hat{H}}\right]^k f$$
$$= \left[e^{-i\,[(t/k)/\hbar]\,T_{\mathcal{V}}}e^{-i\,[(t/k)/\hbar]\hat{H}}\right]^k f \ ,$$

for every $t \geqslant 0$, $k \in \mathbb{N}^*$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, providing a unitary linear approximation to $e^{-i\,(t/\hbar)\,(\hat{H}+T_{\mathcal{V}})}$.

6.1 A Connection Between the Solutions of the Schrödinger and the Heat Equation

Finally, we are going to make the connection between the Schrödinger equation and the heat or diffusion equation. The heat equation,

$$\frac{\partial T}{\partial t} = \alpha\,\triangle T \ ,$$

describes the temperature distribution T, in a homogeneous body occupying the volume Ω, where $\alpha > 0$ is the thermal diffusivity[2] of the body. The equation is a special case of the differential equation

$$u'(t) = -Au(t) \ , \tag{6.4}$$

$t > 0$, where a A is a densely-defined, linear and positive self-adjoint operator in a non-trivial complex Hilbert space X.[3] The unique solution to (6.4), see Theorem 4.5.1 of [8] and Lemma 12.9.15 in the Appendix, for data $u(0)$ from the domain of A, is given by

$$u(t) = e^{-tA}u(0) \ ,$$

for every $t \geqslant 0$, where

$$e^{-tA}$$

[2] Thermal diffusivities have the dimension l^2/t.

[3] The differential equation (6.4) has unique solutions for a considerably larger class of operators A than the class of linear positive self-adjoint operators in Hilbert spaces, e.g., including non-linear operators, see [5, 8, 26, 34, 35, 52, 57].

is the bounded linear operator on X that is associated by the functional calculus of A to the function

$$(\sigma(A) \to \mathbb{C} \ , \ t \mapsto e^{-t\lambda}) \ ,$$

where $\sigma(A)$ is the spectrum of A. According to (6.1), we have for every $t > 0$, $z \in \mathbb{R} \times (-\infty, 0)$, $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ that

$$e^{-i\,(t/\hbar)\,z\hat{H}} f = \left(4\pi i\,\frac{\varepsilon_0 t}{\hbar}\,z\right)^{-n/2} e^{i\,|\ |^2/\left(4\,\frac{\varepsilon_0 t}{\hbar}\,z\right)} * f \ ,$$

and hence for the case $z = -i$ that

$$e^{-(t/\hbar)\hat{H}} f = \left(4\pi\,\frac{\varepsilon_0 t}{\hbar}\right)^{-n/2} e^{-\,|\ |^2/\left(4\,\frac{\varepsilon_0 t}{\hbar}\right)} * f \ .$$

As described above, the latter corresponds to the diffusion type equation

$$u'(t) = -\frac{1}{\hbar}\,\hat{H}u(t) \ , \tag{6.5}$$

$t > 0$ associated with the thermal diffusivity

$$\alpha = \frac{\hbar}{2m} \ .$$

For instance, for the case of an electron, we have that

$$\frac{\hbar}{2m} \approx 5.79 \cdot 10^{-5}\,\frac{\mathrm{m}^2}{\mathrm{s}} \ ,$$

leading to a thermal diffusivity of an order of magnitude similar to the thermal diffusivities of metals.

According to Corollary 12.9.16, for $f \in D(\hat{H})$, the map that associates with every t from the closed lower half-plane of the complex plane, $\mathbb{R} \times (-\infty, 0]$, the element

$$e^{-i\,(t/\hbar)\,\hat{H}} f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$$

is a continuous function whose restriction to the open lower half-plane of the complex plane, $\mathbb{R} \times (-\infty, 0)$, is holomorphic (Fig. 6.1).

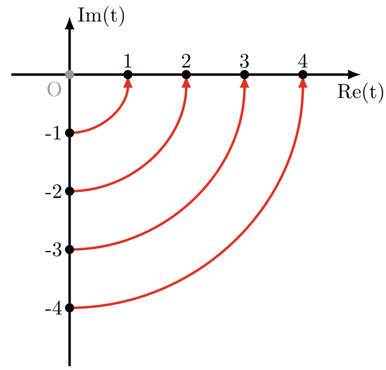


Fig. 6.1 A connection between the solutions of the Schrödinger and a diffusion type equation. Black dots indicate $e^{-i\,(t/\hbar)\,\hat{H}} f$ for the given value of t. Red arrows indicate analytic continuation

A connection between the solutions of the Schrödinger and a diffusion type equation

Hence the solution of the Schrödinger equation for $t \geqslant 0$, corresponding to data f at time $t = 0$ from the domain of $\hat{H}$, is given by the boundary values on the positive real axis, of the analytic extension of the solution, on the purely imaginary axis in the lower half-plane, to the open lower half-plane of the complex plane, corresponding to same data, of the equation of diffusion type (6.5).

7 Conclusion

The purpose of the book is to introduce the reader to quantum mechanics through the analysis of basic quantum mechanical systems. As there is no Newtonian mechanics without Calculus, there is no quantum theory without operator theory. The use of the latter language is a necessity on the way to achieve physical understanding. Therefore, the book teaches in detail how to use the methods of operator theory for analyzing quantum mechanical systems, starting from the determination of the deficiency subspaces of (densely-defined, linear) symmetric operators in complex Hilbert spaces, for the purpose of arriving at their self-adjoint extensions, only the latter can be observables of the theory, up to the calculation of the spectra, spectral measures and functional calculi of observables, including the construction of the exponential functions of the involved Hamilton operators that solve the problem of time evolution.

The reader might have noticed that in this book, instead of writing down a formal Schrödinger equation, the first step in the analysis of a closed quantum mechanical system consists in the construction of a Hamilton operator $\hat{H}$, the generator of the time-evolution of the system. Only when this is done, it is possible to write down a well-defined abstract Schrödinger equation. On the other hand, the latter step is redundant, since there are methods for the construction of the exponential function of $\hat{H}$, for instance from the resolvent of $\hat{H}$, that solve the problem of the time evolution of the system. Therefore, Schrödinger equations only appear implicitly in this book. Also, it is not advisable to consider Schrödinger equations as partial differential equations, since the corresponding unknown is not observable, differently from the unknowns of partial differential equations from classical physics.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/978-3-031-49078-1_7.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1_7

This is relevant because at this point quantum mechanics differs from its early competitor "wave mechanics." These 2 theories are incompatible. The mixture of both theories leads to contradictions.

What is gained from acquiring the methods from operator theory, beyond providing a clearer understanding of quantum theory? To the opinion of the author, it might prepare for future physical theories that have to be expected to be even more abstract than quantum theory. Roughly speaking, classical physics, including the theory of general relativity, describe the macroscopic that is close to our perception. This is reflected by the used mathematical methods, from calculus, geometry and the field of partial differential equations. Quantum theories describe a world that can be accessed only by use of special instrumentation. Atomic radii are of the order 10^{-8} cm. Nuclear radii are of the order 10^{-13} cm. This inaccessibility to our natural senses is the quality that makes this world particularly interesting and unsurprisingly is accompanied by a greater abstractness of the needed mathematical methods. Originally, quantum theory provided the first theory of matter. With the advent of quantum field theory, it turned into a theory of matter and fields, testing also our ideas of space and time. Ultimately, it has the potential to turn into a theory of "everything."

References

1. Abramowitz, M., and I.A. Stegun, eds. 1984. *Pocketbook of mathematical functions*. Thun: Harri Deutsch.
2. Adams, R.A., and J.J.F. Fournier. 2003. *Sobolev spaces*, 2nd ed. New York: Academic.
3. Baez, J.C., I.E. Segal, and Z. Zhou. 1992. *Introduction to algebraic and constructive quantum field theory*. Princeton: Princeton University Press.
4. Beals, R., and R. Wong. 2016. *Special functions and orthogonal polynomials*. Cambridge: Cambridge University Press.
5. Belleni-Morante, A., and A.C. McBride. 1998. *Applied nonlinear semigroups: An introduction*. New York: Wiley.
6. Bellman, R. 1949. *A survey of the theory of the boundedness, stability, and asymptotic behaviour of solutions of linear and nonlinear differential and difference equations, NAVEXOS P-596*. Washington, DC: Office of Naval Research.
7. Beyer, H. 2022. *The reasoning of quantum mechanics: Operator theory and the harmonic oscillator*. Cham: Springer Nature.
8. Beyer, H.R. 2007. *Beyond partial differential equations: On linear and quasi-linear abstract hyperbolic evolution equations*, vol. 1898. Lecture notes in mathematics. Berlin: Springer.
9. Beyer, H.R. 1991. Remarks on Fulling's quantization. *Classical and Quantum Gravity* 8: 1091–1112.
10. Beyer, H.R. 1999. On the completeness of the quasinormal modes of the Pöschl-Teller potential. *Communications in Mathematical Physics* 204: 397–423.
11. Bjorken, J.D., and S.D. Drell. 1964. *Relativistic quantum mechanics*. New York: McGraw-Hill.
12. Bjorken, J.D., and S.D. Drell. 1965. *Relativistic quantum fields*. New York: McGraw-Hill.
13. Born, M., W. Heisenberg, and P. Jordan. 1926. Zur Quantenmechanik II. *Zeitschrift für Physik* 35: 557–615.
14. Born, M., and P. Jordan. 1930. *Elementare Quantenmechanik*. Berlin: Springer.
15. Brezis, H. 1983. *Analyse fonctionnelle: Théorie et applications*. Paris: Collection Mathématiques Appliquées pour la Maîtrise, Masson.
16. Buchholz, D. 2000. Algebraic quantum field theory: A status report. In *Plenary talk given at XIIIth International Congress on Mathematical Physics*, London. http://xxx.lanl.gov/abs/math-ph/0011044.

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1

17. Chernoff, P.R. 1968. Note on product formulas for operator semigroups. *Journal of Functional Analysis* 2: 238–242.
18. Chihara, T.S. 1978. *An introduction to orthogonal polynomials*. New York: Gordon and Breach.
19. Cohen-Tannoudji, C., B. Diu, and F. Laloe. 1978. *Quantum mechanics*, vol. 1. New York: Wiley & Sons.
20. Davisson, C.J., and L.H. Germer. 1928. Reflection of electrons by a crystal of Nickel. *Proceedings of the National Academy of Sciences of the USA* 14: 317–322.
21. Dirac, P.A.M. 2019. *The principles of quantum mechanics*. New York: BN Publishing.
22. Dixmier, J. 1977. $\mathbb{C}^*$-Algebras. Amsterdam: North-Holland.
23. Dunford, N., and J.T. Schwartz. 1957. *Linear operators, Part I: General theory*. New York: Wiley.
24. Dunford, N., and J.T. Schwartz. 1963. *Linear operators, Part II: Spectral theory: Self adjoint operators in Hilbert space theory*. New York: Wiley.
25. Dunkel, O. 1912–1913. Regular singular points of a system of homogeneous linear differential equations of the first order. *American Academy of Arts and Sciences Proceedings* 38: 341–370.
26. Engel, K.-J., and R. Nagel. 2000. *One-parameter semigroups for linear evolution equations*. New York: Springer.
27. Eckart, C. 1930. The penetration of a potential barrier by electrons. *Physical Review* 35: 1303–1309.
28. Erdelyi, A., ed. 1981. *Higher transcendental functions,* vol. II. Florida: Robert Krieger.
29. Feynman, R.P. 1948. Space-time approach to non-relativistic quantum mechanics. *Reviews of Modern Physics* 20: 367–387.
30. Feynman, R.P., and A.R. Hibbs. 1965. *Quantum mechanics and path integrals*. New York: McGraw-Hill.
31. Fulling, S.A. 1989. *Aspects of quantum field theory in curved spacetime*. Cambridge: Cambridge University Press.
32. Galilei, G., ed. 1864. *Il Saggitatore*. Firenze: G. Barbèra.
33. Goldberg, S. 1985. *Unbounded linear operators*. New York: Dover.
34. Goldstein, J.A. 1985. *Semigroups of linear operators and applications*. New York: Oxford University Press.
35. Goldstein, J.A. 1972. *Lectures on semigroups of nonlinear operators*. New Orleans: Tulane University.
36. Haag, R. 1996. *Local quantum physics: Fields, particles, algebras*. New York: Springer.
37. Heisenberg, W. 1925. Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen. *Zeitschrift für Physik* 33: 879–893.
38. Heisenberg, W. 1927. Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik. *Zeitschrift für Physik* 43: 172–198.
39. Hille, E. 1969. *Lectures on ordinary differential equations*. Reading: Addison-Wesley.
40. Hirzebruch, F., and W. Scharlau. 1971. *Einführung in die Funktionalanalysis*. BI: Mannheim.
41. Hutson, V., J.S. Pym, and M.J. Cloud. 2005. *Applications of functional analysis and operator theory*, 2nd ed. Amsterdam: Elsevier.
42. Joergens, K., and F. Rellich. 1976. *Eigenwerttheorie gewoehnlicher Differentialgleichungen*. Berlin, Heidelberg: Springer.
43. Kato, T. 1966. *Perturbation theory for linear operators*. New York: Springer.
44. Landau, L.D., and E.M. Lifshitz. 1991. *Quantum mechanics: Non-relativistic theory*, 3rd ed. Oxford: Pergamon Press.
45. Lang, S. 1996. *Real and functional analysis*, 3rd ed. New York: Springer.
46. Lebedev, N.N. 1965. *Special functions and their applications*. Englewood Cliffs: Prentice-Hall.
47. Levinson, N. 1948. The asymptotic nature of the solutions of linear systems of differential equations. *Duke Mathematical Journal* 15: 111–126.

48. Mackey, G.W. 2004. *Mathematical foundations of quantum mechanics*. Dover: Dover Publications.
49. Mermin, D. 2004. What is wrong with this pillow. *Nature* 505: 153–155.
50. Messiah, A. 2014. *Quantum mechanics*. New York: Dover Publication.
51. Meyenn, K. 1996. *Wolfgang Pauli: Scientific correspondence with Bohr, Einstein, Heisenberg, a.o.*, vol. II, Part I: 1950–1952. Berlin: Springer.
52. Miyadera, I. 1992. *Nonlinear semigroups*. Providence: AMS.
53. Von Neumann, J. 1930. Allgemeine Eigenwerttheorie Hemitescher Funktionaloperatoren. *Mathematische Annalen* 102: 49–131.
54. Von Neumann, J. 1932. *Mathematische Grundlagen der Quantenmechanik*. Berlin: Springer.
55. Olver, F.W.J., D.W. Lozier, R.F. Boisvert, and C.W. Clark, eds. 2010. *NIST handbook of mathematical functions*. New York: Cambridge University Press.
56. Olver, F.W.J., A.B. Olde Daalhuis, D.W. Lozier, B.I. Schneider, R.F. Boisvert, C.W. Clark, B.R. Miller, B.V. Saunders, H.S. Cohl, and M.A. McClain, eds. 2022. *NIST digital library of mathematical functions*. http://dlmf.nist.gov/, Release 1.1.6 of 2022-06-30.
57. Pazy, A. 1983. *Semigroups of linear operators and applications to partial differential equations*. New York: Springer.
58. Pöschl, G., and E. Teller. 1933. Bemerkungen zur Quantenmechanik des harmonischen Oszillators. *Zeitschrift für Physik* 83: 143–151.
59. Prugovecki, E. 1981. *Quantum mechanics in Hilbert space*. New York: Academic.
60. Reed, M., and B. Simon. 1980, 1975, 1979, 1978. *Methods of modern mathematical physics*, vol. I, II, III, IV. New York: Academic.
61. Rejto, P.A. 1966. On the essential spectrum of the hydrogen energy and related operators. *Pacific Journal of Mathematics* 19: 109–140.
62. Renardy, M., and R.C. Rogers. 1993. *An introduction to partial differential equations*. New York: Springer.
63. Riesz, F., and B. Sz-Nagy. 1955. *Functional analysis*. New York: Unger.
64. Rosen, N., and P.M. Morse. 1932. On the vibrations of polyatomic Molecules. *Physical Review* 42: 210–217.
65. Rudin, W. 1991. *Functional analysis*, 2nd ed. New York: MacGraw-Hill.
66. Sakurai, J.J. 1967. *Advanced quantum mechanics*. Reading: Addison-Wesley.
67. Schäfke, W. 1963. *Einführung in die Theorie der speziellen Funktionen der mathematischen Physik*. Berlin: Springer.
68. Schechter, M. 2003. *Operator methods in quantum mechanics*. New York: Dover Publication.
69. Schiff, L.I. 1968. *Quantum mechanics*, 3Rev ed. New York: McGraw-Hill Education.
70. Schroer, B. 2001. *Lectures on algebraic quantum field theory and operator algebras*. http://xxx.lanl.gov/abs/math-ph/0102018.
71. Simon, B. 2015. *A comprehensive course in analysis Part 4: Operator theory*. Providence: AMS.
72. Shankar, R. 1994. *Principles of quantum mechanics*, 2nd ed. New York: Springer.
73. Stein, E.M., and R. Shakarchi. 2003. *Fourier analysis: An introduction*. Princeton and Oxford: Princeton University Press.
74. Streater, R.F., and A.S. Wightman. 2000. *PCT, Spin and statistics, and all that*. Princeton: Princeton University Press.
75. Szegö, G. 1939. *Orthogonal polynomials*. Providence: AMS.
76. Taylor, J.R. 1972. *Scattering theory*. New York: Wiley.
77. Thirring, W. 1981. *A course in mathematical physics 3: Quantum mechanics of atoms and molecules*. New York: Springer.
78. Young, T. 1802. On the theory of light and colours. *Philosophical Transactions of the Royal Society* 92: 12–48.

79. Wald, R.M. 1994. *Quantum field theory in curved spacetime and black hole thermodynamics*. Chicago: University of Chicago Press.
80. Weidmann, J. 1980. *Linear operators in Hilbert spaces*. New York: Springer.
81. Weidmann, J. 2000. *Lineare Operatoren in Hilberträumen: Teil I: Grundlagen*. Stuttgart: Teubner.
82. Weidmann, J. 2003. *Lineare Operatoren in Hilberträumen: Teil II: Anwendungen*. Stuttgart: Teubner.
83. Yosida, K. 1968. *Functional analysis*, 2nd ed. Berlin: Springer.
84. Ziemer, W.P. 1989. *Weakly differentiable functions*. New York: Springer.

Index

H. R. Beyer, *Introduction to Quantum Mechanics*, Synthesis Lectures on Engineering, Science, and Technology, https://doi.org/10.1007/978-3-031-49078-1

Contents

12 Appendix

In the following, we introduce prerequisites for and basics of the language of Operator Theory that can also be found in most textbooks on Functional Analysis [34, 36, 37, 43, 46]. For the convenience of the reader, we also include corresponding proofs, but encourage readers of acquiring a more complete picture, e.g., from the above cited sources.

12.1 Normed Vector Spaces and Banach Spaces

Definition 12.1.1. (**Normed vector spaces, Banach spaces**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. A pair $(X, \| \ \|)$

a) is called a normed vector space over $\mathbb{K}$ if X is a vector space over $\mathbb{K}$ and $\| \ \| : X \to [0, \infty)$ is map such that

   (i) $\|f\| = 0$ if and only if $f = 0$ (*i.e.* , $\| \ \|$ *is positive definite*),

   (ii) $\|\lambda f\| = |\lambda| \, \|f\|$ for every $f \in X$ and $\lambda \in \mathbb{K}$ (*i.e.* , $\| \ \|$ *is homogeneous*),

   (iii) $\|f + g\| \leqslant \|f\| + \|g\|$ for all $f, g \in X$ (*i.e.* , $\| \ \|$ *satisfies triangle inequalities*).

b) is called a Banach space over $\mathbb{K}$ or a $\mathbb{K}$-Banach space if $(X, \| \ \|)$ is a complete normed vector space over $\mathbb{K}$, i.e., if every Cauchy-sequence in X is convergent to an element of X.

Remark 12.1.2. If $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \| \ \|)$ and D is a subspace of X, then $(D, \| \ \||_D)$ is a normed vector space, too. Therefore, unless indicated otherwise, we consider every subspace to be automatically equipped with the corresponding restriction of $\| \ \|$.

Example 12.1.3. (L^1**-Spaces**) Let $n \in \mathbb{N}^*$, $E \subset \mathbb{R}^n$ be non-empty and measurable, where v^n denotes the Lebesgue measure in n dimensions. We define

$$\mathcal{L}^1_{\mathbb{C}}(E) := \{f : E \to \mathbb{C} : \mathrm{Re}(f), \mathrm{Im}(f) \text{ are } v^n\text{-measurable} \\ \text{and } |\mathrm{Re}(f)|, |\mathrm{Im}(f)| \text{ are } v^n\text{-integrable}\}$$

and for every $f \in \mathcal{L}^1_{\mathbb{C}}(E)$

$$\|f\|_1 := \int_E |f| \, dv^n \ .$$

Then *according to Functional Analysis*

> $\left(L^1_{\mathbb{C}}(E), +, ., \|\ \|_1\right)$ is a complex Banach space,

where

$$L^1_{\mathbb{C}}(E) := \mathscr{L}^1_{\mathbb{C}}(E)/_\sim\ ,$$

the equivalence relation $\sim$ on $\mathscr{L}^1_{\mathbb{C}}(E)$ is defined by[1]

$$f \sim g :\Leftrightarrow f = g \text{ a.e. on } E\ ,$$

for all $f, g \in \mathscr{L}^1_{\mathbb{C}}(E)$, and $L^1_{\mathbb{C}}(E)$ is *equipped with the operations* $+, .$ *and the* L^1*-norm* $\|\ \|_1$*, defined by*

$$\begin{aligned}[f] + [g] &:= [f + g]\ ,\ \lambda.[f] := [\lambda.f]\ ,\\ \|[f]\|_1 &:= \|f\|_1\end{aligned}$$

for all $f, g \in \mathscr{L}^1_{\mathbb{C}}(E)$ and $\lambda \in \mathbb{C}$.

Example 12.1.4. (L^∞**-Spaces**) Let $n \in \mathbb{N}^*$, $E \subset \mathbb{R}^n$ be non-empty and measurable, where v^n denotes the Lebesgue measure in n dimensions. We define

$$\begin{aligned}\mathscr{L}^\infty_{\mathbb{C}}(E) := \{f : E \to \mathbb{R} : \mathrm{Re}(f), \mathrm{Im}(f) \text{ are measurable, and there is}\\ C \in [0, \infty) \text{ such that } |f| \leqslant C \text{, a.e. on } E\}\end{aligned}$$

and for every $f \in \mathscr{L}^\infty_{\mathbb{C}}(E)$

$$\|f\|_\infty := \inf\{C \in [0, \infty) : |f| \leqslant C \text{, a.e. on } E\}\ .$$

Then *according to Functional Analysis*

> $(L^\infty_{\mathbb{C}}(E), +, ., \|\ \|_\infty)$ is a complex Banach space,

where

$$L^\infty_{\mathbb{C}}(E) := \mathscr{L}^\infty_{\mathbb{C}}(E)/_\sim\ ,$$

the equivalence relation $\sim$ on $\mathscr{L}^\infty_{\mathbb{C}}(E)$ is defined by[2]

$$f \sim g :\Leftrightarrow f = g \text{ a.e. on } E\ ,$$

---

[1] a.e. stands for *almost everywhere*, i.e., $\{x \in E : f(x) \neq g(x)\}$ is set of Lebesgue measure 0.
[2] a.e. stands for *almost everywhere*, i.e., $\{x \in E : f(x) \neq g(x)\}$ is set of Lebesgue measure 0.

for all $f, g \in \mathcal{L}^\infty_{\mathbb{C}}(E)$, and $L^\infty_{\mathbb{C}}(E)$ is *equipped with the operations* $+, .$ *and the* L^∞*-norm* $\| \ \|_\infty$*, defined by*

$$[f] + [g] := [f + g] \ , \ \lambda.[f] := [\lambda.f] \ ,$$
$$\|[f]\|_\infty := \| f \|_\infty$$

for all $f, g \in \mathcal{L}^\infty_{\mathbb{C}}(E)$ and $\lambda \in \mathbb{C}$.

As is standard practice, we are not going to indicate that we are working with equivalence classes, rather than functions. Normally, this does not lead to complications, since in applications, usually, the equivalence classes in question, have a unique distinguished, e.g., continuous, representative, which is the basis for considerations. On the other hand, occasionally, it is necessary to remember this fact.

12.2 Linear Operators in Banach Spaces

12.2.1 Bounded Linear Operators

Definition 12.2.1. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $(X, \| \ \|_X)$ and $(Y, \| \ \|_Y)$ be normed vector spaces over $\mathbb{K}$. We define the subset $L(X, Y)$ of Y^X to consist of all linear continuous maps from X to Y.

Theorem 12.2.2. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \| \ \|_X)$ a non-trivial normed vector space over $\mathbb{K}$, $(Y, \| \ \|_Y)$ a normed vector space over $\mathbb{K}$ and $A : X \to Y$ be linear.

(i) Then A is continuous if and only if $A(S^1)$ is bounded.

(ii) $(L(X, Y), \| \ \|_{\text{Op}})$,

where $\| \ \|_{\text{Op}} : L(X, Y) \to [0, \infty)$ is defined by

$$\|A\|_{\text{Op}} := \sup\{\|Af\|_Y : f \in S^1\}$$

for every $A \in L(X, Y)$, is a normed vector space over $\mathbb{K}$, where $L(X, Y)$ is equipped with the usual operations of pointwise addition and pointwise scalar multiplication by elements of $\mathbb{K}$. In particular, if Y is complete, then this space is complete, too.

Proof. “Part (i)": If A is continuous, there is $\delta > 0$ such that

$$\|Af\|_Y = \|Af - A0\|_Y < 1$$

for all $f \in B_\delta(0)$. Hence it follows for $f \in S^1$ that

$$\|Af\|_Y = \frac{1}{\delta}\|A\delta f\|_Y < \frac{1}{\delta}$$

and that $A(S^1)$ is bounded. If $A(S^1)$ is bounded, it follows for different elements $f, g \in X$ that

$$\begin{aligned}\|Ag - Af\|_Y &= \|A(g-f)\|_Y = \|g-f\|_X \cdot \|A\,\|g-f\|_X^{-1}.(g-f)\|_Y \\ &\leqslant \left[\sup\{\|Af\|_Y : f \in S^1\}\right] \|g-f\|_X\end{aligned}$$

and hence the continuity of A.
"Part (ii)": Since for $A, B \in L(X, X), \lambda \in \mathbb{K}$ and $f \in S^1$

$$\begin{aligned}&\|0f\|_Y = 0\ , \\ &\|(A+B)f\|_Y \leqslant \|Af\|_Y + \|Bf\|_Y \\ &\leqslant \sup\{\|Af\|_Y : f \in S^1\} + \sup\{\|Bf\|_Y : f \in S^1\}\ , \\ &\|(\lambda.A)f\|_Y = \|\lambda.Af\|_Y = |\lambda| \cdot \|Af\|_Y \leqslant |\lambda| \sup\{\|Af\|_Y : f \in S^1\}\ ,\end{aligned}$$

it follows from (i) that $L(X, Y)$ is a subspace of Y^X, where the latter is equipped with the usual operations of pointwise addition and pointwise scalar multiplication by elements of $\mathbb{K}$. Further, if $A \in L(X, Y)$ is such that $\|A\|_{\text{Op}} = 0$, then

$$\|Af\|_Y = \|f\|_X \|A\|f\|_X^{-1}.f\|_Y \leqslant \|f\|_X \cdot 0 = 0$$

for every $f \in X \setminus \{0\}$. The latter implies that $Af = 0_Y$ for every $f \in X$. If $A = 0_{L(X,Y)}$, then $\|A\|_{\text{Op}} = 0$. If $A \in L(X, Y)$ and $\lambda \in \mathbb{K}$, then

$$\|(\lambda.A)f\|_Y = |\lambda|\|Af\|_Y \leqslant |\lambda|\|A\|_{\text{Op}}$$

for every $f \in S^1$ and hence

$$\|\lambda A\|_{\text{Op}} \leqslant |\lambda|\|A\|_{\text{Op}}\ .$$

Also, if $\lambda \neq 0$, then

$$\|Af\|_Y = \frac{1}{|\lambda|}\|(\lambda A)f\|_Y \leqslant \frac{1}{|\lambda|}\|\lambda A\|_{\text{Op}}$$

for every $f \in S^1$ and hence

$$\|A\|_{\text{Op}} \leqslant \frac{1}{|\lambda|}\|\lambda A\|_{\text{Op}}\ .$$

As a consequence,

$$\|\lambda A\|_{\text{Op}} = |\lambda|\|A\|_{\text{Op}}\ .$$

If $A, B \in L(X, Y)$, then

$$\|(A+B)f\|_Y = \|Af + Bf\|_Y \leqslant \|Af\|_Y + \|Bf\|_Y \leqslant \|A\|_{\text{Op}} + \|B\|_{\text{Op}}$$

for every $f \in S^1$. The latter implies that

$$\|A+B\|_{\text{Op}} \leqslant \|A\|_{\text{Op}} + \|B\|_{\text{Op}}\ .$$

Hence it follows that $(L(X,Y), \| \,\|_{\mathrm{Op}})$ is a normed vector space over $\mathbb{K}$. If Y is complete, we conclude the completeness of $(L(X,Y), \| \,\|_{\mathrm{Op}})$ as follows. For this, let $A_1, A_2, \dots$ be Cauchy-sequence in $(L(X,Y), \| \,\|_{\mathrm{Op}})$. Since for $f \in X$ and $k, l \in \mathbb{N}^*$

$$\|A_k f - A_l f\|_Y = \|(A_k - A_l)f\|_Y \leqslant \|A_k - A_l\|_{\mathrm{Op}} \cdot \|f\|_X$$

it follows for every $f \in X$ that $A_1 f, A_2 f, \dots$ is a Cauchy-sequence and hence convergent. Hence we can define a map $A : X \to Y$ by

$$Af = \lim_{k\to\infty} A_k f \ .$$

Obviously, A is linear. Further, since

$$|\|A_k\|_{\mathrm{Op}} - \|A_l\|_{\mathrm{Op}}| \leqslant \|A_k - A_l\|_{\mathrm{Op}}$$

for all $k, l \in \mathbb{N}^*$, $\|A_1\|_{\mathrm{Op}}, \|A_2\|_{\mathrm{Op}}, \dots$ is a Cauchy-sequence in $\mathbb{R}$. Hence the latter sequence is also convergent. Therefore, we conclude that

$$\|Af\|_Y = \|\lim_{k\to\infty} A_k f\|_Y = \lim_{k\to\infty} \|A_k f\|_Y \leqslant \lim_{k\to\infty} \|A_k\|_{\mathrm{Op}}$$

for every $f \in S^1$ and hence that $A \in L(X,Y)$. In the following, let $\varepsilon > 0$ and $N \in \mathbb{N}^*$ such that

$$\|A_k - A_l\|_{\mathrm{Op}} < \frac{\varepsilon}{2}$$

for all $k, l \in \mathbb{N}^*$ such that $k, l \geqslant N$. In addition, let $g \in S^1$ and $k_0 \in \mathbb{N}^*$ such that $k_0 \geqslant N$ and

$$\|(A_k - A)g\|_Y < \frac{\varepsilon}{2}$$

for $k \in \mathbb{N}^*$ such that $k \geqslant k_0$. Then it follows for $k \in \mathbb{N}^*$ such that $k \geqslant N$ that

$$\begin{aligned}\|(A_k - A)g\|_Y &= \|(A_k - A_{k_0} + A_{k_0} - A)g\|_Y \\ &\leqslant \|(A_k - A_{k_0})g\|_Y + \|(A_{k_0} - A)g\|_Y < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon\end{aligned}$$

and hence, since $g \in S^1$ is otherwise arbitrary, that

$$\|A_k - A\|_{\mathrm{Op}} < \varepsilon \ .$$

As a consequence, $A_1, A_2, \dots$ converges in $(L(X,Y), \| \,\|_{\mathrm{Op}})$ to A. □

Corollary 12.2.3. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \| \,\|_X)$, $(Y, \| \,\|_Y)$ be non-trivial normed vector spaces over $\mathbb{K}$, $(Z, \| \,\|_Z)$ a normed vector space over $\mathbb{K}$ and $A \in L(X,Y)$, $B \in L(Y,Z)$.

(i) Then

$$\|Af\|_Y \leqslant \|A\|_{\mathrm{Op}} \|f\|_X$$

for every $f \in X$, and

(ii)
$$\|B \circ A\|_{\text{Op}} \leqslant \|B\|_{\text{Op}}\|A\|_{\text{Op}} \ .$$

Proof. "Part (i)': First we note that, as a consequence of the linearity of A, $A\,0 = 0_Y$ and hence that

$$0 = \|0_Y\|_Y = \|A0\|_Y \leqslant 0 = \|A\|_{\text{Op}}\,\|0\|_X \ .$$

Further, for $f \in X \setminus \{0\}$, it follows that $\|f\|_X^{-1} f \in S^1$ and hence that

$$\|Af\|_Y = \| \|f\|_X A\|f\|_X^{-1} f\|_Y = \|f\|_X \|A\|f\|_X^{-1} f\|_Y \leqslant \|A\|_{\text{Op}}\|f\|_X \ .$$

"Part (ii)": From (i), it follows for $f \in X$ with $\|f\|_X = 1$ that

$$\|(B \circ A)(f)\|_Z = \|B(A(f))\|_Z \leqslant \|B\|_{\text{Op}}\|A(f)\|_Y \leqslant \|B\|_{\text{Op}}\|A\|_{\text{Op}}$$

and hence that
$$\|B \circ A\|_{\text{Op}} \leqslant \|B\|_{\text{Op}}\|A\|_{\text{Op}} \ .$$

□

Remark 12.2.4. In the following, we will call a *vector space together with an additional bilinear mapping* $\cdot$, usually called "multiplication," an *algebra*. Further, if $\cdot$ is associative, the algebra is called associative, if the algebra contains a multiplicative unit element, the algebra is called with unit element, if the underlying vector space is normed (with norm $|\ |$) and the multiplication satisfies

$$|a \cdot b| \leqslant |a| \cdot |b| \ ,$$

for all elements a, b of the algebra, the algebra is called a *normed algebra*. A complete normed algebra is called a *Banach algebra*. We note that, as a consequence, $(L(X,X), +, . , \circ, \|\ \|_{\text{Op}})$ *is an associative Banach algebra with unit element*.

Theorem 12.2.5. (Small Perturbations of the Unit in Associative Banach Algebras with Unit) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, +, . , \cdot, \|\ \|)$ a non-trivial (i.e., $1 \neq 0$,) associative Banach algebra over $\mathbb{K}$ with unit element 1 and $a \in X$ such that $\|a\| < 1$. Then $1 - a$ is invertible with inverse given by

$$(1-a)^{-1} = \sum_{k=0}^{\infty} a^k \ ,$$

where $a^0 := 1$, $a^{k+1} := a \cdot a^k$ for every $k \in \mathbb{N}$. In addition,

$$\left\|(1-a)^{-1} - 1\right\| \leqslant \frac{\|a\|}{1 - \|a\|} \ .$$

Proof. First, we conclude by induction the auxiliary result that for $k \in \mathbb{N}$

$$a^{k+1} = a^k \cdot a \ . \tag{12.1}$$

Indeed, for $k = 0$

$$a^1 = a \cdot a^0 = a \cdot 1 = a = 1 \cdot a = a^0 \cdot a \ .$$

Also, if (12.1) is valid for $k \in \mathbb{N}$, it follows that

$$a^{k+2} = a \cdot a^{k+1} = a \cdot a^k \cdot a = a^{k+1} \cdot a$$

and hence the validity of (12.1) with k replaced $k+1$. Further, for $k \in \mathbb{N}$, we conclude that

$$\|a^{k+1}\| = \|a \cdot a^k\| \leqslant \|a\| \cdot \|a^k\|$$

and hence by induction that

$$\|a^k\| \leqslant \|a\|^k$$

for every $k \in \mathbb{N}^*$. Since $\|a\| < 1$, the latter implies that

$$\lim_{k \to \infty} a^k = 0$$

and that $(a^k)_{k \in \mathbb{N}} \in X^{\mathbb{N}}$ is absolutely summable. Note that here we use the fact that X is complete. Further,

$$\begin{aligned}
&(1-a) \cdot \sum_{k=0}^{n} a^k = \sum_{k=0}^{n} a^k - \sum_{k=0}^{n} a^{k+1} = 1 - a^{n+1} \ , \\
&\left(\sum_{k=0}^{n} a^k \right) \cdot (1-a) = \sum_{k=0}^{n} a^k \cdot (1-a) = \sum_{k=0}^{n} (a^k - a^{k+1}) \\
&= \sum_{k=0}^{n} a^k - \sum_{k=0}^{n} a^{k+1} = 1 - a^{n+1}
\end{aligned}$$

for $n \in \mathbb{N}$. Hence, we conclude that

$$(1-a) \cdot \sum_{k=0}^{\infty} a^k = \left(\sum_{k=0}^{\infty} a^k \right) \cdot (1-a) = 1 \ .$$

Finally, it follows that

$$\begin{aligned}
\big\|(1-a)^{-1} - 1\big\| &= \left\| \sum_{k=1}^{\infty} a^k \right\| \leqslant \sum_{k=1}^{\infty} \|a^k\| \leqslant \sum_{k=1}^{\infty} \|a\|^k \\
&= \|a\| \cdot \sum_{k=0}^{\infty} \|a\|^k = \frac{\|a\|}{1 - \|a\|} \ .
\end{aligned}$$

$\square$

Theorem 12.2.6. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, +, \,.\,, \cdot, \| \ \|)$ a non-trivial (i.e., $1 \neq 0$,) associative Banach algebra over $\mathbb{K}$ with unit element 1. The set of invertible elements U is open in X, and the map

$$\text{Inv} : U \to X \ ,$$

for every $a \in U$, defined by

$$\text{Inv}(a) := a^{-1} \ ,$$

is continuous.

Proof. We note that $U \neq \emptyset$, since $1 \in U$, and that $\|1\| \neq 0$, since according to the assumptions, $1 \neq 0$. Also, if $a \in U$, then

$$\|1\| = \|a \cdot a^{-1}\| \leqslant \|a\| \cdot \|a^{-1}\| \ .$$

Hence $\|a\|$ and $\|a^{-1}\|$ are both non-vanishing. Further, if $b \in U_{1/\|a^{-1}\|}(a)$, then

$$b = a - (a - b) = a \cdot [1 - a^{-1} \cdot (a - b)]$$

and

$$\|a^{-1} \cdot (a - b)\| \leqslant \|a^{-1}\| \cdot \|b - a\| < \|a^{-1}\| \cdot \frac{1}{\|a^{-1}\|} = 1 \ .$$

Hence according to Theorem 12.2.5, $1 - a^{-1} \cdot (a - b)$ and therefore also b are invertible. Also, if $b_1, b_2, \dots$ is a sequence in U that is convergent to a and $\nu_0 \in \mathbb{N}^*$ is such that $b_\nu \in U_{1/\|a^{-1}\|}(a)$, for every $\nu \in \mathbb{N}^*$ satisfying $\nu \geqslant \nu_0$, then it follows with the help of Theorem 12.2.5 for such ν that

$$\begin{aligned}
&\|b_\nu^{-1} - a^{-1}\| = \|[1 - a^{-1} \cdot (a - b_\nu)]^{-1} \cdot a^{-1} - a^{-1}\| \\
&\leqslant \|a^{-1}\| \cdot \|[1 - a^{-1} \cdot (a - b_\nu)]^{-1} - 1\| \\
&\leqslant \|a^{-1}\| \cdot \frac{\|a^{-1} \cdot (a - b_\nu)\|}{1 - \|a^{-1} \cdot (a - b_\nu)\|} \leqslant \frac{\|a^{-1}\|^2 \cdot \|b_\nu - a\|}{1 - \|a^{-1}\| \cdot \|b_\nu - a\|}
\end{aligned}$$

and hence that

$$\lim_{\nu \to \infty} b_\nu^{-1} = a^{-1} \ .$$

□

12.2.2 Unbounded Operators

Lemma 12.2.7. (**Direct sums of Banach and Hilbert spaces**)

(i) Let $(X, \| \ \|_{\mathrm{X}})$ and $(Y, \| \ \|_{\mathrm{Y}})$ be Banach spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $\| \ \|_{\mathrm{X} \times \mathrm{Y}} : X \times Y \to \mathbb{R}$ be defined by

$$\|(f, g)\|_{\mathrm{X} \times \mathrm{Y}} := \sqrt{\|f\|_{\mathrm{X}}^2 + \|g\|_{\mathrm{Y}}^2}$$

for all $(f, g) \in \mathrm{X} \times \mathrm{Y}$. Then $(X \times Y, \| \ \|_{\mathrm{X} \times \mathrm{Y}})$ is a Banach space.

(ii) Let $(X, \langle\,|\,\rangle_{\mathrm{X}})$ and $(Y, \langle\,|\,\rangle_{\mathrm{Y}})$ be Hilbert spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $\langle\,|\,\rangle_{\mathrm{X}\times\mathrm{Y}} : (X \times Y)^2 \to \mathbb{K}$ be defined by

$$\langle (f,g)|(h,k)\rangle_{\mathrm{X}\times\mathrm{Y}} := \langle f|h\rangle_{\mathrm{X}} + \langle g|k\rangle_{\mathrm{Y}}$$

for all $(f,g),(h,k) \in \mathrm{X} \times \mathrm{Y}$. Then $(X \times Y, \langle\,|\,\rangle_{\mathrm{X}\times\mathrm{Y}})$ is a Hilbert space.

Proof. '(i)': Obviously, $\|\,\|_{\mathrm{X}\times\mathrm{Y}}$ is positive definite and homogeneous. Further, it follows for $(f,g),(h,k) \in X \times Y$ by the Cauchy-Schwarz inequality for the Euclidean scalar product for $\mathbb{R}^2$ that

$$\begin{aligned}
&\|(f,g)+(h,k)\|^2_{\mathrm{X}\times\mathrm{Y}} = \|f+h\|^2_{\mathrm{X}} + \|g+k\|^2_{\mathrm{Y}} \\
&\leqslant (\,\|f\|_{\mathrm{X}} + \|h\|_{\mathrm{X}})^2 + (\,\|g\|_{\mathrm{Y}} + \|k\|_{\mathrm{Y}})^2 = (a+a')^2 + (b+b')^2 \\
&= a^2 + b^2 + a'^2 + b'^2 + 2\,(a\,a' + b\,b') \\
&\leqslant a^2 + b^2 + a'^2 + b'^2 + 2\,\sqrt{a^2+b^2}\cdot\sqrt{a'^2+b'^2} \\
&= \left(\sqrt{a^2+b^2} + \sqrt{a'^2+b'^2}\right)^2 = (\,\|(f,g)\|_{\mathrm{X}\times\mathrm{Y}} + \|(h,k)\|_{\mathrm{X}\times\mathrm{Y}})^2 \ ,
\end{aligned}$$

where $a := \|f\|_{\mathrm{X}}, a' := \|h\|_{\mathrm{X}}, b := \|g\|_{\mathrm{Y}}, b' := \|k\|_{\mathrm{Y}}$, and hence that

$$\|(f,g)+(h,k)\|_{\mathrm{X}\times\mathrm{Y}} \leqslant \|(f,g)\|_{\mathrm{X}\times\mathrm{Y}} + \|(h,k)\|_{\mathrm{X}\times\mathrm{Y}} \ .$$

The completeness of $(X \times Y, \|\,\|_{\mathrm{X}\times\mathrm{Y}})$ is an obvious consequence of the completeness of X and Y.
'(ii)': Obviously, $\langle\,|\,\rangle_{\mathrm{X}\times\mathrm{Y}}$ is a positive definite symmetric bilinear, positive definite symmetric sesquilinear form, respectively. Further, the induced norm on $X \times Y$ coincides with the norm defined in (i). □

Definition 12.2.8. (Linear Operators) Let $(X, \|\,\|_{\mathrm{X}})$ and $(Y, \|\,\|_{\mathrm{Y}})$ be Banach spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. Then we define

(i) A map A is called a *Y-valued linear operator in* X if its *domain* $D(A)$ is a subspace of X, Ran $A \subset Y$ and A is linear. If $(Y, \|\,\|_{\mathrm{Y}}) = (X, \|\,\|_{\mathrm{X}})$ such a map is also called a *linear operator in* X.

(ii) If in addition A is a Y-valued linear operator in X:

a) The *graph* $G(A)$ of A by

$$G(A) := \{(f, Af) \in X \times Y : f \in D(A)\} \ .$$

Note that $G(A)$ is a subspace of $X \times Y$.

b) A is *densely-defined* if $D(A)$ is in particular dense in X.

c) A is *closed* if $G(A)$ is a closed subspace of $(X \times Y, \|\,\|_{\mathrm{X}\times\mathrm{Y}})$.

d) A Y-valued linear operator B in X is said to be an *extension* of A, symbolically denoted by

$$A \subset B \quad \text{or} \quad B \supset A \ ,$$

if $G(A) \subset G(B)$.

e) A is *closable* if there is a closed extension. In this case,

$$\bigcap_{B \supset A, B \text{ closed}} G(B)$$

is a closed subspace of $X \times Y$ which, obviously, is the graph of a unique Y-valued closed linear extension $\bar{A}$ of A, called the *closure* of A. By definition, every closed extension B of A satisfies $B \supset \bar{A}$.

f) If A is closed, a *core* of A is a subspace D of its domain such that the closure of $A|_D$ coincides with A, i.e., if

$$\overline{A|_D} = A \ .$$

Theorem 12.2.9. (Elementary properties of linear operators) Let $(X, \| \ \|_{\text{X}})$, $(Y, \| \ \|_{\text{Y}})$ be Banach spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, A a *Y-valued linear operator in* X and $B \in L(X, Y)$.

(i) $(D(A), \| \ \|_{\text{A}})$, where $\| \ \|_{\text{A}} : D(A) \to \mathbb{R}$ is defined by

$$\|f\|_{\text{A}} := \|(f, Af)\|_{\text{X}\times\text{Y}} = \sqrt{\|f\|_{\text{X}}^2 + \|Af\|_{\text{Y}}^2}$$

for every $f \in D(A)$, is a normed vector space. Further, the inclusion $\iota_{\text{A}} : (D(A), \| \ \|_{\text{A}}) \hookrightarrow X$ is continuous and $A \in L((D(A), \| \ \|_{\text{A}}), Y)$.

(ii) A is closed if and only if $(D(A), \| \ \|_{\text{A}})$ is complete.

(iii) If A is closable, then $G(\bar{A}) = \overline{G(A)}$.

(iv) (*Bounded inverse theorem*) If A is closed and bijective, then $A^{-1} \in L(Y, X)$.

(v) (*Closed graph theorem*) In addition, let $D(A) = X$. Then A is bounded if and only if A is closed.

(vi) If A is closable, then $A + B$ is also closable and

$$\overline{A + B} = \bar{A} + B \ .$$

Proof. '(i)': Obviously, $(D(A), \| \ \|_{\text{A}})$ is a normed vector space. Further, because of

$$\|\iota_{\text{A}} f\|_{\text{X}} = \|f\|_{\text{X}} \leqslant \sqrt{\|f\|_{\text{X}}^2 + \|Af\|_{\text{Y}}^2} = \|f\|_{\text{A}}$$

and

$$\|Af\|_{\mathrm{Y}} \leqslant \sqrt{\|f\|_{\mathrm{X}}^2 + \|Af\|_{\mathrm{Y}}^2} = \|f\|_{\mathrm{A}}$$

for every $f \in D(A)$, it follows that $\iota_{\mathrm{A}} \in L((D(A), \| \,\|_{\mathrm{A}}), X)$ and $A \in L((D(A), \| \,\|_{\mathrm{A}}), Y)$.

'(ii)': Let A be closed and $f_0, f_1, \dots$ a Cauchy sequence in $(D(A), \| \,\|_{\mathrm{A}})$. Then $(f_0, Af_0), (f_1, Af_1), \dots$ is a Cauchy sequence in $G(A)$ and hence by Lemma 12.2.7 along with the closedness of $G(A)$ convergent to some $(f, Af) \in G(A)$. This implies that

$$\lim_{\nu\to\infty} \|f_\nu - f\|_{\mathrm{A}} = 0 \ .$$

Let $(D(A), \| \,\|_{\mathrm{A}})$ be complete and $(f, g) \in \overline{G(A)}$. Then there is a sequence $(f_0, Af_0), (f_1, Af_1), \dots$ in $G(A)$ which is convergent to (f, g). Hence $(f_0, Af_0), (f_1, Af_1), \dots$ is a Cauchy sequence in $X \times Y$. As a consequence, $f_0, f_1, \dots$ is a Cauchy sequence in $(D(A), \| \,\|_{\mathrm{A}})$ and therefore convergent to some $h \in D(A)$. In particular,

$$\lim_{\nu\to\infty} \|(f_\nu, Af_\nu) - (h, Ah)\|_{\mathrm{X}\times\mathrm{Y}} = 0$$

and hence $(f, g) = (h, Ah) \in G(A)$.

'(iii)': Let A be closable. Then the closed graph of every closed extension of A contains $G(A)$ and hence also $\overline{G(A)}$. Therefore $G(\bar{A}) \supset \overline{G(A)}$. This implies in particular that $\overline{G(A)}$ is the graph of a map $\tilde{A}$. Further, $D(\tilde{A}) = \mathrm{pr}_1 \overline{G(A)}$, where $\mathrm{pr}_1 := (X \times Y \to X, (f, g) \mapsto f)$, is a subspace of X and $\tilde{A}$ is in particular a linear closed extension of A. Hence $\tilde{A} \supset \bar{A}$ and $\overline{G(A)} = G(\tilde{A}) \supset G(\bar{A})$.

'(iv)': Let A be closed and bijective. Then it follows by (ii) that $(D(A), \| \,\|_{\mathrm{A}})$ is a Banach space and that $A \in L((D(A), \| \,\|_{\mathrm{A}}), Y)$. Hence it follows by the 'bounded inverse theorem theorem', for e.g. see Theorem III.11 in Vol. I of [34], that $A^{-1} \in L(Y, (D(A), \| \,\|_{\mathrm{A}}))$ and by the continuity of ι_{A} that $A^{-1} \in L(Y, X)$.

'(v)': Let $D(A) = X$. If A is bounded and $f_0, f_1, \dots$ is some Cauchy sequence in $(X, \| \,\|_{\mathrm{A}})$, it follows by the continuity of ι_{A} that $f_0, f_1, \dots$ is a Cauchy sequence in X and hence convergent to some $f \in X$. Since A is continuous, it follows the convergence of $Af_0, Af_1, \dots$ to Af and therefore also the convergence of $f_0, f_1, \dots$ in $(X, \| \,\|_{\mathrm{A}})$ to f. Hence $(X, \| \,\|_{\mathrm{A}})$ is complete and A is closed by (ii). If A is closed, it follows by (ii) that $(X, \| \,\|_{\mathrm{A}})$ is a Banach space and that the bijective X-valued linear operator ι_{A} is continuous. Hence ι_{A} is closed by the previous part of the proof. Therefore, the inverse of ι_{A} is continuous by (iv) and hence A is bounded.

'(vi)': Let A be closable. In a first step, we prove that $\bar{A} + B$ is closed. For this, let $(f, g) \in \overline{G(\bar{A} + B)}$. Then there is a sequence $f_0, f_1, \dots$ in $D(\bar{A})$ which is convergent to f and such that $(\bar{A} + B)f_0, (\bar{A} + B)f_1, \dots$ is convergent to g. Since B is continuous, it follows that $\bar{A}f_0, \bar{A}f_1, \dots$ is convergent to $g - Bf$. Since $\bar{A}$ is closed, it follows that $f \in D(\bar{A})$ as well as $\bar{A}f = g - Bf$ and hence that $f \in D(\bar{A} + B)$ as well as $(\bar{A} + B)f = g$. Hence $\bar{A} + B$ is closed, and therefore $A + B$ is closable such that $\bar{A} + B \supset \overline{A + B}$. Further, it follows by the previous part of the proof that $\overline{A+B}-B$ is a closed extension of A. Hence $\overline{A+B}-B \supset \bar{A}$ and therefore also $\overline{A+B} \supset \bar{A}+B$. Finally, it follows that $\overline{A+B} = \bar{A}+B$. $\square$

Theorem 12.2.10. (**An application of the closed graph theorem**) Let $(X, \| \,\|_{\mathrm{X}})$, $(Y, \| \,\|_{\mathrm{Y}})$, $(Z, \| \,\|_{\mathrm{Z}})$ be Banach spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, A a closed bijective Y-valued linear operator in X and B a *closable* Z-valued linear operator in X such that $D(B) \supset D(A)$. Then there is $C \in [0, \infty)$ such that

$$\|B\xi\|_{\mathrm{Z}} \leqslant C \, \|A\xi\|_{\mathrm{Y}}$$

for all $\xi \in D(A)$ and hence in particular $B|_{D(A)} \in L((D(A), \| \,\|_{\mathrm{A}}), Z)$.

Proof. First, it follows by Theorem 12.2.9 (iv) that $A^{-1} \in L(Y, X)$. Further, $B \circ A^{-1}$ is a Z-valued linear operator on Y since A^{-1} maps into the domain of B. Let $(\eta, \zeta) \in G(\overline{B \circ A^{-1}})$. Then there is a sequence $(\eta_0, B(A^{-1}\eta_0)), (\eta_1, B(A^{-1}\eta_1)), \dots$ in $G(B \circ A^{-1})$ converging to (η, ζ). In particular,

$$\lim_{\nu \to \infty} \eta_\nu = \eta$$

and therefore also

$$\lim_{\nu \to \infty} A^{-1}\eta_\nu = A^{-1}\eta \ .$$

Since B is closable, it follows that $(A^{-1}\eta, \zeta) \in G(\bar{B})$ and hence because of $A^{-1}\eta \in D(A) \subset D(B)$ that $(A^{-1}\eta, \zeta) \in G(B)$. Therefore also $BA^{-1}\eta = \zeta$ and $(\eta, \zeta) \in G(B \circ A^{-1})$. Hence $B \circ A^{-1}$ is in addition closed and therefore by Theorem 12.2.9 (v) bounded. As a consequence, it follows

$$\|B\xi\|_{\mathrm{Z}} = \|B \circ A^{-1}A\xi\|_{\mathrm{Z}} \leqslant C \, \|A\xi\|_{\mathrm{Y}}$$

for every $\xi \in D(A)$ where $C \in [0, \infty)$ is some bound for $B \circ A^{-1}$. $\square$

Example 12.2.11. Apart from the unitary Fourier transform F_2, the text uses a related linear Fourier transformation which is denoted by F_1,

$$\mathrm{F}_1 : \mathrm{L}^1_{\mathbb{C}}(\mathbb{R}^n) \to \mathrm{C}_\infty(\mathbb{R}^n, \mathbb{C}) \ ,$$

which for every $f \in \mathrm{L}^1_{\mathbb{C}}(\mathbb{R}^n)$, is defined by

$$(\mathrm{F}_1 f)(k) := \int_{-\infty}^{\infty} e^{-ik \cdot u} f(u) \, du$$

for every $k \in \mathbb{R}^n$. Here, $\mathrm{C}_\infty(\mathbb{R}^n, \mathbb{C})$ denotes the vector space of continuous complex-valued functions on the real numbers that vanish at $\pm\infty$, which, equipped with the norm $\| \,\|_\infty$, defined by

$$\|f\|_\infty := \sup_{k \in \mathbb{R}^n} |f(k)| \ ,$$

for every $f \in C_\infty(\mathbb{R}^n, \mathbb{C})$, is a complex Banach space. In particular,

$$\|F_1 f\|_\infty \leqslant \|f\|_\infty \ ,$$

for every $f \in C_\infty(\mathbb{R}^n, \mathbb{C})$, implying that F_1 is continuous.

12.2.3 Spectra and Resolvents

Theorem 12.2.12. (Elementary properties of the resolvent) Let $(X, \| \,\|_X)$ be a non-trivial Banach space over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and A a densely-defined closed linear operator in X.

(i) We define the *resolvent set* $\rho(A) \subset \mathbb{K}$ of A by

$$\rho(A) := \{\lambda \in \mathbb{K} : A - \lambda \text{ is bijective}\} \ .$$

Then $\rho(A)$ is an *open* subset of $\mathbb{K}$. Therefore, its complement $\sigma(A) := \mathbb{K} \setminus \rho(A)$, which is called the *spectrum* of A, is a *closed* subset of $\mathbb{K}$.

(ii) We define the *resolvent* $R_A : \rho(A) \to L(X, X)$ of A by

$$R_A(\lambda) := (A - \lambda)^{-1}$$

for every $\lambda \in \rho(A)$. Then R_A is continuous, satisfies the *first resolvent formula*

$$R_A(\mu) - R_A(\lambda) = (\mu - \lambda)\, R_A(\mu) R_A(\lambda) \tag{12.2}$$

for every $\lambda, \mu \in \rho(A)$ and the *second resolvent formula*

$$R_A(\lambda) - R_B(\lambda) = R_A(\lambda)(B - A) R_B(\lambda) \tag{12.3}$$

for every $\lambda \in \rho(A) \cap \rho(B)$, where B is some closed linear operator in X having the *same domain* as A, i.e., $D(B) = D(A)$.

(iii) For every $f \in X, \omega \in L(X, \mathbb{K})$, the corresponding function

$$\omega \circ R_A f$$

is *real-analytic/holomorphic*. Here $R_A f : \rho(A) \to X$ is defined by $(R_A f)(\lambda) := R_A(\lambda) f$.

Proof. Let $\lambda_0 \in \rho(A)$. Then $A - \lambda_0$ is a closed densely-defined bijective linear operator in X and hence $R_A(\lambda_0) \in L(X, X) \setminus \{0\}$. Then it follows for every $\lambda \in U_{1/\|R_A(\lambda_0)\|}(\lambda_0)$

$$A - \lambda = \left[1 - (\lambda - \lambda_0).R_A(\lambda_0)\right](A - \lambda_0)$$

and therefore, since

$$1 - (\lambda - \lambda_0).R_A(\lambda_0)$$

is bijective as a consequence of

$$\|(\lambda - \lambda_0).R_A(\lambda_0)\| < 1 \ ,$$

that $A - \lambda$ is bijective, as a composition of bijective maps, hence $\lambda \in \rho(A)$ and

$$R_A(\lambda) = \sum_{k=0}^{\infty} (\lambda - \lambda_0)^k \, [R_A(\lambda_0)]^{k+1} \ .$$

Further, it follows for every $f \in X, \omega \in L(X, \mathbb{K})$ that

$$(\omega \circ R_A f)(\lambda) = \sum_{k=0}^{\infty} \omega \left([R_A(\lambda_0)]^{k+1} f \right) (\lambda - \lambda_0)^k \ .$$

In addition, if $\lambda \in U_{1/(2\|R_A(\lambda_0)\|)}(\lambda_0)$, then

$$\|R_A(\lambda)\| \leqslant \sum_{k=0}^{\infty} |\lambda - \lambda_0|^k \, \|R_A(\lambda_0)\|^{k+1} \leqslant \sum_{k=0}^{\infty} (2\|R_A(\lambda_0)\|)^{-k} \, \|R_A(\lambda_0)\|^{k+1}$$
$$= \|R_A(\lambda_0)\| \sum_{k=0}^{\infty} 2^{-k} = 2 \, \|R_A(\lambda_0)\| \ ,$$

i.e., $\|R_A\|$ is bounded in a neighborhood of λ_0. Further, for $\lambda, \mu \in \rho(A)$ and every $f \in D(A)$, it follows that

$$(A - \mu)f = (A - \lambda)f + (\lambda - \mu)f$$

and hence for every $g \in X$

$$(A - \mu)R_A(\lambda)g = g + (\lambda - \mu)R_A(\lambda)g \ .$$

The latter implies that

$$R_A(\lambda) = R_A(\mu) + (\lambda - \mu)R_A(\mu)R_A(\lambda)$$

and hence (12.2). We note that this implies the continuity of R_A, since $\|R_A\|$ is bounded in a neighborhood of every $\lambda \in \rho(A)$. Finally, let $B : D(A) \to X$ be some closed linear operator in X. Then it follows for every $\mu \in \rho(A)$, $\lambda \in \rho(B)$ and every $f \in D(A)$ that

$$(A - \mu)f = (A - B)f + (B - \lambda)f + (\lambda - \mu)f$$

and hence for every $g \in X$ that

$$(A - \mu)R_B(\lambda)g = (A - B)R_B(\lambda)g + g + (\lambda - \mu)R_B(\lambda)g \ .$$

The latter implies that

$$R_B(\lambda) = R_A(\mu)(A - B)R_B(\lambda) + R_A(\mu) + (\lambda - \mu)R_A(\mu)R_B(\lambda)$$

and hence (12.3). □

12.3 Hilbert Spaces

12.3.1 Elementary Properties

Definition 12.3.1. (**$\mathbb{K}$-Sesquilinear forms**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and X a vector space over $\mathbb{K}$.

(i) s is called a $\mathbb{K}$-Sesquilinear form on X if s is a map from $X \times X$ to $\mathbb{K}$ such that $s(f, \cdot)$ is linear for every $f \in X$ and $s(\cdot, g)$ is linear and anti-linear[1] for every $g \in X$ if $\mathbb{K} = \mathbb{R}$ and $\mathbb{K} = \mathbb{C}$, respectively.

(ii) If s is a $\mathbb{K}$-Sesquilinear form on X, we call the function $(X \to \mathbb{K}, f \mapsto s(f, f))$ the quadratic form that is generated by s.

(iii) A $\mathbb{K}$-Sesquilinear form s on X is called symmetric if $s(f, g) = s(g, f)$ and $s(g, f) = (s(f, g))^*$ for all $f, g \in X$ if $\mathbb{K} = \mathbb{R}$ and $\mathbb{K} = \mathbb{C}$, respectively, where $*$ denotes complex conjugation on $\mathbb{C}$.

(iv) s is called a semi-scalar product and scalar product on X if s is a symmetric $\mathbb{K}$-Sesquilinear form on X such that $s(f, f) \geqslant 0$ for every $f \in X$[2] and $s(f, f) > 0$ for every $f \in X \setminus \{0\}$[3], respectively.

Remark 12.3.2. Note that Definition 12.3.1 (iv) uses that the quadratic forms that are associated with $\mathbb{K}$-sesquilinear forms are real-valued.

Theorem 12.3.3. (**Basic properties of $\mathbb{K}$-Sesquilinear forms**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, X a vector space over $\mathbb{K}$ and s a $\mathbb{K}$-Sesquilinear form on X. Then

(i) (**Parallelogram law**)

$$s(f + g, f + g) + s(f - g, f - g) = 2[s(f, f) + s(g, g)]$$

for all $f, g \in X$.

(ii) (**Polarization identity for $\mathbb{C}$-Sesquilinear forms**) if $\mathbb{K} = \mathbb{C}$,

$$\begin{aligned} s(f, g) = &\frac{1}{4}\,[s(f + g, f + g) - s(f - g, f - g) - is(f + ig, f + ig) \\ &+ is(f - ig, f - ig)] \end{aligned}$$

for all $f, g \in X$.

Proof. "(i)":

$$s(f + g, f + g) + s(f - g, f - g) = s(f, f) + s(g, f) + s(f, g) + s(g, g)$$

[1] I.e., $s(f_1 + f_2, g) = s(f_1, g) + s(f_2, g)$ and $s(\lambda f, g) = \lambda^* s(f, g)$ for all $f_1, F, f \in X$ and $\lambda \in \mathbb{C}$, where $*$ denotes complex conjugation on $\mathbb{C}$.

[2] A symmetric $\mathbb{K}$-Sesquilinear form on X with this property is also called positive semi-definite.

[3] A symmetric $\mathbb{K}$-Sesquilinear form on X with this property is also called positive definite.

$$+ s(f,f) - s(g,f) - s(f,g) + s(g,g) = 2[s(f,f) + s(g,g)]$$

for all $f, g \in X$.
"(ii)": First it follows that

$$s(f+g, f+g) = s(f,f) + s(g,f) + s(f,g) + s(g,g) \ ,$$
$$s(f-g, f-g) = s(f,f) - s(g,f) - s(f,g) + s(g,g)$$

and hence that

$$s(f+g, f+g) - s(f-g, f-g) = 2[s(f,g) + s(g,f)]$$

for all $f, g \in X$. This implies that

$$-i[s(f+ig, f+ig) - s(f-ig, f-ig)] = 2[s(f,g) - s(g,f)]$$

for all $f, g \in X$. By addition of the last two equations and multiplication of the resulting equation by $1/4$, we arrive at the statement. □

Remark 12.3.4. As a consequence of part (ii) of Theorem 12.3.3, a $\mathbb{C}$-Sesquilinear form is uniquely determined by its corresponding quadratic form. That the analogous is not true for $\mathbb{R}$-Sesquilinear forms can be seen from the existence of non-trivial skew-symmetric bilinear forms. The quadratic forms corresponding to the latter vanish.

Theorem 12.3.5. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, X a vector space over $\mathbb{K}$ and $\langle\,|\,\rangle$ a semi-scalar product on X and $\|\ \| : X \to [0, \infty)$ defined by $\|f\| := \langle f|f\rangle^{1/2}$ for every $f \in X$. Then

(i) (**Cauchy-Schwarz inequality**) For all $f, g \in X$, the following *Cauchy-Schwarz inequality* holds

$$|\langle f|g\rangle| \leqslant \|f\|\|g\| \ . \tag{12.4}$$

(ii) (**Triangle inequality**) For all $f, g \in X$

$$\|f + g\| \leqslant \|f\| + \|g\| \ . \tag{12.5}$$

(iii) $N := \{f \in X : \|f\| = 0\}$ is subspace of X, the so called null space of $\langle\,|\,\rangle$.

(iv) (**Cauchy-Schwarz equality**)

$$|\langle f|g\rangle| = \|f\|\|g\| \tag{12.6}$$

for some $f, g \in X$ if and only if

$$\|f\|^2 g - \langle f|g\rangle\, f \in N \ .$$

Proof. "(i)": For arbitrary $f, g \in X$, it follows that

$$\begin{aligned} 0 &\leqslant \langle \|f\|^2 g - \langle f|g\rangle\, f, \|f\|^2 g - \langle f|g\rangle\, f\rangle \\ &= \|f\|^2(\|f\|^2\|g\|^2 + |\,\langle f|g\rangle\,|^2 - |\,\langle f|g\rangle\,|^2 - |\,\langle f|g\rangle\,|^2) \\ &= \|f\|^2(\|f\|^2\|g\|^2 - |\,\langle f|g\rangle\,|^2) \end{aligned} \tag{12.7}$$

and hence also that

$$0 \leqslant \|g\|^2(\|f\|^2\|g\|^2 - |\,\langle f|g\rangle\,|^2)\ .$$

As a consequence, we conclude the validity of (12.4) if $\|f\| \neq 0$ and/or $\|g\| \neq 0$. Further, if $\|f\| = \|g\| = 0$, it follows that

$$\begin{aligned} 0 &\leqslant \langle -af + \frac{1}{2}\, g| - af + \frac{1}{2}\, g\rangle = -\frac{1}{2}\,(\langle af|g\rangle + \langle g|af\rangle) = -\mathrm{Re}(a\,\langle g|f\rangle) \\ &= -|\,\langle f|g\rangle\,|\ , \end{aligned}$$

where $a \in \mathbb{K}$ is such that $|a| = 1$ and

$$a\,\langle g|f\rangle = |\,\langle f|g\rangle\,|\ ,$$

and hence that

$$\langle f|g\rangle = 0\ .$$

As a consequence, we conclude also in this case the validity of (12.4).
"(ii)": With the help of (i), it follows for arbitrary $f, g \in X$ that

$$\begin{aligned} \|f+g\|^2 &= |\,\langle f+g|f+g\rangle\,| = |\,\|f\|^2 + \|g\|^2 + \langle f|g\rangle + \langle g|f\rangle\,| \\ &\leqslant \|f\|^2 + \|g\|^2 + 2\|f\|\|g\| = (\|f\| + \|g\|)^2\ . \end{aligned}$$

and hence (12.5).
"(iii)": First, as a consequence of the linearity of $\langle 0|\cdot\rangle$, $\|0\| = \langle 0|0\rangle^{1/2} = 0$ and hence $0 \in N$. Further, if $f, g \in N$, it follows by (12.5) that $\|f+g\| = 0$ and hence that $f + g \in N$. Finally, for $f \in N$ and $\lambda \in \mathbb{K}$, it follows that

$$\|\lambda f\|^2 = \langle \lambda f|\lambda f\rangle = |\lambda|^2\|f\|^2 = 0$$

and hence that $\lambda f \in N$.
"(iv)": If (12.6) is valid for some $f, g \in X$, it follows from (12.7) that $\|f\|^2 g - \langle f|g\rangle\, f \in N$. If $\|f\|^2 g - \langle f|g\rangle\, f \in N$, it follows from (12.7) that

$$\|f\|^2(\|f\|^2\|g\|^2 - |\,\langle f|g\rangle\,|^2) = 0\ .$$

If $\|f\| = 0$, it follows by (12.4) the validity of (12.6).

□

Theorem 12.3.6. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, X vector space over $\mathbb{K}$, $\langle\,|\,\rangle$ a scalar product on X and $\|\;\| : X \to [0, \infty)$ defined by $\|f\| := \langle f|f\rangle^{1/2}$ for every $f \in X$. Then

(i) $(X, \|\;\|)$ is a normed vector space over $\mathbb{K}$. In the following, we call $\|\;\|$ the norm that is induced on X by $\langle\,|\,\rangle$.

(ii) The maps $\langle f|\cdot\rangle$ and $\langle\cdot|f\rangle$, interpreted as maps from $(X, \|\;\|)$ to $(\mathbb{K}, |\;|)$, are continuous for every $f \in X$. In particular, if X is non-trivial, $\|\,\langle f|\cdot\rangle\,\| = \|f\|$ for every $f \in X$.

Proof. "(i)": First, $\|0\| = \langle 0|0\rangle^{1/2} = 0$, as a consequence of the linearity of $\langle 0|\cdot\rangle$. Also, since $\|f\| = \langle f|f\rangle^{1/2} > 0$ for every $f \in X \setminus \{0\}$, from $\|f\| = 0$ for some $f \in X$, it follows that $f = 0$. Second, $\|\lambda f\| = \langle \lambda f|\lambda f\rangle^{1/2} = (|\lambda|^2 \langle f|f\rangle)^{1/2} = |\lambda|\,\langle f|f\rangle^{1/2} = |\lambda|\,\|f\|$ for every $f \in X$ and $\lambda \in \mathbb{K}$. Finally, according to Theorem 12.3.5 (ii), $\|f + g\| \leqslant \|f\| + \|g\|$ for all $f, g \in X$. Hence $(X, \|\;\|)$ is a normed vector space over $\mathbb{K}$.
"(ii)": Let $f \in X$. Then, we conclude by help of the Cauchy-Schwarz inequality, Theorem 12.3.5 (i), that

$$|\,\langle f|g_1\rangle - \langle f|g_2\rangle\,| = |\,\langle f|g_1 - g_2\rangle\,| \leqslant \|f\|\|g_1 - g_2\|$$
$$|\,\langle g_1|f\rangle - \langle g_2|f\rangle\,| = |\,\langle g_1 - g_2|f\rangle\,| \leqslant \|f\|\|g_1 - g_2\|$$

for all $g_1, g_2 \in X$. The latter implies the continuity of $\langle f|\cdot\rangle$ and $\langle\cdot|f\rangle$. Further, if X is non-trivial, the latter implies that $\|\,\langle f|\cdot\rangle\,\|_{Op} \leqslant \|f\|$. In this case , it also follows that $|\,\langle f|\cdot\rangle\,(\|f\|^{-1}f)| = |\,\langle f|\|f\|^{-1}f\rangle\,| = \|f\|$ and hence that $\|\,\langle f|\cdot\rangle\,\|_{Op} \geqslant \|f\|$. □

Definition 12.3.7. (**Pre-Hilbert spaces and Hilbert spaces**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. A pair $(X, \langle\,|\,\rangle)$ is called a pre-Hilbert space over $\mathbb{K}$ if X is a vector space over $\mathbb{K}$ and $\langle\,|\,\rangle : X^2 \to \mathbb{K}$ is a scalar product on X. If moreover, $(X, \|\;\|)$ is complete, where $\|\;\|$ is the norm that is induced on X by $\langle\,|\,\rangle$, we call $(X, \langle\,|\,\rangle)$ a Hilbert space.

Example 12.3.8. Let $n \in \mathbb{N}^*$, $\langle\,|\,\rangle : \mathbb{C}^n \times \mathbb{C}^n \to \mathbb{C}$ be the *canonical scalar product*, defined for all $u = (u_1, \ldots, u_n), v = (v_1, \ldots, v_n) \in \mathbb{C}^n$ by

$$\langle u|v\rangle_c := u_1^* \cdot v_1 + \cdots + u_n^* \cdot v_n\ .$$

Then, *according to Linear Algebra and Analysis*,

> $(\mathbb{C}^n, \langle\,|\,\rangle_c)$ is a complex Hilbert space,

Example 12.3.9. (L^2**-Spaces**) Let $n \in \mathbb{N}^*$, $E \subset \mathbb{R}^n$ be non-empty and v^n-measurable, where v^n denotes the Lebesgue measure in n dimensions. We define

$$\mathcal{L}^2_{\mathbb{C}}(E) := \{f : E \to \mathbb{C} : \mathrm{Re}(f), \mathrm{Im}(f) \text{ are } v^n\text{-measurable}$$

and $|\mathrm{Re}(f)|^2, |\mathrm{Im}(f)|^2$ are v^n-integrable$\}$

and for all $f, g \in \mathcal{L}^2_{\mathbb{C}}(E)$

$$\langle f|g\rangle_2 := \int_E f^* \cdot g \, dv^n \ .$$

Then *according to Functional Analysis*

> $\left(L^2_{\mathbb{C}}(E), +, ., \langle\,|\,\rangle_2\right)$ is a complex Hilbert space,

where

$$L^2_{\mathbb{C}}(E) := \mathcal{L}^2_{\mathbb{C}}(E)/_{\sim} \ ,$$

the equivalence relation $\sim$ on $\mathcal{L}^2_{\mathbb{C}}(E)$ is defined by[1]

$$f \sim g :\Leftrightarrow f = g \text{ a.e. on } E \ ,$$

for all $f, g \in \mathcal{L}^2_{\mathbb{C}}(E)$, and $L^2_{\mathbb{C}}(E)$ is *equipped with the operations* $+, .$ *and the scalar product* $\langle\,|\,\rangle_2$*, defined by*

$$\begin{aligned} &[f] + [g] := [f + g] \ , \ \lambda.[f] := [\lambda.f] \ , \\ &\langle [f] | [g] \rangle_2 := \langle f | g \rangle_2 \end{aligned}$$

for all $f, g \in \mathcal{L}^2_{\mathbb{C}}(E)$ and $\lambda \in \mathbb{C}$.

As is standard practice, we are not going to indicate that we are working with equivalence classes, rather than functions. Normally, this does not lead to complications, since in applications, usually, the equivalence classes in question, have a unique distinguished, e.g., continuous, representative, which is the basis for considerations. On the other hand, occasionally, it is necessary to remember this fact.

12.3.2 Projections on Closed Subspaces

Definition 12.3.10. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a pre-Hilbert space, $f, g \in X$ and $S, T \subset X$.

(i) We say that f is perpendicular to g and indicate this symbolically by $f \perp g$ if $\langle f|g\rangle = 0$.

(ii) We say that S is perpendicular to T and indicate this symbolically by $S \perp T$ if $\langle f|g\rangle = 0$ for all $f \in S$ and $g \in T$.

[1] a.e. stands for *almost everywhere*, i.e., $\{x \in E : f(x) \neq g(x)\}$ is set of Lebesgue measure 0.

(iii) We define the orthogonal complement $S^{\perp}$ of S by

$$S^{\perp} := \{g \in X : \langle g|f\rangle = 0 \text{ for all } f \in S\} \ .$$

Theorem 12.3.11. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a pre-Hilbert space and $S, T \subset X$. Then

(i) $\{0\}^{\perp} = X$ and $X^{\perp} = \{0\}$,

(ii) $S^{\perp}$ is a closed subspace of X,

(iii) $S \subset T \Rightarrow T^{\perp} \subset S^{\perp}$,

(iv) $S^{\perp} = (\,\text{Span}\, S\,)^{\perp} = (\,\overline{\text{Span}\, S}\,)^{\perp}$.

Proof. “(i)": For every $f \in X$, as a consequence of the linearity of $\langle f|\cdot\rangle$, it follows that $\langle f|0\rangle = 0$ and hence that $X \subset \{0\}^{\perp} \subset X$. Further, for every $f \in X$, it follows as a consequence of the linearity of $\langle f|\cdot\rangle$ and the Hermiticity of $\langle\,|\,\rangle$ that $\langle 0|f\rangle = 0$ and hence that $0 \in X^{\perp}$. Finally, for every $f \in X \setminus \{0\}$, since $\langle\,|\,\rangle$ is a scalar product, it follows that $\langle f|f\rangle > 0$ and hence that $f \notin X^{\perp}$.
“(ii)": First, it follows for every $f \in S$ as well as a consequence of the linearity of $\langle f|\cdot\rangle$ and the Hermiticity of $\langle\,|\,\rangle$ that $\langle 0|f\rangle = 0$ and hence that $0 \in S^{\perp}$. Further, if $f_1, f_2 \in S^{\perp}$ and $\lambda \in \mathbb{K}$, then

$$\langle f_1 + f_2|f\rangle = \langle f_1|f\rangle + \langle f_2|f\rangle = 0 \ , \ \langle \lambda f_1|f\rangle = 0$$

for every $f \in S$. Hence, $S^{\perp}$ is a subspace of X. In addition, if $g_1, g_2, \dots$ is a sequence in $S^{\perp}$ that is convergent to $g \in X$, we conclude that

$$\langle g|f\rangle = \langle \lim_{\nu\to\infty} g_{\nu}|f\,\rangle = \lim_{\nu\to\infty} \langle g_{\nu}|f\rangle = 0$$

for every $f \in S$ and hence that $g \in S^{\perp}$. As a consequence, $S^{\perp}$ is a closed subspace of X.
“(iii)": If $S \subset T$ and $g \in T^{\perp}$, it follows that $\langle g|f\rangle = 0$ for every $f \in S$ and hence that $g \in S^{\perp}$.
“(iv)": Since $S \subset \text{Span}\, S \subset \overline{\text{Span}\, S}$, we conclude by (iii) that $S^{\perp} \supset (\,\text{Span}\, S\,)^{\perp} \supset (\,\overline{\text{Span}\, S}\,)^{\perp}$. Further, for every $f \in S^{\perp}$, it follows from the linearity of $\langle f|\cdot\rangle$ that $f \in (\,\text{Span}\, S\,)^{\perp}$ and hence that $S^{\perp} \subset (\,\text{Span}\, S\,)^{\perp}$. Finally, for every $f \in (\,\text{Span}\, S\,)^{\perp}$, it follows from the continuity of $\langle f|\cdot\rangle$ that $f \in (\,\overline{\text{Span}\, S}\,)^{\perp}$ and hence that $(\,\text{Span}\, S\,)^{\perp} \subset (\,\overline{\text{Span}\, S}\,)^{\perp}$. □

Theorem 12.3.12. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a Hilbert space and $S \subset X$ non-empty, closed and convex[1]. Then for every $f \in X$, there is a unique $f_S \in S$ such that

$$\|f - f_S\| = d(f, S) := \inf\{\|f - g\| : g \in S\} \ ,$$

where $\|\ \|$ denotes the norm that is induced on X by $\langle\,|\,\rangle$.

[1] I.e., such that $\alpha f + (1-\alpha)g \in S$ for all $f, g \in S$ and $\alpha \in [0, 1]$.

Proof. Let $f \in X$. Then

$$D := \{\|f - g\| : g \in S\}$$

is a non-empty subset of $\mathbb{R}$ that is bounded from below by 0. Hence the largest lower bound, $\inf D$, of D exists and is ≥ 0. Further, since for $\nu \in \mathbb{N}^*$, $\inf D + \nu^{-1}$ is no lower bound of D, there is $f_\nu \in S$ such that

$$\inf D \leq \|f - f_\nu\| < \inf D + \nu^{-1} \ .$$

As a consequence,

$$\lim_{\nu \to \infty} \|f - f_\nu\| = \inf D \ . \tag{12.8}$$

Further, it follows by application of the Parallelogram law, Theorem 12.3.3 (i) for $\langle\,|\,\rangle$, that

$$\begin{aligned}
&\|f_\mu - f_\nu\|^2 = \|f_\mu - f - (f_\nu - f)\|^2 \\
&= \|f_\mu - f - (f_\nu - f)\|^2 + \|f_\mu - f + (f_\nu - f)\|^2 - \|f_\mu - f + (f_\nu - f)\|^2 \\
&= 2[\|f_\mu - f\|^2 + \|f_\nu - f\|^2] - 4\,\|2^{-1} f_\mu + 2^{-1} f_\nu - f\|^2 \\
&\leq 2[\|f_\mu - f\|^2 + \|f_\nu - f\|^2] - 4(\inf D)^2
\end{aligned}$$

for $\mu, \nu \in \mathbb{N}^*$ and hence by (12.8) that $f_1, f_2, \dots$ is a Cauchy-sequence in X. Note that the last step uses the convexity of S. Since $(X, \|\ \|)$ is complete and S is closed, it follows the convergence of $f_1, f_2, \dots$ to a $f_S \in S$. Furthermore, (12.8) implies that

$$\|f - f_S\| = \inf D \ .$$

If $f'_S \in S$ is such that

$$\|f - f'_S\| = \inf D \ ,$$

we conclude by application of the Parallelogram law, Theorem 12.3.3 (i) for $\langle\,|\,\rangle$, that

$$\begin{aligned}
\|f'_S - f_S\|^2 &= 2[\|f'_S - f\|^2 + \|f_S - f\|^2] - 4\,\|2^{-1} f'_S + 2^{-1} f_S - f\|^2 \\
&\leq 2[\|f'_S - f\|^2 + \|f_S - f\|^2] - 4(\inf D)^2 = 0
\end{aligned}$$

and hence that $f'_S = f_S$. □

Theorem 12.3.13. (**Projection Theorem**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a Hilbert space with induced norm $\|\ \|$, Y a closed subspace of X and $P_Y : X \to X$ defined by

$$P_Y f := f_Y \ ,$$

where is f_Y is the unique element of Y such that

$$\|f - f_Y\| = d(f, Y) := \inf\{\|f - g\| : g \in Y\} \ .$$

Then

(i) $f - P_Y f \in Y^{\perp}$ for every $f \in X$. For this reason, we call P_Y "the orthogonal projection of X onto Y".

(ii) $X = Y \otimes Y^{\perp}$, i.e., for every $f \in X$ there is a unique pair $(g_1, g_2) \in Y \times Y^{\perp}$ such that $f = g_1 + g_2$. This pair is given by $(g_1, g_2) = (P_Y f, f - P_Y f)$.

(iii) P_Y is linear, continuous, symmetric[1] such that

$$\|P_Y f\| \leq \|f\|$$

for every $f \in X$ and $P_Y^2 = P_Y$.

Proof. We note that, as a consequence of Theorem 12.3.12, since Y is a non-empty, closed and convex subset of X, P_Y is well-defined.
"(i)": Let $f \in X$ and $g \in Y$ with $\|g\| = 1$. Then

$$f - P_Y f = f - P_Y f - \langle g|f - P_Y f\rangle \; g + \langle g|f - P_Y f\rangle \; g$$

and

$$\begin{aligned} &\langle f - P_Y f - \langle g|f - P_Y f\rangle \; g| \, \langle g|f - P_Y f\rangle \; g\rangle \\ &= |\, \langle g|f - P_Y f\rangle \,|^2 - |\, \langle g|f - P_Y f\rangle \,|^2 \|g\|^2 = 0 \; . \end{aligned}$$

As a consequence,

$$\|f - P_Y f\|^2 = \|f - P_Y f - \langle g|f - P_Y f\rangle \; g\|^2 + \|\langle g|f - P_Y f\rangle \; g\|^2$$

Hence it follows from the definition of $P_Y f$ that $(f - P_Y f) \perp g$. Note that here it has been used that $P_Y f + \langle g|f - P_Y f\rangle \; g \in Y$.
"(ii)": Let $f \in X$. From (i) follows that $(P_Y f, f - P_Y f) \in Y \times Y^{\perp}$. Also, $f = P_Y f + f - P_Y f$. If $(g_1, g_2) \in Y \times Y^{\perp}$ is such that $f = g_1 + g_2$, then

$$0 = g_1 - P_Y f + g_2 - (f - P_Y f) \; .$$

Since $g_1 - P_Y f \perp g_2 - (f - P_Y f)$, we conclude that

$$0 = \|g_1 - P_Y f\|^2 + \|g_2 - (f - P_Y f)\|^2$$

and hence that $(g_1, g_2) = (P_Y f, f - P_Y f)$.
"(iii)" For $f, f_1, f_2 \in X$ and $\lambda \in \mathbb{K}$, it follows that

$$\begin{aligned} f_1 + f_2 &= P_Y f_1 + P_Y f_2 + f_1 - P_Y f_1 + f_2 - P_Y f_2 \\ &= P_Y(f_1 + f_2) + f_1 + f_2 - P_Y(f_1 + f_2) \\ \lambda f &= \lambda P_Y f + \lambda(f - P_Y f) = P_Y \lambda f + (\lambda f - P_Y \lambda f) \; . \end{aligned}$$

and hence by (ii) that

$$P_Y(f_1 + f_2) = P_Y f_1 + P_Y f_2 \; , \; P_Y \lambda f = \lambda P_Y f \; .$$

[1] I.e., $\langle f|P_Y g\rangle = \langle P_Y f|g\rangle$ for all $f, g \in X$.

Further, for $f \in X$, we conclude that

$$\|f\|^2 = \|P_Y f\|^2 + \|f - P_Y f\|^2$$

and hence that $\|P_Y f\| \leq \|f\|$. In particular, the latter implies that P_Y is continuous. Also, for $f, g \in X$, it follows that

$$\begin{aligned}\langle f|P_Y g\rangle &= \langle P_Y f + f - P_Y f|P_Y g\rangle = \langle P_Y f|P_Y g\rangle \\ &= \langle P_Y f|P_Y g + g - P_Y g\rangle = \langle P_Y f|g\rangle \ .\end{aligned}$$

Finally, for every $f \in Y$, $\|f - f\| = 0$ and hence $P_Y f = f$. The latter implies that $P_Y \circ P_Y = P_Y$. □

Corollary 12.3.14. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a Hilbert space and $S \subset X$. Then

(i)
$$S^{\perp\perp} = \overline{\text{Span}S} \ , \tag{12.9}$$
i.e., $S^{\perp\perp}$ is the smallest closed subspace of X containing S.

(ii) $S^{\perp} = \{0\}$ if and only if Span$S$ is dense in X, i.e., if and only if
$$\overline{\text{Span}S} = X \ .$$

Proof. “(i)": From Theorem 12.3.11, we conclude that

$$S^{\perp\perp} = (\,\overline{\text{Span}S}\,)^{\perp\perp} \ .$$

Further, from Theorems 12.3.11, 12.3.13, it follows that

$$X = \overline{\text{Span}S} \otimes (\,\overline{\text{Span}S}\,)^{\perp} = (\,\overline{\text{Span}S}\,)^{\perp} \otimes (\,\overline{\text{Span}S}\,)^{\perp\perp} \ .$$

Hence it follows (12.9).
“(ii)": If $S^{\perp} = \{0\}$, we conclude from (i) and Theorem 12.3.11 that

$$\overline{\text{Span}S} = S^{\perp\perp} = \{0\}^{\perp} = X \ .$$

If $\overline{\text{Span}S} = X$, it follows from Theorem 12.3.11 that

$$S^{\perp} = (\,\overline{\text{Span}S}\,)^{\perp} = X^{\perp} = \{0\} \ .$$

□

12.3.3 Riesz’ Lemma, Hilbert Bases

Theorem 12.3.15. (**Riesz’ lemma**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $(X, \langle\,|\,\rangle)$ a Hilbert space with induced norm $\|\ \|$. For every $\omega \in L(X, \mathbb{K})$, there is a unique $f \in X$ such that $\omega = \langle f|\cdot\rangle$. In particular, if X is non-trivial, $\|\omega\|_{Op} = \|f\|$.

Proof. Let $\omega \in L(X, \mathbb{K})$. Then $\ker \omega$ is a closed subspace of X. In case that $\ker \omega = X$, $\omega = \langle 0|\cdot\rangle$. Further, if $f \in X$ is such that $\omega = \langle f|\cdot\rangle$, then $0 = \omega(f) = \|f\|^2$ and hence $f = 0$. Finally, if X is non-trivial $0 = \|\omega\|_{Op} = \|0\|$. In case that $\ker \omega \neq X$, $(\ker \omega)^{\perp}$ is non-trivial. Let $f_0 \in (\ker \omega)^{\perp}$ such that $\|f_0\| = 1$. Then

$$\begin{aligned} \omega(g) &= \omega\left(g - \frac{\omega(g)}{\omega(f_0)}\, f_0 + \frac{\omega(g)}{\omega(f_0)}\, f_0\right) \\ &= \langle (\omega(f_0))^* f_0 | g - \frac{\omega(g)}{\omega(f_0)}\, f_0\rangle + \langle (\omega(f_0))^* f_0 | \frac{\omega(g)}{\omega(f_0)}\, f_0\rangle = \langle (\omega(f_0))^* f_0 | g\rangle \end{aligned}$$

for every $g \in X$ and hence

$$\omega = \langle (\omega(f_0))^* f_0 | \cdot\rangle \ .$$

Further, if $f \in X$ is such that $\omega = \langle f|\cdot\rangle$, it follows that

$$\langle f - (\omega(f_0))^* f_0 | \cdot\rangle = 0 \ .$$

The latter implies that

$$0 = \langle f - (\omega(f_0))^* f_0 | f - (\omega(f_0))^* f_0\rangle = \|f - (\omega(f_0))^* f_0\|^2$$

and hence that $f = (\omega(f_0))^* f_0$. In particular, if X is non-trivial, $\|\omega\|_{Op} = \|\,\langle (\omega(f_0))^* f_0|\cdot\rangle\,\|_{Op} = \|(\omega(f_0))^* f_0\|\ (= |\omega(f_0)|\,)$. □

Definition 12.3.16. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $(X, \langle\,|\,\rangle)$ a non-trivial Hilbert space.

(i) An object M is called an orthonormal system in X if M is a non-empty subset of X such that $\langle e|e'\rangle = 1$ if $e = e'$ and $\langle e|e'\rangle = 0$ if $e \neq e'$.

(ii) An object M is called a Hilbert basis of X if M is an orthonormal system in X and Span$M$ is dense in X.

Theorem 12.3.17. Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a non-trivial Hilbert space with induced norm $\|\ \|$, and M an orthonormal system in X. Then

(i) a) M is linearly independent.

b) M is a Hilbert basis of X if and only if M is a maximal orthonormal system in X, i.e., for every orthonormal system M' in X satisfying $M' \supset M$, it follows that $M' = M$.

(ii) a) If $n \in \mathbb{N}^*$ and $e_1, \dots e_n$ a sequence of pairwise different elements of M, then

$$d(f, \text{Span}\{e_1, \dots e_n\}) = \|f - \sum_{i=1}^{n} \langle e_i|f\rangle\, e_i\| \ . \tag{12.10}$$

for every $f \in X$.

b) (**Bessel inequality**) For every $f \in X$,

$$M(f) := \{e \in M : \langle e|f\rangle \neq 0\} \subset M$$

is at most countable and the corresponding sequence

$$(|\langle e|f\rangle|^2)_{e \in M(f)}$$

is summable such that

$$\sum_{e \in M(f)} |\langle e|f\rangle|^2 \leq \|f\|^2 \ ,$$

where the sum is defined as 0 if $M(f) = \phi$.

c) (**Parseval equality**)

1) M is a Hilbert basis of X if and only if for every $f \in X$

$$\sum_{e \in M(f)} |\langle e|f\rangle|^2 = \|f\|^2 \ .$$

2) If M is a Hilbert basis of X, for every $f \in X$ and every bijection $e : I \to M(f)$, where I is finite or $I = \mathbb{N}^*$,

$$(\langle e_i|f\rangle \, e_i)_{i \in I} \in X^I$$

is summable such that

$$f = \sum_{i \in I} \langle e_i|f\rangle \, e_i \ ,$$

where the last sum is defined by 0 if $I = \phi$.

(iii) In addition, let M be infinite. If $(e_n)_{n \in \mathbb{N}^*} \in M^{\mathbb{N}^*}$ is a sequence of pairwise different elements of M and $(a_n)_{n \in \mathbb{N}^*} \in \mathbb{K}^{\mathbb{N}^*}$, then $(\sum_{n=1}^m a_n e_n)_{m \in \mathbb{N}^*}$ is convergent if and only if $(\sum_{n=1}^m |a_n|^2)_{m \in \mathbb{N}^*}$ is convergent.

Proof. "(i)a)": Let $e_1, \dots, e_n$, where $n \in \mathbb{N}^*$, be a sequence of pairwise different elements of M and $a_1, \dots, a_n$ elements of $\mathbb{K}$ such that

$$\sum_{i=1}^n a_i e_i = 0 \ .$$

Then

$$0 = \left\| \sum_{i=1}^n a_i e_i \right\|^2 = \langle \sum_{i=1}^n a_i e_i | \sum_{j=1}^n a_j e_j \rangle = \sum_{i,j=1}^n a_i^* a_j \, \langle e_i|e_j\rangle = \sum_{i,j=1}^n |a_i|^2 \ ,$$

and hence $a_i = 0$ for every $i \in \{1, \dots, n\}$.
"(i)b)": If M is in particular a Hilbert basis of X and $M' \supsetneqq M$ an orthonormal system in X. Then it follows for $f \in M' \setminus M$ that

$$f \in M^\perp = (\,\overline{\text{Span}M}\,)^\perp = X^\perp = \{0\}$$

in contradiction to $\|f\| = 1$.↯ If M is maximal, it follows that $M^\perp = \{0\}$ and hence that

$$\overline{\text{Span}M} = \overline{\text{Span}M}^{\perp\perp} = (M^\perp)^\perp = \{0\}^\perp = X \ .$$

Therefore, M is a Hilbert basis.
"(ii)a)": If $n \in \mathbb{N}^*$ and $e_1, \dots, e_n$ is a sequence of pairwise different elements of M, it follows for $f \in X$, $a_1, \dots, a_n \in \mathbb{K}$ that

$$\left\| f - \sum_{i=1}^n a_i e_i \right\|^2 = \langle f - \sum_{i=1}^n a_i e_i | f - \sum_{j=1}^n a_j e_j \rangle \tag{12.11}$$
$$= \|f\|^2 - \sum_{i=1}^n a_i^* \langle e_i|f\rangle - \sum_{i=1}^n a_i \langle f|e_i\rangle + \sum_{i=1}^n |a_i|^2$$
$$= \|f\|^2 - \sum_{i=1}^n |\langle e_i|f\rangle|^2 + \sum_{i=1}^n (a_i - \langle e_i|f\rangle)^*(a_i - \langle e_i|f\rangle)$$
$$= \|f\|^2 - \sum_{i=1}^n \langle e_i|f\rangle^* \langle e_i|f\rangle - \sum_{i=1}^n \langle e_i|f\rangle \langle f|e_i\rangle + \sum_{i=1}^n |\langle e_i|f\rangle|^2$$
$$+ \sum_{i=1}^n |a_i - \langle e_i|f\rangle|^2$$
$$= \left\| f - \sum_{i=1}^n \langle e_i|f\rangle e_i \right\|^2 + \sum_{i=1}^n |a_i - \langle e_i|f\rangle|^2 \geq \left\| f - \sum_{i=1}^n \langle e_i|f\rangle e_i \right\|^2 ,$$

where $^* := \text{id}_{\mathbb{R}}$ if $\mathbb{K} = \mathbb{R}$, and hence the validity of (12.10).
"(ii)b)": Let $f \in X$. If $n \in \mathbb{N}^*$ and $e_1, \dots, e_n$ is a sequence of pairwise different elements of M, it follows from (12.11) that

$$\|f\|^2 = \sum_{i=1}^n |\langle e_i|f\rangle|^2 + \left\| f - \sum_{i=1}^n \langle e_i|f\rangle e_i \right\|^2 \geq \sum_{i=1}^n |\langle e_i|f\rangle|^2 \ . \tag{12.12}$$

As a consequence, for every $\nu \in \mathbb{N}^*$,

$$\{e \in M : |\langle e|f\rangle| > \frac{1}{\nu}\}$$

is a finite, possibly empty, subset of M. Hence

$$M(f) := \{e \in M : \langle e|f\rangle \neq 0\} = \bigcup_{\nu \in \mathbb{N}^*} \{e \in M : |\langle e|f\rangle| > \frac{1}{\nu}\}$$

is at most countable. If $M(f)$ is finite, (12.12) implies that

$$\sum_{e \in M(f)} |\langle e|f\rangle|^2 \leq \|f\|^2 .$$

If $M(f)$ is infinite and $e : \mathbb{N}^* \to M(f)$ a bijection, then

$$\left(\sum_{i=1}^{n} |\langle e_i|f\rangle|^2 \right)_{n \in \mathbb{N}^*}$$

is an increasing sequence of real numbers that, as a consequence of (12.12), is bounded from above by $\|f\|^2$. Hence this sequence is convergent such that

$$\sum_{i=1}^{\infty} |\langle e_i|f\rangle|^2 \leq \|f\|^2 .$$

"(ii)c)1)": If M is Hilbert Basis and $f \in X$, then $f \in \overline{\text{Span}M} = X$. We note that from (12.11), it follows for $n \in \mathbb{N}^*$, a sequence $e_1, \dots, e_n$ of pairwise different elements of M and $a_1, \dots, a_n \in \mathbb{K}$ that

$$\left\| f - \sum_{i=1}^{n} a_i e_i \right\|^2 \geq \left\| f - \sum_{i=1}^{n} \langle e_i|f\rangle\, e_i \right\|^2 = \|f\|^2 - \sum_{i=1}^{n} |\langle e_i|f\rangle|^2$$
$$\geq \|f\|^2 - \sum_{e \in M(f)} |\langle e|f\rangle|^2 .$$

From this, we conclude for every $\varepsilon > 0$ that

$$\|f\|^2 - \sum_{e \in M(f)} |\langle e|f\rangle|^2 \leq \varepsilon$$

and hence that

$$\|f\|^2 \leq \sum_{e \in M(f)} |\langle e|f\rangle|^2 .$$

The latter and part ii)b) imply that

$$\sum_{e \in M(f)} |\langle e|f\rangle|^2 = \|f\|^2 .$$

If $f \in X$ and

$$\sum_{e \in M(f)} |\langle e|f\rangle|^2 = \|f\|^2 ,$$

we conclude as follows. First, we note that from (12.11) follows for $n \in \mathbb{N}^*$ and a sequence $e_1, \dots, e_n$ of pairwise different elements of M that

$$\left\| f - \sum_{i=1}^{n} \langle e_i|f\rangle\, e_i \right\|^2 = \|f\|^2 - \sum_{i=1}^{n} |\langle e_i|f\rangle|^2 .$$

Hence, if I is a finite, possibly empty, set or $I = \mathbb{N}^*$ and $e : I \to M(f)$ a bijection, we conclude from the latter that

$$f = \sum_{i \in I}^{n} \langle e_i | f \rangle \, e_i$$

and hence that $f \in \overline{\text{Span} M}$.
"(ii)c)2)": See the previous proof of (ii)c)1).
"(iii)": If M be infinite, $(e_n)_{n \in \mathbb{N}^*} \in M^{\mathbb{N}^*}$ is a sequence of pairwise different elements of M and $(a_n)_{n \in \mathbb{N}^*} \in \mathbb{K}^{\mathbb{N}^*}$, then

$$\left\| \sum_{n=1}^{m} a_n e_n - \sum_{n=1}^{m'} a_n e_n \right\|^2 = \left| \sum_{n=1}^{m} |a_n|^2 - \sum_{n=1}^{m'} |a_n|^2 \right|$$

for $m, m' \in \mathbb{N}^*$. Hence

$$\left(\sum_{n=1}^{m} a_n e_n \right)_{m \in \mathbb{N}^*}$$

is a Cauchy-sequence in X if and only if

$$\left(\sum_{n=1}^{m} |a_n|^2 \right)_{m \in \mathbb{N}^*}$$

is a Cauchy-sequence in $\mathbb{R}$. Since X and $\mathbb{R}$ are complete, the latter implies that $(\sum_{n=1}^{m} a_n e_n)_{m \in \mathbb{N}^*}$ is convergent if and only if $(\sum_{n=1}^{m} |a_n|^2)_{m \in \mathbb{N}^*}$ is convergent. □

Theorem 12.3.18. (**Existence of Hilbert bases**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a non-trivial Hilbert space with induced norm $\|\ \|$, and M_0 an orthonormal system in X. Then there is an extension of M_0 to a Hilbert basis of X.

Proof. We define

$$\mathscr{P} := \{M \text{ orthonormal system in } X \text{ and } M \supset M_0\} \ .$$

Then, the restriction of $\subset$ to $\mathscr{P} \times \mathscr{P}$ defines a partial order in $\mathscr{P}$. If $\mathscr{P}'$ is a totally ordered subset of $\mathscr{P}$, then

$$\bigcup_{M \in \mathscr{P}'} M$$

is an upper bound for $\mathscr{P}'$ in $\mathscr{P}$. Hence according to Zorn's lemma, $\mathscr{P}$ contains a maximal element. According to Theorem 12.3.17 (i)b) such a maximal element is a Hilbert basis. □

12.4 Linear Operators in Hilbert Spaces

12.4.1 Bounded Operators

Definition 12.4.1. (Adjoint Operators, Self-Adjointness) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a non-trivial Hilbert space, and $A \in L(X, X)$. We note for every $f \in X$, since for every $g \in X$

$$|\langle f|A\,g\rangle| \leqslant \left[\|f\| \cdot \|A\|_{\text{Op}}\right] \|g\| \ ,$$

that

$$\langle f|A\,\cdot\rangle \in L(X, \mathbb{K})$$

and hence according to Riesz' lemma, Theorem 12.3.15, that there is a unique f' such that

$$\langle f|A\,\cdot\rangle = \langle f'|\cdot\rangle \ .$$

Therefore, we can and do define a so called adjoint $A^* : X \to X$ to A, for every $f \in X$ by

$$\langle f|A\,\cdot\rangle = \langle A^* f|\cdot\rangle \ .$$

In particular, we call A self-adjoint if $A^* = A$. Also, we define

$$L_s(X, X) := \{A \in L(X, X) : A \text{ is self-adjoint}\} \ .$$

Theorem 12.4.2. (**Elementary Properties of the Adjoint**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, $(X, \langle\,|\,\rangle)$ a non-trivial Hilbert space, and $A, B \in L(X, X), \alpha \in \mathbb{K}$.

(i) Then $A^* \in L(X, X)$,

$$\|A^*\|_{\text{Op}} = \|A\|_{\text{Op}} \ ,$$

(ii)

$$(A^*)^* = A \ , \ (A + B)^* = A^* + B^* \ ,$$
$$(\alpha.A)^* = \alpha^*.A^* \ , \ (A \circ B)^* = B^* \circ A^* \ ,$$

(iii)

$$\|A^* \circ A\|_{\text{Op}} = \|A\|_{\text{Op}}^2 \ .$$

Proof. Parts (i), (iii): First, we note that for $f, g \in X$, $\lambda \in \mathbb{K}$ that

$$\begin{aligned}\langle A^*(f+g)|\cdot\rangle &= \langle f+g|A\,\cdot\rangle = \langle f|A\,\cdot\rangle + \langle g|A\,\cdot\rangle = \langle A^* f|\cdot\rangle + \langle A^* g|\cdot\rangle \\ &= \langle A^* f + A^* g|\cdot\rangle \ , \\ \langle A^*\lambda.f|\cdot\rangle &= \langle\lambda.f|A\,\cdot\rangle = \lambda^*\langle f|A\,\cdot\rangle = \lambda^*\langle A^* f|\cdot\rangle = \langle\lambda.A^* f|\cdot\rangle\end{aligned}$$

and hence that A is linear. Also, for $f \in X$

$$\|A^* f\|^2 = \langle A^* f|A^* f\rangle = \langle f|AA^* f\rangle \leqslant \|f\| \cdot \|A\|_{\text{Op}} \cdot \|A^* f\|$$

and hence
$$\|A^* f\| \leqslant \|A\|_{\text{Op}} \cdot \|f\| \ .$$
As a consequence, $A^* \in L(X,X)$ and
$$\|A^*\|_{\text{Op}} \leqslant \|A\|_{\text{Op}} \ .$$
In addition, for $f \in X$
$$\|Af\|^2 = \langle Af|Af\rangle = \langle A^*Af|f\rangle \leqslant \|A^*\|_{\text{Op}} \cdot \|Af\| \cdot \|f\|$$
and hence
$$\|Af\| \leqslant \|A^*\|_{\text{Op}} \cdot \|f\| \ .$$
As a consequence,
$$\|A\|_{\text{Op}} \leqslant \|A^*\|_{\text{Op}} \ .$$
Finally,
$$\|A^*A\|_{\text{Op}} \leqslant \|A^*\|_{\text{Op}} \cdot \|A\|_{\text{Op}} = \|A\|_{\text{Op}}^2 \ ,$$
and for $f \in X$
$$\|Af\|^2 = \langle Af|Af\rangle = \langle A^*Af|f\rangle \leqslant \|A^*A\|_{\text{Op}} \cdot \|f\|^2 \ ,$$
implying that
$$\|Af\| \leqslant \sqrt{\|A^*A\|_{\text{Op}}} \cdot \|f\|$$
and that
$$\|A\|_{\text{Op}} \leqslant \sqrt{\|A^*A\|_{\text{Op}}} \ .$$
Part (ii): For $f \in X$,
$$\begin{aligned}
\langle (A^*)^* f|\cdot\rangle &= \langle f|A^* \cdot\rangle = \langle A^* \cdot |f\rangle^* = \langle \cdot|Af\rangle^* = \langle Af|\cdot\rangle \ , \\
\langle (A+B)^* f|\cdot\rangle &= \langle f|(A+B)\cdot\rangle = \langle f|A\cdot\rangle + \langle f|B\cdot\rangle \\
&= \langle A^* f|\cdot\rangle + \langle B^* f|\cdot\rangle = \langle (A^*+B^*) f|\cdot\rangle \ , \\
\langle (\alpha.A)^* f|\cdot\rangle &= \langle f|(\alpha.A)\cdot\rangle = \alpha \langle f|A\cdot\rangle = \alpha \langle A^* f|\cdot\rangle = \langle \alpha^* A^* f|\cdot\rangle \ , \\
\langle (A\circ B)^* f|\cdot\rangle &= \langle f|(A\circ B)\cdot\rangle = \langle A^* f|B\cdot\rangle = \langle (B^*\circ A^*) f|\cdot\rangle \ .
\end{aligned}$$

□

Remark 12.4.3. A map $*$ on an algebra satisfying Theorem 12.4.2 (ii) is called an *involution* and such algebra an *involutive algebra*. A Banach algebra with involution, where the involution satisfies Theorem 12.4.2 (i) is called an *involutive Banach algebra*. An involutive Banach algebra over $\mathbb{C}$, where the involution satisfies Theorem 12.4.2 (iii), is called a $\mathbb{K}^*$-*algebra*. Since, according to Remark 12.2.4, $(L(X,X),+,.,\circ,\| \ \|_{\text{Op}})$ is an associative Banach algebra with unit element, $(L(X,X),+,.,\circ,{}^*,\| \ \|_{\text{Op}})$ *is an associative* $\mathbb{K}^*$-*algebra with unit element*.

12.4.2 Unbounded Operators

Theorem 12.4.4. (**Definition and elementary properties of the adjoint**) Let $(X, \langle\,|\,\rangle_{\mathrm{X}})$ and $(Y, \langle\,|\,\rangle_{\mathrm{Y}})$ be Hilbert spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, A a *densely-defined* Y-valued linear operator in X and $U : X \times Y \to Y \times X$ the Hilbert space isomorphism defined by $U(f, g) := (-\,g, f)$ for all $(f, g) \in X \times Y$.

(i) Then the closed subspace

$$[U(G(A))]^{\perp} = \{(f, h) \in Y \times X : \langle f|Ag\rangle_{\mathrm{Y}} = \langle h|g\rangle_{\mathrm{X}} \\ \text{for all } g \in D(A)\}$$

of $Y \times X$ is the graph of an uniquely determined X-valued linear operator A^* in Y which is in particular closed and called the *adjoint* of A. *If in addition* $(X, \langle\,|\,\rangle_{\mathrm{X}}) = (Y, \langle\,|\,\rangle_{\mathrm{Y}})$, we call A *symmetric* if $A^* \supset A$ and *self-adjoint* if $A^* = A$.

(ii) If B is a Y-valued linear operator in X such that $B \supset A$, then

$$B^* \subset A^* \ .$$

(iii) If A^* is densely-defined, then $A \subset A^{**} := (A^*)^*$ and hence A is in particular closable.

(iv) If A is closed, then A^* is densely-defined and $A^{**} = A$.

(v) If A is closable, then $\bar{A} = A^{**}$.

(vi) If $B \in L(X, X)$, then $(A + B)^* = A^* + B^*$.

If in addition $(X, \langle\,|\,\rangle_{\mathrm{X}}) = (Y, \langle\,|\,\rangle_{\mathrm{Y}})$:

(vii) (*Maximality of self-adjoint operators*) If A is self-adjoint and $B \supset A$ is symmetric, then $B = A$.

(viii) If A is symmetric, then $\bar{A}$ is symmetric, too. Therefore, we call a symmetric A *essentially self-adjoint* if $\bar{A}$ is self-adjoint.

(ix) (*Hellinger-Toeplitz*) If $D(A) = X$ and A is self-adjoint, then $A \in L(X, X)$.

Proof. '(i)': First, it follows that

$$[U(G(A))]^{\perp} = \{(g, f) \in Y \times X : \langle (g, f)|U(h, Ah)\rangle_{\mathrm{Y}\times\mathrm{X}} = 0 \text{ for all } h \in D(A)\}$$

and hence that

$$[U(G(A))]^{\perp} = \{(g, f) \in Y \times X : \langle g|Ah\rangle_{\mathrm{Y}} = \langle f|h\rangle_{\mathrm{X}} \text{ for all } h \in D(A)\} \ .$$

In particular, it follows for $(g, f_1), (g, f_2) \in [U(G(A))]^{\perp}$ that

$$\langle f_1 - f_2|h\rangle_{\mathrm{X}} = 0$$

for all $h \in D(A)$ and hence that $f_1 = f_2$ since $D(A)$ is dense in X. As a consequence, by

$$A^* : \text{pr}_1[U(G(A))]^{\perp} \to X \ ,$$

where $\text{pr}_1 := (Y \times X \to Y, (g, f) \mapsto g)$, defined by

$$A^* g := f \ ,$$

for all $g \in \text{pr}_1[U(G(A))]^{\perp}$, where $f \in X$ is the unique element such that $(g, f) \in [U(G(A))]^{\perp}$, there is defined a map such that

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

Note that the domain of A^* is a subspace of Y. In particular, it follows for all $g, k \in D(A^*)$ and $\lambda \in \mathbb{K}$

$$\begin{aligned}
&\langle g + k | Ah \rangle_{\text{Y}} = \langle g | Ah \rangle_{\text{Y}} + \langle k | Ah \rangle_{\text{Y}} = \langle A^* g | h \rangle_{\text{X}} + \langle A^* k | h \rangle_{\text{X}} \\
&= \langle A^* g + A^* k | h \rangle_{\text{X}} \\
&\langle \lambda . g | Ah \rangle_{\text{Y}} = \lambda^{(*)} \cdot \langle g | Ah \rangle_{\text{Y}} = \lambda^{(*)} \cdot \langle A^* g | h \rangle_{\text{X}} = \langle \lambda . A^* g | h \rangle_{\text{X}}
\end{aligned}$$

for all $h \in D(A)$ and hence also the linearity of A^*.
'(ii)': Since

$$U(G(B)) \supset U(G(A)) \ ,$$

it follows that

$$G(B^*) = [U(G(B))]^{\perp} \subset [U(G(A))]^{\perp} = G(A^*) \ .$$

'(iii)': For this, let A^* be densely-defined. Then, it follows

$$\big(Y \times X \to X \times Y, (g, f) \mapsto (-f, g)\big) = -U^{-1}$$

and hence

$$\begin{aligned}
&G(A^{**}) = \big[-U^{-1}(G(A^*)) \big]^{\perp} = \big[U^{-1}(G(A^*)) \big]^{\perp} = \big[U^{-1}[U(G(A))]^{\perp} \big]^{\perp} \\
&= \big[[U^{-1}U(G(A))]^{\perp} \big]^{\perp} = G(A)^{\perp\perp} = \overline{G(A)} \supset G(A) \ .
\end{aligned} \tag{12.13}$$

'(iv)': For this, let A be closed. Then, it follows for $g \in [D(A^*)]^{\perp}$

$$\begin{aligned}
&(0, g) \in \big[U^{-1}(G(A^*)) \big]^{\perp} = \big[U^{-1}[U(G(A))]^{\perp} \big]^{\perp} = \big[[U^{-1}U(G(A))]^{\perp} \big]^{\perp} \\
&= G(A)^{\perp\perp} = \overline{G(A)} = G(A)
\end{aligned}$$

and hence $g = 0$. Hence $D(A^*)$ is dense in X, and it follows by (12.13) that $G(A^{**}) = \overline{G(A)} = G(\bar{A}) = G(A)$.
'(v)': For this, let A be closable. Since $\bar{A}$ is densely defined and closed, it follows

by (iv) that $\bar{A}^*$ is densely-defined. Because of $A \subset \bar{A}$, this implies that $A^* \supset \bar{A}^*$ and hence that A^* is densely-defined, too. Therefore, it follows by (iii) that $A \subset A^{**}$ and by (12.13) that $G(A^{**}) = \overline{G(A)} = G(\bar{A})$ and hence, finally, that $A^{**} = \bar{A}$.
'(vi)': Note that, by Riesz' representation theorem, $D(B^*) = Y$. '$A^* + B^* \supset (A+B)^*$': If $f \in D((A+B)^*), g \in D(A)$, then

$$\langle (A+B)^* f | g \rangle_{\mathrm{X}} = \langle f | (A+B) g \rangle_{\mathrm{Y}} = \langle f | A g \rangle_{\mathrm{Y}} + \langle B^* f | g \rangle_{\mathrm{X}} \ .$$

The latter implies that

$$\langle f | A g \rangle_{\mathrm{Y}} = \langle (A+B)^* f - B^* f | g \rangle_{\mathrm{X}}$$

and hence that $f \in D(A^*)$ and

$$A^* f = (A+B)^* f - B^* f \ .$$

The latter implies that

$$(A+B)^* f = (A^* + B^*) f \ .$$

'$(A+B)^* \supset A^* + B^*$': If $f \in D(A^*), g \in D(A)$, then

$$\begin{aligned} \langle f | (A+B) g \rangle_{\mathrm{Y}} &= \langle f | A g \rangle_{\mathrm{Y}} + \langle f | B g \rangle_{\mathrm{Y}} = \langle A^* f | g \rangle_{\mathrm{X}} + \langle B^* f | g \rangle_{\mathrm{X}} \\ &= \langle (A^* + B^*) f | g \rangle_{\mathrm{X}} \ . \end{aligned}$$

Hence $f \in D((A+B)^*)$ and

$$(A+B)^* f = (A^* + B^*) f \ .$$

In the following, it is assumed that $(X, \langle\,|\,\rangle_{\mathrm{X}}) = (Y, \langle\,|\,\rangle_{\mathrm{Y}})$.
'(vii)': For this, let A be self-adjoint and B a symmetric extension of A. Then, it follows by using $G(B) \supset G(A)$ that

$$G(B) \subset G(B^*) = [U(G(B))]^{\perp} \subset [U(G(A))]^{\perp} = G(A^*) = G(A)$$

and hence $B \subset A \subset B$ and therefore, finally, that $B = A$.
'(viii)': For this, let A be symmetric. Then $A^* \supset A$ and hence also $A^* \supset \bar{A}$.

$$\begin{aligned} G(\bar{A}^*) &= [U(G(\bar{A}))]^{\perp} = [U\,\overline{G(A)}\,]^{\perp} = [\,\overline{U(G(A))}\,]^{\perp} = \big[[U(G(A))]^{\perp\perp}\big]^{\perp} \\ &= \overline{[U(G(A))]^{\perp}} = \overline{G(A^*)} = G(A^*) \supset G(\bar{A}) \ . \end{aligned}$$

Hence it follows that $\bar{A}^* \supset \bar{A}$.
'(ix)': For this, let A be self-adjoint and $D(A) = X$. Then, $A = A^*$ is in particular closed and hence by Theorem 12.2.9 (v) bounded. □

Example 12.4.5. The text uses the Fourier transform F_2, which is a linear unitary transformation and hence the special case of a Hilbert space isomorphism. The transformation

$$\mathrm{F}_2 : \mathrm{L}^2_{\mathbb{C}}(\mathbb{R}^n) \to \mathrm{L}^2_{\mathbb{C}}(\mathbb{R}^n)$$

is defined for every rapidly decreasing test function $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R}^n)$ by

$$(\mathrm{F}_2 f)(k) := \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ik\cdot u} f(u)\, du \ ,$$

for every $k \in \mathbb{R}^n$.

12.4.3 Basic Criteria for Self-Adjointness

Theorem 12.4.6. (**Basic criteria for essential self-adjointness**) Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space and $A : D(A) \to X$ be a densely-defined, linear and symmetric Operator in X.

(i) If Ran A is dense in X and there is $a \in (0, \infty)$ such

$$\|Af\| \geqslant a\|f\|$$

for every $f \in D(A)$, then A is essentially self-adjoint.

(ii) If A is semi-bounded from below with lower bound $\gamma \in \mathbb{R}$, i.e.,

$$\langle f|Af\rangle \geqslant \gamma\,\langle f|f\rangle$$

for every $f \in D(A)$, and there is $\gamma' < \gamma$ such that Ran$(A - \gamma')$ is dense in X, then A is essentially self-adjoint.

Proof. '(i)': For this, let Ran A be dense in X and $a \in (0, \infty)$ be such

$$\|Af\| \geqslant a\|f\|$$

for every $f \in D(A)$. First, since $\bar{A}$ is symmetric, it follows that $\bar{A}^* \supset \bar{A}$. In the following, we show that

$$\bar{A}^* \subset \bar{A}\ . \tag{12.14}$$

For this, let $f \in D(\bar{A}^*)$. Since Ran A is dense in X, there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

$$\lim_{\nu\to\infty} Af_\nu = \bar{A}^* f.$$

Since

$$\|Af_\mu - Af_\nu\| \geqslant a\|f_\mu - f_\nu\|$$

for all $\nu, \mu \in \mathbb{N}^*$, $f_1, f_2, \dots$ is a Cauchy sequence in X and hence, by the completeness of X, also convergent. Hence it follows for every $g \in D(A)$ that

$$\langle \lim_{\nu\to\infty} f_\nu - f|Ag\,\rangle = \lim_{\nu\to\infty} \langle f_\nu|Ag\rangle - \langle f|Ag\rangle$$

$$= \lim_{\nu \to \infty} \langle A f_\nu | g \rangle - \langle f | \bar{A} g \rangle = \langle \bar{A}^* f | g \rangle - \langle f | \bar{A} g \rangle = 0$$

and hence, since Ran A is dense in X, that

$$\lim_{\nu \to \infty} f_\nu = f \ .$$

Hence it follows that $(f, \bar{A}^* f) \in G(\bar{A})$ and also (12.14). Finally, we conclude that $\bar{A}^* = \bar{A}$.
'(ii)': For this, let $\gamma \in \mathbb{R}$ be such that

$$\langle f | A f \rangle \geqslant \gamma \, \langle f | f \rangle$$

for every $f \in D(A)$ and such that there is $\gamma' < \gamma$ such that $\mathrm{Ran}(A - \gamma')$ is dense in X. Then

$$\|f\| \cdot \|(A - \gamma')f\| \geqslant | \, \langle f | (A - \gamma') f \rangle \, | \geqslant (\gamma - \gamma') \|f\|^2$$

for every $f \in D(A)$ and hence

$$\|(A - \gamma')f\| \geqslant (\gamma - \gamma') \|f\|$$

for every $f \in D(A)$. Since $A - \gamma'$ is a densely-defined, linear and symmetric operator in X, it follows by (i) that $A - \gamma'$ is essentially self-adjoint. This implies that

$$\bar{A} - \gamma' = \overline{A - \gamma'} = (\,\overline{A - \gamma'}\,)^* = (\bar{A} - \gamma')^* = \bar{A}^* - \gamma'$$

and hence that A is essentially self-adjoint. □

Theorem 12.4.7. (Rank-nullity theorem for linear operators) Let $(X, \langle \, | \, \rangle_{\mathrm{X}})$ and $(Y, \langle \, | \, \rangle_{\mathrm{Y}})$ be Hilbert spaces over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, and A be a densely-defined and linear Y-valued operator in X. Then

$$\ker A^* = (\mathrm{Ran} A)^{\perp} \ .$$

Proof. '$\subset$': For this, let $g \in \ker A^*$. Then, it follows that

$$0 = \langle A^* g | f \rangle_{\mathrm{X}} = \langle g | A f \rangle_{\mathrm{Y}}$$

for all $f \in D(A)$ and hence that $g \in (\mathrm{Ran} A)^{\perp}$.
'$\supset$': For this, let $g \in (\mathrm{Ran} A)^{\perp}$. Then, it follows that

$$0 = \langle g | A f \rangle_{\mathrm{Y}}$$

for all $f \in D(A)$ and hence that $g \in D(A^*)$ as well as that $A^* g = 0$. □

The following lemma is an application of the rank-nullity theorem for linear operators.

Lemma 12.4.8. (**Inverses of self-adjoint operators**) Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space and $A : D(A) \to X$ be a densely-defined, linear and symmetric and essentially self-adjoint operator in X, $\bar{A} : D(\bar{A}) \to X$ the closure of A and $I \in L(X, X)$.

(i) If $IAf = f$, for every $f \in D(A)$, then $\bar{A}$ is injective and $\mathrm{Ran}(\bar{A})$ is dense in X.

(ii) If there is a dense subspace D of X such that $AIg = g$, for every $g \in D$. Then, $\bar{A}$ is bijective and $\bar{A}^{-1} = I$.

Proof. For the proof of Part (i), let $f \in D(\bar{A})$. Since $\bar{A}$ is the closure of A, there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

$$\lim_{\nu\to\infty} f_\nu = f \ , \ \lim_{\nu\to\infty} Af_\nu = \bar{A}f \ .$$

Further, since $I \in L(X, X)$,

$$f = \lim_{\nu\to\infty} f_\nu = \lim_{\nu\to\infty} IAf_\nu = I\bar{A}f \ .$$

Hence $\ker \bar{A} = \{0\}$, and it follows from Theorem 12.4.7 that

$$(\mathrm{Ran}\,\bar{A}\,)^{\perp\perp} = \{0\}^{\perp} = X \ .$$

Since $(\mathrm{Ran}\,\bar{A}\,)^{\perp\perp}$ coincides with the closure of $\mathrm{Ran}\,\bar{A}$, $\mathrm{Ran}\,\bar{A}$ is dense in X. For the proof of Part (ii), let D be as stated and $\bar{g} \in X$. Since D is dense in X, there is a sequence $g_1, g_2, \dots$ in X such that

$$\lim_{\nu\to\infty} g_\nu = \bar{g} \ .$$

Hence,

$$\lim_{\nu\to\infty} AIg_\nu = \bar{g} \ .$$

Since I is continuous, we have that

$$\lim_{\nu\to\infty} Ig_\nu = I\bar{g} \ .$$

As a consequence, $I\bar{g} \in D(\bar{A})$ and

$$\bar{A}I\bar{g} = \bar{g} \ . \tag{12.15}$$

Therefore, $\bar{A}$ is surjective and according to Theorem 12.4.7 also injective. Hence, it follows that $\bar{A}$ is bijective and from (12.15) that $I = \bar{A}^{-1}$. □

Theorem 12.4.9 (**A characterization of essential self-adjointness**). Let $(X, \langle\,|\,\rangle)$ be a complex Hilbert space and $A : D(A) \to X$ be a densely-defined, linear, symmetric operator in X. Then A is essentially self-adjoint if and only if $\mathrm{Ran}(A - i)$ and $\mathrm{Ran}(A + i)$ are dense in X.

Proof. For this, we note that for $\lambda \in \{-i, i\}$ and $f \in D(A)$ it follows that

$$\begin{aligned}&\|(A-\lambda)f\|^2 = \langle Af - \lambda f | Af - \lambda f\rangle \\ &= \|Af\|^2 + |\lambda|^2\|f\|^2 - \lambda^* \langle f|Af\rangle - \lambda \langle Af|f\rangle \\ &= \|Af\|^2 + |\lambda|^2\|f\|^2 - \lambda^* \langle f|Af\rangle - \lambda \langle f|Af\rangle = \|f\|_A^2 \geqslant \|f\|^2\end{aligned}$$

and hence that

$$\|(A-\lambda)f\| = \|f\|_A \geqslant \|f\| \ . \tag{12.16}$$

In particular, the latter implies that

$$\ker(A-\lambda) = \{0\} \ .$$

'$\Rightarrow$': For this, let A be essentially self-adjoint and $\lambda \in \{-1, 1\}$. Then according to the Theorem 12.4.7,

$$[\mathrm{Ran}(\bar{A}+\lambda)]^{\perp} = \ker(\bar{A}-\lambda) = \{0\} \ .$$

Since $\mathrm{Ran}(A+\lambda)$ is dense in $\mathrm{Ran}(\bar{A}+\lambda)$, the latter also implies that

$$[\mathrm{Ran}(A+\lambda)]^{\perp} = \{0\}$$

and hence that

$$\overline{\mathrm{Ran}(A+\lambda)} = [\mathrm{Ran}(A+\lambda)]^{\perp\perp} = X \ .$$

'$\Leftarrow$': For this, let $\mathrm{Ran}(A-\lambda)$ be dense in X for $\lambda \in \{-i, i\}$. In a first step, we show, for $\lambda \in \{-i, i\}$, that

$$\mathrm{Ran}(\bar{A}-\lambda) = X \ . \tag{12.17}$$

Since $\mathrm{Ran}(A-\lambda)$ is dense in X, for $g \in X$, there is a sequence $f_1, f_2, \dots$ of elements of $D(A)$ such that

$$\lim_{\nu\to\infty} (A-\lambda)f_\nu = g \ .$$

Hence it follows from (12.16) that $f_1, f_2, \dots$ is a Cauchy sequence in X and hence, by the completeness of X, convergent to some $f \in X$. In particular, this implies that $f \in D(\bar{A})$ as well as that

$$(\bar{A}-\lambda)f = g \ .$$

Hence it follows (12.17). Since $\bar{A}$ is symmetric, i.e., $\bar{A}^* \supset \bar{A}$, for the proof of self-adjointness of $\bar{A}$, it is sufficient to show that $D(\bar{A}^*) \subset D(\bar{A})$. For this, let $f \in D(\bar{A}^*)$. Then according to (12.17), there is $g \in D(\bar{A})$ such that

$$(\bar{A}-\lambda)g = (\bar{A}^*-\lambda)f \ .$$

Hence it follows by Theorem 12.4.7 that

$$f - g \in \ker(\bar{A}^*-\lambda) = [\mathrm{Ran}(\bar{A}+\lambda)]^{\perp} = \{0\}$$

and hence that $f = g \in D(\bar{A})$. $\square$

Corollary 12.4.10 (A characterization of self-adjointness). Let $(X, \langle | \rangle)$ be a complex Hilbert space and $A : D(A) \to X$ be a densely-defined, linear, symmetric operator in X. Then A is self-adjoint if and only if $\text{Ran}(A - i) = X$ and $\text{Ran}(A + i) = X$.

Proof. If A is self-adjoint, then A is essentially self-adjoint and closed. From Theorem 12.4.9, we conclude that $\text{Ran}(A - i)$ and $\text{Ran}(A + i)$ are dense in X. According the proof of Theorem 12.4.9, this implies that

$$\text{Ran}(A - \lambda) = \text{Ran}(\bar{A} - \lambda) = X$$

for $\lambda \in \{-i, i\}$. If $\text{Ran}(A - i) = X$ and $\text{Ran}(A + i) = X$, we conclude from Theorem 12.4.9 and the corresponding proof that A is essentially self-adjoint as well as that $A - i$ and $A + i$ are bijective. As a consequence, $(A - i)^{-1}, (A + i)^{-1} \in L(X, X)$. Further, for $f \in D(\bar{A})$, there is a sequence $f_0, f_1, \dots$ in $D(A)$ such that

$$\lim_{\nu \to \infty} f_\nu = f \ , \ \lim_{\nu \to \infty} A f_\nu = \bar{A} f \ .$$

Hence also

$$\lim_{\nu \to \infty} (A - i) f_\nu = (\bar{A} - i) f$$

and

$$f = \lim_{\nu \to \infty} f_\nu = (A - i)^{-1} (\bar{A} - i) f \in D(A).$$

Therefore, it follows that $\bar{A} = A$ and that A is self-adjoint. □

Theorem 12.4.11. (Relatively bounded perturbations of self-adjoint operators, Rellich-Kato theorem) Let $(X, \langle | \rangle)$ be a complex Hilbert space, A, B be densely-defined, linear, symmetric operators in X and $0 \leqslant a < 1$, $b \geqslant 0$ such that $D(B) \supset D(A)$ and

$$\|Bf\|^2 \leqslant a^2 \|Af\|^2 + b^2 \|f\|^2 \tag{12.18}$$

for every $f \in D(A)$. If A is in addition essentially self-adjoint, then $A + B$ is densely-defined, linear and essentially self-adjoint such that

$$\overline{A + B} = \bar{A} + \bar{B} \ .$$

Proof. For this, let A be in addition essentially self-adjoint. In first step, we show that $D(\bar{B}) \supset D(\bar{A})$ and that

$$\|\bar{B} f\|^2 \leqslant a^2 \|\bar{A} f\|^2 + b^2 \|f\|^2 \tag{12.19}$$

for every $f \in D(\bar{A})$. For this, let $f \in D(\bar{A})$ and $f_1, f_2, \dots$ be a sequence in $D(A)$ converging to f and such that $A f_1, A f_2, \dots$ converges to $\bar{A} f$. As a consequence of (12.18), $B f_1, B f_2, \dots$ is a Cauchy sequence in X and hence convergent to an element in X. Hence it follows that $f \in D(\bar{B})$,

$$\lim_{\nu \to \infty} B f_\nu = \bar{B} f$$

and (12.19). In particular, we note that this also implies that

$$\lim_{\nu\to\infty}(f_\nu, (A+B)f_\nu) = (f, (\bar{A}+\bar{B})f)$$

and hence that $f \in D(\overline{A+B})$ and

$$\overline{A+B}\, f = (\bar{A}+\bar{B})f \ .$$

As a consequence, $\overline{A+B}$ is a symmetric extension of $\bar{A}+\bar{B}$. Further, let $0 < \varepsilon < 1-a$ and

$$A_\varepsilon := \frac{a+\varepsilon}{b+\varepsilon}\,\bar{A} \ , \ B_\varepsilon := \frac{a+\varepsilon}{b+\varepsilon}\,\bar{B} \ .$$

Then $A_\varepsilon, B_\varepsilon$ are densely-defined, linear and symmetric operators in X. Further, A_ε is self-adjoint and

$$\begin{aligned}&\|B_\varepsilon f\|^2 \leqslant a^2\|A_\varepsilon f\|^2 + \frac{(a+\varepsilon)^2}{(b+\varepsilon)^2}\,b^2\|f\|^2 \leqslant (a+\varepsilon)^2\left[\|A_\varepsilon f\|^2 + \|f\|^2\right]\\ &= (a+\varepsilon)^2\|(A_\varepsilon-\lambda)f\|^2\end{aligned}$$

for every $f \in D(\bar{A})$, where $\lambda \in \{-i, i\}$. Since, according to the Corollary to Theorem 12.4.9, $A_\varepsilon - \lambda$ is bijective, from the latter it follows that

$$B_\varepsilon \circ (A_\varepsilon - \lambda)^{-1} \in L(X, X)$$

and that

$$\|B_\varepsilon \circ (A_\varepsilon - \lambda)^{-1}\| < 1 \ .$$

Therefore

$$1 + B_\varepsilon \circ (A_\varepsilon - \lambda)^{-1}$$

is bijective, and hence also

$$A_\varepsilon + B_\varepsilon - \lambda = [1 + B_\varepsilon \circ (A_\varepsilon - \lambda)^{-1}](A_\varepsilon - \lambda)$$

is bijective. According to Theorem 12.4.9, from this follows that $A_\varepsilon + B_\varepsilon$ and hence also $\bar{A}+\bar{B}$ are self-adjoint. Since, $\overline{A+B}$ is a symmetric extension of $\bar{A}+\bar{B}$, this implies that $A+B$ is essentially self-adjoint. □

12.5 Spectra of Linear Operators in Hilbert Spaces

Theorem 12.5.1. (A characterization of the spectra of closed linear operators) Let $(X, \langle\,|\,\rangle)$ be a complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and closed operator in X and $\lambda \in \mathbb{C}$. Then $\lambda \in \sigma(A)$ if and only if at least one of the following cases applies.

(i) There is a sequence $f_1, f_2, \ldots$ of unit vectors in $D(A)$ such that

$$\lim_{\nu\to\infty} (A-\lambda) f_\nu = 0 \ ,$$

(ii) λ^* is an eigenvalue of A^*.

Proof. "$\Leftarrow$": If there is a sequence $f_1, f_2, \ldots$ of unit vectors in $D(A)$ such that

$$\lim_{\nu\to\infty} (A-\lambda) f_\nu = 0 \ ,$$

then $A-\lambda$ is not bijective, and hence λ is a spectral value. Otherwise, it would follow from the boundedness of $(A-\lambda)^{-1}$ that

$$0 = (A-\lambda)^{-1} \lim_{\nu\to\infty} (A-\lambda) f_\nu = \lim_{\nu\to\infty} f_\nu$$

and hence also that

$$\lim_{\nu\to\infty} \|f_\nu\| = 0 \ . \lightning$$

If λ^* is an eigenvalue of A^* and $f \in D(A^*)$ a corresponding eigenvector, then

$$\langle f|(A-\lambda)g\rangle = \langle A^* f|g\rangle - \lambda \langle f|g\rangle = \langle \lambda^* f|g\rangle - \lambda \langle f|g\rangle = 0$$

for every $g \in D(A)$, and hence $A-\lambda$ is not surjective. "$\Rightarrow$": Suppose that there is no sequence $f_1, f_2, \ldots$ of unit vectors in $D(A)$ such that

$$\lim_{\nu\to\infty} (A-\lambda) f_\nu = 0 \ .$$

Then, there is $C > 0$ such that

$$\|(A-\lambda)f\| \geq C\|f\| \tag{12.20}$$

for every $f \in D(A)$. Otherwise, for every $\nu \in \mathbb{N}^*$, there is $f_\nu \in D(A) \setminus \{0\}$ such that

$$\|(A-\lambda)f_\nu\| < \frac{1}{\nu} \|f_\nu\|$$

and hence

$$\lim_{\nu\to\infty} (A-\lambda)\|f_\nu\|^{-1} f_\nu = 0 \ . \lightning$$

Hence $A-\lambda$ is injective and $\mathrm{Ran}(A-\lambda)$ is a closed subspace. The closedness of the latter space can be seen as follows. For g in the closure of $\mathrm{Ran}(A-\lambda)$, there is a sequence $f_0, f_1, \ldots$ in $D(A)$ such that

$$g = \lim_{\nu\to\infty} (A-\lambda) f_\nu \ .$$

As a consequence of (12.20), $f_0, f_1, \ldots$ is a Cauchy-sequence in X and hence convergent to some $f \in X$. Hence

$$\lim_{\nu\to\infty} (f_\nu, Af_\nu) = (f, g+\lambda f) \ .$$

Since A is closed, $f \in D(A)$ and $(A - \lambda)f = g$, i.e., $g \in \text{Ran}(A - \lambda)$. As a consequence of $\lambda \in \sigma(A)$ and the fact that $\text{Ran}(A - \lambda)$ is a closed subspace of X, it follows that $\text{Ran}(A - \lambda)$ is a proper closed subspace of X. Hence there is $f \in [\text{Ran}(A - \lambda)]^{\perp} \setminus \{0\}$. Therefore, $\langle f|\cdot\rangle$ vanishes on $\text{Ran}(A - \lambda)$ and

$$\langle \lambda^* f|g\rangle = \langle f|\lambda g\rangle + \langle f|(A - \lambda)g\rangle = \langle f|Ag\rangle$$

for every $g \in D(A)$. Hence $f \in D(A^*)$ and λ^* is an eigenvalue of A^*. $\square$

Theorem 12.5.2. Let $(X, \langle\,|\,\rangle)$ be a complex Hilbert space and $A : D(A) \to X$ a linear operator in X. Then the following is true.

(i) (**Toeplitz-Hausdorff**) The numerical range $N(A)$ of A, defined by

$$N(A) := \{\, \langle f|Af\rangle : f \in D(A) \wedge \|f\| = 1\} \ ,$$

is convex.

(ii) If in addition one of the following applies to A,

a) A is densely-defined, linear, closed and A^* has no eigenvalues,

b) A is densely-defined, linear and self-adjoint,

c) $A \in L(X, X)$,

then

$$\sigma(A) \subset \overline{N(A)} \ .$$

Proof. "(i)": For this, in a first step, let $f_1, f_2 \in D(A)$ be such that

$$\|f_1\| = \|f_2\| = 1 \ , \ \langle f_1|Af_1\rangle = 0 \ , \ \langle f_2|Af_2\rangle = 1 \ .$$

In the following, we show that for every $t \in (0, 1)$, there is $g \in D(A)$ such that $\|g\| = 1$ and $\langle g|Ag\rangle = t$. For this, we define the continuous map $g : \mathbb{R}^2 \to X$ by

$$g(\varphi, s) := f_1 + se^{i\varphi} f_2$$

for every $\varphi, s \in \mathbb{R}$. Note that $g(\varphi, s) \neq 0$ for all $\varphi, s \in \mathbb{R}$, since the assumption that there are $\varphi, s \in \mathbb{R}$ is such that $g(\varphi, s) = 0$ leads to

$$1 = \|f_1\| = \| - se^{i\varphi} f_2\| = |s| \ ,$$
$$0 = \langle f_1|Af_1\rangle = \langle -se^{i\varphi} f_2| - se^{i\varphi} Af_2\rangle = s^2 \ . \lightning$$

Further,

$$\langle g(\varphi, s)|Ag(\varphi, s)\rangle = \langle f_1 + se^{i\varphi} f_2|Af_1 + se^{i\varphi} Af_2\rangle = s^2 + f(\varphi)s \ ,$$
$$\|g(\varphi, s)\|^2 = \langle f_1 + se^{i\varphi} f_2|f_1 + se^{i\varphi} f_2\rangle = 1 + s^2$$
$$+ s \left[e^{i\varphi} \langle f_1|f_2\rangle + e^{-i\varphi} \langle f_2|f_1\rangle\right]$$

for all $\varphi, s \in \mathbb{R}$, where

$$f(\varphi) := e^{i\varphi} \langle f_1|Af_2\rangle + e^{-i\varphi} \langle f_2|Af_1\rangle$$

for every $\varphi \in \mathbb{R}$. Since f is continuous and $f(\pi) = -f(0)$, it follows by the intermediate value theorem the existence of $\varphi_0 \in [0, \pi]$ such that $f(\varphi_0)$ is real. Hence

$$F := \left(\mathbb{R} \to \mathbb{R}, s \mapsto \frac{\langle g(\varphi_0, s)|Ag(\varphi_0, s)\rangle}{\|g(\varphi_0, s)\|^2}\right)$$

is well-defined. Further, it follows that

$$F(0) = 0 \ , \ \lim_{s\to\infty} F(1) = 1 \ .$$

Hence it follows, by the intermediate theorem and for every $t \in (0, 1)$, the existence of $s \in (0, \infty)$ such that $F(s) = t$ and hence that

$$\langle \|g(\varphi_0, s)\|^{-1} g(\varphi_0, s)|A\|g(\varphi_0, s)\|^{-1} g(\varphi_0, s)\rangle = t \ .$$

For the final step, let $f_1, f_2 \in D(A)$ such that $\|f_1\| = \|f_2\| = 1$. If $\langle f_1|Af_1\rangle = \langle f_2|Af_2\rangle$, then

$$(1 - s) \langle f_1|Af_1\rangle + s \langle f_2|Af_2\rangle = \langle f_1|Af_1\rangle$$

for every $s \in [0, 1]$. If $\langle f_1|Af_1\rangle \neq \langle f_2|Af_2\rangle$, we define an auxiliary linear operator $\tilde{A} : D(A) \to X$ by

$$\tilde{A} := [\langle f_2|Af_2\rangle - \langle f_1|Af_1\rangle]^{-1}(A - \langle f_1|Af_1\rangle) \ .$$

As a consequence,

$$\langle f_1|\tilde{A}f_1\rangle = 0 \ , \ \langle f_2|\tilde{A}f_2\rangle = 1 \ .$$

Hence, according to the result from the first step, for every $t \in (0, 1)$, there is $g \in D(A)$ such that $\|g\| = 1$ and

$$t = \langle g|\tilde{A}g\rangle = [\langle f_2|Af_2\rangle - \langle f_1|Af_1\rangle]^{-1}(\langle g|Ag\rangle - \langle f_1|Af_1\rangle) \ .$$

This also implies that

$$\langle g|Ag\rangle = \langle f_1|Af_1\rangle + t\,[\langle f_2|Af_2\rangle - \langle f_1|Af_1\rangle] \ .$$

Hence it follows the convexity of $N(A)$. '(ii)': If A is also densely-defined, linear, closed and λ is an element of the spectrum of A, according to Lemma 12.5.1, we need to consider only two cases. In the first case, there is a sequence of unit vectors $f_1, f_2, \dots$ in $D(A)$ such that

$$\lim_{\nu\to\infty} (A - \lambda) f_\nu = 0 \ .$$

Hence it follows also that

$$0 = \lim_{\nu\to\infty} \langle f_\nu|(A - \lambda) f_\nu\rangle = -\lambda + \lim_{\nu\to\infty} \langle f_\nu|Af_\nu\rangle$$

and hence that $\lambda \in \overline{N(A)}$. In the second case, λ^* is an eigenvalue of A^*. If $f \in D(A^*)$ is a corresponding normed eigenvector of A^*, we conclude that

$$\langle f|Ag\rangle = \langle A^* f|g\rangle = \lambda \langle f|g\rangle$$

for every $g \in D(A)$. Hence if in addition A is self-adjoint and/or $A \in L(X, X)$, it follows that $f \in D(A)$ and hence that $\lambda = \langle f|Af\rangle \in N(A)$. □

Theorem 12.5.3. (A characterization of the spectra of self-adjoint linear operators) Let $(X, \langle\,|\,\rangle)$ be a complex Hilbert space and $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $\lambda \in \mathbb{R}$. Then

(i) $\sigma(A) \subset \mathbb{R}$,

(ii) $\lambda \in \sigma(A)$ if and only if there is a sequence $f_1, f_2, \dots$ of unit vectors in $D(A)$ such that
$$\lim_{\nu\to\infty} (A - \lambda) f_\nu = 0 \ .$$

Proof. "(i)": Since $A^* = A$,

$$(\langle f|Af\rangle)^* = \langle Af|f\rangle = \langle A^* f|f\rangle = \langle f|Af\rangle$$

for every $f \in D(A)$ and hence the numerical range of A and its closure are part of the real numbers. Hence it follows from Theorem 12.5.2 that $\sigma(A) \subset \mathbb{R}$.
"(ii)": Since $A^* = A$ and λ is real, the case that λ^* is an eigenvalue of A^*, implies that λ is an eigenvalue of A. If $f \in D(A)$ is a corresponding eigenvector of length 1, then
$$\lim_{\nu\to\infty} (A - \lambda) f_\nu = 0 \ ,$$
where $f_\nu := f$ for every $\nu \in \mathbb{N}^*$. Hence the statement of (ii) follows from Theorem 12.5.1. □

Theorem 12.5.4 (Spectral properties of densely-defined, linear and positive self-adjoint operators). Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space and $A : D(A) \to X$ a densely-defined, linear and symmetric operator in X. We call A positive, if
$$\langle f|Af\rangle \geqslant 0 \ ,$$
for every $f \in D(A)$. Then, the following holds:

(i) If A is positive, the $\bar{A}$ is positive.

(ii) If A is self-adjoint, then A is positive if and only if

$$\sigma(A) \subset [0, \infty) \ ,$$

where $\sigma(A)$ denotes the spectrum of A.

Proof. "Part (i):" If A is positive, then for $f \in D(\bar{A})$, there is a sequence $f_1, f_2, \dots$ such that

$$\lim_{\nu\to\infty} f_\nu = f \ , \text{ and } \lim_{\nu\to\infty} Af_\nu = \bar{A}f \ .$$

Since $\langle \, | \, \rangle : X^2 \to \mathbb{C}$, as a consequence of the sesquilinearity of $\langle \, | \, \rangle$ and the Cauchy-Schwartz inequality, is continuous, it follows that

$$\langle f|\bar{A}f\rangle = \lim_{\nu\to\infty} \langle f_\nu|Af_\nu\rangle \geqslant 0 \ .$$

Since $\bar{A}$ is also symmetric, we conclude that $\bar{A}$ is positive.
"Part (ii):" In the following, let A be in addition self-adjoint and $\sigma(A)$ denote the spectrum of A.
"$\Rightarrow$:" If A is positive, it follows for $\lambda < 0$ and $f \in D(A)$ that

$$\begin{aligned}
&\|(A-\lambda)f\|^2 = \langle (A-\lambda)f|(A-\lambda)f\rangle \\
&= \|Af\|^2 - \lambda\,\langle f|Af\rangle - \lambda\,\langle Af|f\rangle + \lambda^2 \cdot \|f\|^2 \\
&= \|Af\|^2 + (-2\lambda)\,\langle f|Af\rangle + \lambda^2 \cdot \|f\|^2 \geqslant \lambda^2 \cdot \|f\|^2
\end{aligned}$$

and hence that

$$\|(A-\lambda)\,f\| \geqslant |\lambda| \cdot \|f\| \ . \tag{12.21}$$

Therefore, $A - \lambda$ is injective. In addition, it follows that $\mathrm{Ran}(A-\lambda)$ is dense in X. This can be seen as follows. If $g \in [\mathrm{Ran}(A-\lambda)]^\perp$, then

$$\langle g|Af\rangle = \langle g|(A-\lambda)f\rangle + \langle \lambda g|f\rangle = \langle \lambda g|f\rangle \ ,$$

for every $f \in D(A)$. Hence $g \in D(A^*) = D(A)$, and

$$Ag = A^*g = \lambda g \ .$$

Since $A - \lambda$ is injective, we conclude that $g = 0$. As a consequence,

$$\overline{\mathrm{Ran}(A-\lambda)} = [\mathrm{Ran}(A-\lambda)]^{\perp\perp} = \{0\}^\perp = X \ ,$$

i.e., $\mathrm{Ran}(A-\lambda)$ is dense in X. In the following, we are going to show that $A-\lambda$ is also surjective. For the proof, we note that, since $A - \lambda$ is an injective linear operator with a dense range satisfying (12.21),

$$(A-\lambda)^{-1} : \mathrm{Ran}(A-\lambda) \to X$$

is a densely-defined, bounded linear map. Hence there is a unique $B \in L(X, X)$ such that $B \supset (A-\lambda)^{-1}$. Since $\mathrm{Ran}(A-\lambda)$ is dense in X, for $g \in X$ there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

$$\lim_{\nu\to\infty} (A-\lambda)f_\nu = g \ .$$

Therefore,

$$Bg = B \lim_{\nu\to\infty} (A-\lambda)f_\nu = \lim_{\nu\to\infty} B(A-\lambda)f_\nu = \lim_{\nu\to\infty} f_\nu \ .$$

Further, it follows that

$$g = \lim_{\nu\to\infty} (A-\lambda) f_\nu = \lim_{\nu\to\infty} A f_\nu - \lambda B g$$

and hence that

$$\lim_{\nu\to\infty} A f_\nu = g + \lambda B g \ .$$

Since A is closed, we conclude that $Bg \in D(A)$, $ABg = g + \lambda Bg$ and hence that

$$(A-\lambda)Bg = g \ .$$

As a consequence, $A - \lambda$ is surjective, hence also bijective and $\lambda \notin \sigma(A)$. We conclude that $\sigma(A) \subset [0,\infty)$.
"$\Rightarrow$:" If $\sigma(A) \subset [0,\infty)$, we conclude as follows. If $f \in D(A)$ and ψ_f the corresponding spectral measure, then $(-\infty, 0)$ is a ψ_f-zero set. Hence it follows from Theorem 12.6.2 that

$$\langle f|Af\rangle = \int_{\mathbb{R}} \mathrm{id}_{\mathbb{R}}\, d\psi_f = \int_{\mathbb{R}} \chi_{[0,\infty)}\, \mathrm{id}_{\mathbb{R}}\, d\psi_f \geqslant 0 \ .$$

Therefore, A is positive. $\square$

Corollary 12.5.5 (Spectral properties of densely-defined, linear and semi-bounded self-adjoint operators). Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space and $A : D(A) \to X$ a densely-defined, linear and symmetric operator in X. We call A semi-bounded (from below) with lower bound $\mu \in \mathbb{R}$ if

$$\langle f|Af\rangle \geqslant \mu\, \|f\|^2 \ ,$$

for every $f \in D(A)$. Then, the following holds:

(i) If A is semi-bounded with lower bound $\mu \in \mathbb{R}$, then $\bar{A}$ is semi-bounded with lower bound μ.

(ii) If A is self-adjoint, then A is semi-bounded with lower bound $\mu \in \mathbb{R}$ if and only if

$$\sigma(A) \subset [\mu, \infty) \ ,$$

where $\sigma(A)$ denotes the spectrum of A.

Proof. "Part (i):" If A is semi-bounded with lower bound $\mu \in \mathbb{R}$, then for $f \in D(\bar{A}\,)$, there is a sequence $f_1, f_2, \dots$ such that

$$\lim_{\nu\to\infty} f_\nu = f \ , \text{ and } \lim_{\nu\to\infty} A f_\nu = \bar{A} f \ .$$

Since $\langle\,|\,\rangle : X^2 \to \mathbb{C}$, as a consequence of the sesquilinearity of $\langle\,|\,\rangle$ and the Cauchy-Schwartz inequality, is continuous, it follows that

$$\langle f|\bar{A}f\rangle = \lim_{\nu\to\infty} \langle f_\nu|Af_\nu\rangle \geqslant \lim_{\nu\to\infty} \mu\, \|f_\nu\|^2 = \mu\, \|f\|^2 \ .$$

Since $\bar{A}$ is also symmetric, we conclude that $\bar{A}$ is semi-bounded with lower bound μ.
"Part (ii):" In the following, let A be in addition self-adjoint and $\sigma(A)$ denote the spectrum of A.
"$\Rightarrow$:" If A is semi-bounded with lower bound $\mu \in \mathbb{R}$, then $A - \mu$ is a densely-defined, linear and positive self-adjoint operator in X, and hence according to Theorem 12.5.4

$$\sigma(A) - \mu = \sigma(A - \mu) \subset [0, \infty) \ ,$$

where $\sigma(A - \mu)$ denotes the spectrum of $A - \mu$. The latter implies that $\sigma(A) \subset [\mu, \infty)$.
"$\Leftarrow$:" If $\sigma(A) \subset [\mu, \infty)$, then, $A - \mu$ is a densely-defined, linear and self-adjoint operator in X such

$$\sigma(A - \mu) = \sigma(A) - \mu \subset [0, \infty) \ ,$$

where $\sigma(A - \mu)$ denotes the spectrum of $A - \mu$, and hence according to Theorem 12.5.4, $A - \mu$ is in particular positive. The latter implies that A is semi-bounded with lower bound μ. □

12.5.1 Compact Operators

Definition 12.5.6. (Compact operators) Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. We call $A \in L(X, X)$ compact if for every bounded sequence $f_1, f_2, \dots$ in X, the corresponding sequence $Af_1, Af_2, \dots$ has a convergent subsequence.

Corollary 12.5.7. Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and A an element of $L(X, X)$ with a finite dimensional range. Then A is compact.

Proof. The statement is a simple consequence of the Bolzano-Weierstrass theorem. □

12.5.2 Essential Spectrum

Definition 12.5.8. Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space and $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X. We define the essential spectrum $\sigma_e(A)$ of A as

$$\sigma_e(A) = \bigcap_{K \in L(X,X), K \text{ self-adjoint and compact}} \sigma(A + K) \ \left(\subset \sigma(A) \right) \ .$$

Theorem 12.5.9. (Characterization of the essential spectrum, I) Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $\lambda \in \mathbb{R}$. Then $\lambda \in \sigma_e(A)$ if and only if there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

a) $\|f_\nu\| = 1$ for every $\nu \in \mathbb{N}^*$,

b) $f_1, f_2, \dots$ has no convergent subsequence,

c) and $\lim_{\nu\to\infty}(A-\lambda)f_\nu = 0$.

Proof. We note that, as a consequence of Theorem 12.4.7,

$$\ker(A-\lambda) = [\text{Ran}(A-\lambda)]^\perp \ , \ [\ker(A-\lambda)]^\perp = \overline{\text{Ran}(A-\lambda)} \ .$$

In particular, $\ker(A-\lambda)$ is a closed subspace of X.
"$\Leftarrow$": Let $f_1, f_2, \dots$ be a sequence in $D(A)$ with properties a)-c). In the following, we lead the assumption that $\lambda \notin \sigma_e(A)$ to a contradiction. If $\lambda \notin \sigma_e(A)$, there is a compact operator $K \in L(X,X)$ such that $A + K - \lambda$ is bijective. In particular, this implies the existence of $C > 0$ such that

$$\|f\| \leqslant C\|(A+K-\lambda)f\|$$

for every $f \in D(A)$. Since K is compact, there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that $Kf_{\nu_1}, Kf_{\nu_2}, \dots$ is convergent. Hence,

$$\begin{aligned} \|\, f_{\nu_{\mu_1}} - f_{\nu_{\mu_2}} \| &\leqslant C\, \|(A+K-\lambda)(f_{\nu_{\mu_1}} - f_{\nu_{\mu_2}})\| \\ &\leqslant C\, \|(A-\lambda)f_{\nu_{\mu_1}}\| + C\, \|(A-\lambda)f_{\nu_{\mu_2}}\| + C\, \|Kf_{\nu_{\mu_1}} - Kf_{\nu_{\mu_2}})\| \end{aligned}$$

for all $\mu_1, \mu_2 \in \mathbb{N}^*$. As a consequence, $f_{\nu_1}, f_{\nu_2}, \dots$ is a Cauchy-sequence in X and hence convergent. The latter is in contradiction to b).$\lightning$ Hence it follows that $\lambda \in \sigma_e(A)$.
"$\Rightarrow$": If $\lambda \in \sigma_e(A)(\subset \sigma(A))$, $A - \lambda$ is not bijective. We consider two cases. If $\ker(A-\lambda)$ is infinite dimensional, there is an orthonormal sequence $f_1, f_2, \dots$ in $\ker(A-\lambda)$. Since

$$\|f_\mu - f_\nu\|^2 = 2$$

for different $\mu, \nu \in \mathbb{N}^*$, every subsequence of such sequence is not Cauchy and hence not convergent. As a consequence, any orthonormal sequence in $\ker(A-\lambda)$ satisfies a)-c). If $\ker(A-\lambda)$ is finite dimensional, there is a sequence $f_1, f_2, \dots$ such that

$$f_\nu \in [\ker(A-\lambda)]^\perp \cap D(A) \ , \ \|f_\nu\| = 1 \ , \ \lim_{\nu\to\infty}(A-\lambda)f_\nu = 0 \qquad (12.22)$$

for every $\nu \in \mathbb{N}^*$. For the proof, let $P \in L(X,X)$ be the orthogonal projection onto $\ker(A-\lambda)$. According to Corollary 12.5.7, P is in particular compact. If there is no $f_1, f_2, \dots$ satisfying (12.22) for every $\nu \in \mathbb{N}^*$, then there is $C \geq 0$ such that

$$\|f\| \leqslant C\|(A-\lambda)f\|$$

for every $f \in [\ker(A-\lambda)]^\perp \cap D(A)$. Otherwise, for every $\nu \in \mathbb{N}^*$, there is $f_\nu \in ([\ker(A-\lambda)]^\perp \cap D(A)) \setminus \{0\}$ such that

$$\|(A-\lambda)f_\nu\| < \frac{1}{\nu}\,\|f_\nu\|$$

and hence

$$\lim_{\nu\to\infty}(A-\lambda)\|f_\nu\|^{-1}f_\nu = 0 \;.\lightning$$

Hence it follows for $f \in D(A)$ that

$$\begin{aligned}
&\|f\|^2 = \|(1-P+P)f\|^2 = \|(1-P)f\|^2 + \|Pf\|^2 \\
&\leqslant C^2\|(A-\lambda)(1-P)f\|^2 + \|Pf\|^2 = C^2\|(1-P)(A-\lambda)f\|^2 + \|Pf\|^2 \\
&\leqslant (1+C)^2[\|(1-P)(A-\lambda)f\|^2 + \|Pf\|^2] \\
&= (1+C)^2\|(1-P)(A-\lambda)f \; + Pf\|^2 \\
&= (1+C)^2\|(A-\lambda)(1-P)f + Pf\|^2 \\
&= (1+C)^2\|(A-\lambda)(P+1-P)f + Pf\|^2 \\
&= (1+C)^2\|(A+P-\lambda)f\|^2 \;. \qquad (12.23)
\end{aligned}$$

[1] Hence $A+P-\lambda$ is injective and $\operatorname{Ran}(A+P-\lambda)$ is a closed subspace. The closedness of the latter space can be seen as follows. For g in the closure of $\operatorname{Ran}(A+P-\lambda)$, there is a sequence $f_0, f_1, \dots$ in $D(A)$ such that

$$g = \lim_{\nu\to\infty}(A+P-\lambda)f_\nu \;.$$

As a consequence of (12.23), $f_0, f_1, \dots$ is a Cauchy-sequence in X and hence convergent to some $f \in X$. Hence

$$\lim_{\nu\to\infty}(f_\nu, (A+P)f_\nu) = (f, g+\lambda f) \;.$$

Since $A+P$ is closed, $f \in D(A)$ and $(A+P-\lambda)f = g$, i.e., $g \in \operatorname{Ran}(A+P-\lambda)$. Further, from Theorem 12.4.7, we conclude that

$$\{0\} = \ker(A+P-\lambda) = [\operatorname{Ran}(A+P-\lambda)]^\perp$$

and hence that

$$X = \overline{\operatorname{Ran}(A+P-\lambda)} = \operatorname{Ran}(A+P-\lambda) \;.$$

As a consequence, $A+P-\lambda$ is bijective and therefore $\lambda \notin \sigma_e(A)$.$\lightning$ Hence it follows the existence of a sequence $f_1, f_2, \dots$ satisfying (12.22) for every $\nu \in \mathbb{N}^*$. Such sequence $f_1, f_2, \dots$ has no convergent subsequence and thus satisfies a)-c). Otherwise, there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that $f_{\nu_1}, f_{\nu_2}, \dots$ is convergent to some $f \in X$. In particular, as a consequence of the closedness of $[\ker(A-\lambda)]^\perp$, $f \in [\ker(A-\lambda)]^\perp$. Since

$$\lim_{\mu\to\infty}(A-\lambda)f_{\nu_\mu} = 0$$

[1] Here it has been used that $P \circ (A-\lambda) \subset (A-\lambda)\circ P$. The latter is a consequence of the spectral theorem for densely-defined, linear and self-adjoint operators in Hilbert spaces.

and $A - \lambda$ is closed, this implies that $f \in \ker(A - \lambda) \cap [\ker(A - \lambda)]^{\perp}$ and hence that $f = 0$. Finally, we arrive at the contradiction that

$$0 = \|f\| = \| \lim_{\mu \to \infty} f_{\nu_\mu} \| = \lim_{\mu \to \infty} \|f_{\nu_\mu}\| = 1 \ . \lightning$$

$\square$

Theorem 12.5.10 (Accumulation points of the spectrum are part of the essential spectrum). Let $(X, \langle | \rangle)$ be a non-trivial Hilbert space and $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X. If $\lambda \in \sigma(A)$ is not an isolated point of $\sigma(A)$, then $\lambda \in \sigma_e(A)$.

Proof. If $\lambda \in \sigma(A)$ is not an isolated point of $\sigma(A)$, then there is a sequence $\lambda_1, \lambda_2, \dots$ in $\sigma(A) \setminus \{\lambda\}$ such that $\lim_{\nu \to \infty} \lambda_\nu = \lambda$. Further, since $\lambda_\nu \in \sigma(A)$, for every $\nu \in \mathbb{N}^*$, there is f_ν such that $\|f_\nu\| = 1$ and

$$\|(A - \lambda_\nu) f_\nu\| < |\lambda_\nu - \lambda| / \nu \ .$$

This implies that

$$\lim_{\nu \to \infty} (A - \lambda_\nu) f_\nu = 0 \ .$$

We claim that there is no convergent subsequence of $f_1, f_2, \dots$. Otherwise, there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that $f_{\nu_1}, f_{\nu_2}, \dots$ is convergent to some $f \in X$. In particular, since

$$\lim_{\mu \to \infty} (A - \lambda) f_{\nu_\mu} = 0$$

and $A - \lambda$ is closed, we conclude that $f \in \ker(A - \lambda)$ and that

$$\|f\| = \| \lim_{\mu \to \infty} f_{\nu_\mu} \| = \lim_{\mu \to \infty} \|f_{\nu_\mu}\| = 1 \ .$$

On the other hand,

$$\langle (A - \lambda_{\nu_\mu}) f_{\nu_\mu} | f \rangle = \langle f_{\nu_\mu} | (A - \lambda_{\nu_\mu}) f \rangle = (\lambda - \lambda_{\nu_\mu}) \, \langle f_{\nu_\mu} | f \rangle$$

and hence

$$|\lambda - \lambda_{\nu_\mu}| \, | \, \langle f_{\nu_\mu} | f \rangle \, | < |\lambda_{\nu_\mu} - \lambda| / \nu_\mu$$

as well as

$$| \, \langle f_{\nu_\mu} | f \rangle \, | < 1/\nu_\mu$$

for every $\mu \in \mathbb{N}^*$. As a consequence, we arrive at the contradiction

$$0 = \lim_{\mu \to \infty} \langle f_{\nu_\mu} | f \rangle = \langle f | f \rangle = \|f\|^2 = 1 \ . \lightning$$

$\square$

12.5.3 Weak Convergence

Definition 12.5.11. (**Weak convergence**) Let $(X, \langle\,|\,\rangle)$ be a Pre-Hilbert space over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. A sequence $f_1, f_2, \dots$ in X is called weakly convergent to $f \in X$ if

$$\lim_{\nu\to\infty} \langle g|f_\nu\rangle = \langle g|f\rangle$$

for every $g \in X$.

Theorem 12.5.12. (**Uniqueness of the limit of weakly convergent sequences**) Let $(X, \langle\,|\,\rangle)$ be a Pre-Hilbert space over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $f_1, f_2, \dots$ a sequence in X that is weakly convergent to $f \in X$ and $g \in X$. Then, $g = f$.

Proof. Since $f_1, f_2, \dots$ is weakly convergent to $f \in X$ and $g \in X$, it follows that

$$\lim_{\nu\to\infty} \langle f - g|f_\nu\rangle = \langle f - g|f\rangle = \langle f - g|g\rangle$$

and hence that $\|f - g\|^2 = 0$. The latter implies that $g = f$. $\square$

Theorem 12.5.13. (**Convergence implies weak convergence**) Let $(X, \langle\,|\,\rangle)$ be a Pre-Hilbert space over $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $f_1, f_2, \dots$ a sequence in X that is convergent to $f \in X$. Then $f_1, f_2, \dots$ is also weakly convergent to f.

Proof. If $f_1, f_2, \dots$ in X is convergent to $f \in X$ and $g \in X$, then $\langle g|\cdot\rangle \in L(X, \mathbb{K})$ and hence

$$\langle g|f\rangle = \langle g|\lim_{\nu\to\infty} f_\nu\rangle = \lim_{\nu\to\infty} \langle g|f_\nu\rangle \ .$$

$\square$

Theorem 12.5.14. (**Weak convergence does not necessarily imply convergence**) Let $(X, \langle\,|\,\rangle)$ be a Pre-Hilbert space and $f_1, f_2, \dots$ an orthonormal sequence. Then $f_1, f_2, \dots$ is weakly convergent to 0, but not convergent.

Proof. First, we note that

$$\|f_\mu - f_\nu\|^2 = \langle f_\mu - f_\nu|f_\mu - f_\nu\rangle = \|f_\mu\|^2 + \|f_\nu\|^2 = 1 + 1 = 2$$

for $\mu, \nu \in \mathbb{N}^*$ such that $\mu \neq \nu$. Hence $f_1, f_2, \dots$ is no Cauchy-sequence in X and therefore also not convergent. On the other hand, for $g \in X$, according to Theorem 12.3.17 (ii)b)[1],

$$M_g := \{\nu \in \mathbb{N}^* : \langle g|f_\nu\rangle \neq 0\}$$

at most countable and the corresponding sequence $(|\langle g|f_\nu\rangle|^2)_{\nu\in M_g}$ is summable such that

$$\sum_{\nu\in M_g} |\langle g|f_\nu\rangle|^2 \leqslant \|g\|^2 \ .$$

[1] Note that the completeness of $(X, \langle\,|\,\rangle)$ does not enter the proof of that statement.

In particular, this implies that

$$\lim_{\nu \to \infty} \langle g | f_\nu \rangle = 0$$

and hence that $f_1, f_2, \dots$ is weakly convergent to 0. □

Theorem 12.5.15. Let X be a finite dimensional vector space and $\langle \, | \, \rangle$ a scalar product on X. Further, let $f_1, f_2, \dots$ be a sequence in X that is weakly convergent to $f \in X$. Then $f_1, f_2, \dots$ is also convergent to f.

Proof. If $X = \{0\}$, the statement is trivially satisfied. In the following, we consider the case that X is non-trivial. According to linear algebra, there is an orthonormal basis $g_1, \dots, g_n$, where $n \in \mathbb{N}^*$, for X. As a consequence, the representation

$$g = \sum_{k=1}^{n} \langle g_k | g \rangle \cdot g_k$$

is valid for every $g \in X$. Hence, we conclude that

$$\|f_\nu - f\|^2 = \left\| \sum_{k=1}^{n} \langle g_k | f_\nu - f \rangle \cdot g_k \right\|^2 = \sum_{k=1}^{n} | \langle g_k | f_\nu - f \rangle |^2$$
$$= \sum_{k=1}^{n} | \langle g_k | f_\nu \rangle - \langle g_k | f \rangle |^2$$

and therefore the convergence of $f_1, f_2, \dots$ to f. □

Theorem 12.5.16. Let $(X, \langle \, | \, \rangle)$ be a Hilbert space and $f_1, f_2, \dots$ a bounded sequence in X. Then, there is weakly convergent subsequence of $f_1, f_2, \dots$.

Proof. Let $f_1, f_2, \dots$ be a bounded sequence in X and $C > 0$ such that $\|f_k\| \leqslant C$ for every $k \in \mathbb{N}^*$. For every $k \in \mathbb{N}^*$, the corresponding sequence $\langle f_k | f_1 \rangle, \langle f_k | f_2 \rangle, \dots$ is bounded. Hence according to the Bolzano-Weierstrass theorem for the real numbers, there is an infinite subset $\mathbb{N}_1$ of $\mathbb{N}^*$, along with a strictly increasing bijection $\nu_1 : \mathbb{N}^* \to \mathbb{N}_1$ such that

$$\langle f_1 | f_{\nu_1(1)} \rangle, \langle f_1 | f_{\nu_1(2)} \rangle, \dots$$

is convergent. We note that

$$\nu_1(k) \geqslant k$$

for every $k \in \mathbb{N}^*$. Continuing this reasoning sucessively, we arrive at a sequence $\mathbb{N}_1, \mathbb{N}_2, \dots$ of infinite subsets of $\mathbb{N}^*$ such that

$$\mathbb{N}^* \supset \mathbb{N}_1 \supset \mathbb{N}_2 \supset \dots$$

along with strictly increasing bijections $\nu_k : \mathbb{N}^* \to \mathbb{N}_k$, where $k \in \mathbb{N}^*$, such that

$$\langle f_l | f_{\nu_k(1)} \rangle, \langle f_l | f_{\nu_k(2)} \rangle, \dots$$

is convergent for every $l \in \mathbb{N}^*$ satisfying $l \leqslant k$. In particular,

$$\nu_{l+1}(k) \geqslant \nu_l(k) \tag{12.24}$$

for all $l, k \in \mathbb{N}^*$. The latter implies that

$$\nu_{k+1}(k+1) > \nu_{k+1}(k) \geqslant \nu_k(k)$$

for every $k \in \mathbb{N}^*$ and hence that the sequence $\nu_1(1), \nu_2(2), \dots$ is strictly increasing. Also, (12.24) implies that

$$\nu_{l+k}(l+k) \geqslant \nu_l(l+k) > \nu_l(k) \tag{12.25}$$

for all $l, k \in \mathbb{N}^*$. We claim that

$$\langle f_l | f_{\nu_1(1)} \rangle , \langle f_l | f_{\nu_2(2)} \rangle , \dots$$

is convergent for every $l \in \mathbb{N}^*$. For the proof, let $\varepsilon > 0$ and $l \in \mathbb{N}^*$. Since, in particular,

$$\langle f_l | f_{\nu_l(1)} \rangle , \langle f_l | f_{\nu_l(2)} \rangle , \dots$$

is a Cauchy-sequence in $\mathbb{K}$, there is $N \in \mathbb{N}^*$ such that

$$| \langle f_l | f_{\nu_l(k)} \rangle - \langle f_l | f_{\nu_l(k')} \rangle | < \varepsilon$$

for all $k, k' \in \mathbb{N}^*$ satisfying $k \geqslant N$ and $k' \geqslant N$. Hence it follows by (12.25) that

$$| \langle f_l | f_{\nu_{l+k}(l+k)} \rangle - \langle f_l | f_{\nu_{l+k'}(l+k')} \rangle | < \varepsilon$$

for all $k, k' \in \mathbb{N}^*$ satisfying $k \geqslant N$ and $k' \geqslant N$. As a consequence,

$$\langle f_l | f_{\nu_1(1)} \rangle , \langle f_l | f_{\nu_2(2)} \rangle , \dots$$

is a Cauchy-sequence in $\mathbb{K}$ and hence convergent. In the following, we define $g_k := f_{\nu_k(k)}$ for every $k \in \mathbb{N}^*$,

$$Y := \text{Span}(\{f_1, f_2, \dots\}) \ .$$

Then $\langle f | g_1 \rangle , \langle f | g_2 \rangle , \dots$ is convergent for every $f \in Y$. The same is true also for every $f \in \bar{Y}$. For the proof, let $f \in \bar{Y}$, $\varepsilon > 0$ and $h \in Y$ such that $\|h - f\| < \varepsilon/(4C)$. Hence if $N \in \mathbb{N}^*$ is such

$$| \langle h | g_k \rangle - \langle h | g_l \rangle | < \frac{\varepsilon}{2}$$

for every $k, l \in \mathbb{N}^*$ satisfying $k \geqslant N$ and $l \geqslant N$, then it follows for such k and l that

$$\begin{aligned} &| \langle f | g_k \rangle - \langle f | g_l \rangle | = | \langle f | g_k - g_l \rangle | \leqslant | \langle f - h | g_k - g_l \rangle | + | \langle h | g_k - g_l \rangle | \\ &\leqslant 2C \|f - h\| + | \langle h | g_k - g_l \rangle | < \varepsilon \ . \end{aligned}$$

Hence

$$\langle f|g_1\rangle\,, \langle f|g_2\rangle\,, \dots$$

is a Cauchy-sequence in $\mathbb{K}$ and hence convergent. Further, it follows for $f \in \bar{Y}^{\perp}$ that

$$\langle f|g_1\rangle\,, \langle f|g_2\rangle\,, \dots$$

is convergent to zero. Finally, since for every $f \in X$ there is a uniquely determined pair $(h_1, h_2) \in \bar{Y} \times \bar{Y}^{\perp}$ such that $f = h_1 + h_2$, we conclude that $g_1, g_2, \dots$ is weakly convergent. $\square$

Theorem 12.5.17. (**A further characterization of the essential spectrum**) Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $\lambda \in \mathbb{R}$. Then $\lambda \in \sigma_e(A)$ if and only if there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

a) $\|f_\nu\| = 1$ for every $\nu \in \mathbb{N}^*$,

b) $f_1, f_2, \dots$ is weakly convergent to 0,

c) and $\lim_{\nu\to\infty}(A - \lambda)f_\nu = 0$.

Proof. "$\Rightarrow$": Let $f_1, f_2, \dots$ be a sequence in $D(A)$ with properties a)-c). Then, there is no convergent subsequence of $f_1, f_2, \dots$. Otherwise, there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that the sequence $f_{\nu_1}, f_{\nu_2}, \dots$ is convergent to some $f \in X$. As a consequence of property b), $f_{\nu_1}, f_{\nu_2}, \dots$ is weakly convergent to 0. Hence,

$$0 = \langle f|0\rangle = \lim_{\mu\to\infty} \langle f|f_{\nu_\mu}\rangle = \|f\|^2 \ ,$$

whereas from property a), we conclude that

$$\|f\| = \|\lim_{\mu\to\infty} f_{\nu_\mu}\| = \lim_{\mu\to\infty} \|f_{\nu_\mu}\| = 1 \ . \lightning$$

Hence, we conclude from Theorem 12.5.9 that $\lambda \in \sigma_e(A)$.
"$\Leftarrow$": Let $\lambda \in \sigma_e(A)$. According, to Theorem 12.5.9, there is a sequence of unit vectors $f_1, f_2, \dots$ in $D(A)$ which has no convergent subsequence and is such that

$$\lim_{\nu\to\infty} (A - \lambda)f_\nu = 0 \ .$$

As a consequence of Theorem 12.5.16, without restriction of generality, we can assume that $f_1, f_2, \dots$ is weakly convergent to some $f \in X$. Also, we note that, since there is no convergent subsequence of $f_1, f_2, \dots$, the value f can be assumed only finitely many times. Hence, without restriction of generality, we can assume that the sequence $f_1, f_2, \dots$ does not assume the value f. As consequence, using the fact that there is no convergent subsequence of $f_1, f_2, \dots$, we conclude that there is $\varepsilon > 0$ such that

$$\|f_\nu - f\| \geqslant \varepsilon \tag{12.26}$$

for every $\nu \in \mathbb{N}^*$. Further,

$$\langle f|(A-\lambda)g\rangle = \lim_{\nu\to\infty} \langle f_\nu|(A-\lambda)g\rangle = \lim_{\nu\to\infty} \langle (A-\lambda)f_\nu|g\rangle = 0$$

for every $g \in D(A)$. Hence, $f \in D(A)$ and

$$(A-\lambda)f = 0 \ .$$

For every $\nu \in \mathbb{N}^*$, we define,

$$g_\nu := \|f_\nu - f\|^{-1}.(f_\nu - f) \ .$$

Then $g_1, g_2, \dots$ is a sequence in $D(A)$ that is weakly convergent to 0, $\|g_\nu\| = 1$ for every $\nu \in \mathbb{N}^*$ and

$$\lim_{\nu\to\infty} (A-\lambda)g_\nu = \lim_{\nu\to\infty} \|f_\nu - f\|^{-1}.(A-\lambda)f_\nu = 0 \ .$$

$\square$

Theorem 12.5.18. Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X. We define, the discrete spectrum $\sigma_d(A)$ of A by

$$\sigma_d(A) := \{\lambda \in \sigma(A) : \lambda \text{ is an isolated point of } \sigma(A) \\ \text{as well as an eigenvalue of } A \text{ of finite multiplicity}\} \ .$$

Then

$$\sigma(A) = \sigma_e(A) \mathbin{\dot\cup} \sigma_d(A) \ .$$

Proof. In first step, we prove that

$$\sigma(A) \backslash \sigma_e(A) \subset \sigma_d(A)$$

and hence that

$$\sigma(A) = \sigma_e(A) \cup \sigma_d(A) \ .$$

If $\lambda \in \sigma(A)\backslash\sigma_e(A)$, then λ is an isolated point of $\sigma(A)$, since otherwise, according to Theorem 12.5.10, $\lambda \in \sigma_e(A)$. Also, there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that $\|f_\nu\| = 1$ for every $\nu \in \mathbb{N}^*$ and such that

$$\lim_{\nu\to\infty} (A-\lambda)f_\nu = 0 \ .$$

Since $\lambda \notin \sigma_e(A)$, this sequence has a convergent subsequence, $f_{\nu_1}, f_{\nu_2}, \dots$, where $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ is strictly monotonically increasing, that is convergent to some $f \in X$. Since A is closed, $f \in \ker(A-\lambda)$. Moreover,

$$\|f\| = \|\lim_{\mu\to\infty} f_{\nu_\mu}\| = \lim_{\mu\to\infty} \|f_{\nu_\mu}\| = 1 \ .$$

Hence $f \neq 0$ and λ is an eigenvalue of A. In addition, $\ker(A-\lambda)$ is finite dimensional. This can be seen as follows. If $\ker(A-\lambda)$ is infinite dimensional, there is a orthonormal sequence $f_1, f_2, \dots$ of elements $\ker(A-\lambda)$. As consequence of Theorem 12.5.16, we can assume that this sequence is weakly convergent to some $f \in X$. Also, according to Theorem 12.3.18, there is an extension of the orthonormal system $M_0 := \{f_1, f_2, \dots\}$ to a Hilbert basis M of X. Then

$$\lim_{\nu\to\infty} \langle g|f_\nu\rangle = \langle g|f\rangle = 0 \ ,$$

for every $g \in M$ and hence $f = 0$. Since

$$\lim_{\nu\to\infty} (A-\lambda)f_\nu = 0 \ ,$$

it follows from Theorem 12.5.17 that $\lambda \in \sigma_e(A)$.↯ Hence $\ker(A-\lambda)$ is finite dimensional. Finally, we prove that

$$\sigma_e(A) \cap \sigma_d(A) = \phi \ . \tag{12.27}$$

For this purpose, let $\lambda \in \sigma_e(A) \cap \sigma_d(A)$, then

$$\operatorname{Ran}\left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A)$$

is infinite dimensional, for every $\varepsilon > 0$. Otherwise, there is $\varepsilon > 0$ such that

$$\operatorname{Ran}\left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A)$$

is finite dimensional. Hence, it follows from Corollary 12.5.7 that

$$\left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A)$$

is compact. If $f_1, f_2, \dots$ is a sequence of unit vectors in $D(A)$ that is weakly convergent to 0 and such that

$$\lim_{\nu\to\infty} (A-\lambda)f_\nu = 0 \ ,$$

then

$$\lim_{\nu\to\infty} \left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A)f_\nu = 0$$

leading to

$$\lim_{\nu\to\infty} \|(A-\lambda)f_\nu\|^2 = 0 \tag{12.28}$$

and

$$\lim_{\nu\to\infty} \left\|\left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A)f_\nu\right\|^2 = 0 \ .$$

As consequence,

$$\|(A-\lambda)f_\nu\|^2 = \int_{\sigma(A)} \left(\mathrm{id}_{\sigma(A)} - \lambda\right)^2 d\psi_{f_\nu}$$

$$
\begin{aligned}
&\geqslant \int_{\sigma(A)\cap(\mathbb{R}\setminus U_\varepsilon(\lambda))} \left(\mathrm{id}_{\sigma(A)} - \lambda\right)^2 d\psi_{f_\nu} \\
&\geqslant \varepsilon^2 \int_{\sigma(A)\cap(\mathbb{R}\setminus U_\varepsilon(\lambda))} d\psi_{f_\nu} = \varepsilon^2 \left[\|f_\nu\|^2 - \int_{\sigma(A)\cap U_\varepsilon(\lambda)} d\psi_{f_\nu}\right] \\
&= \varepsilon^2 \left[1 - \left\|\left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A) f_\nu\right\|^2\right] ,
\end{aligned}
$$

where ψ_{f_ν} denotes the spectral measure that is associated with A and f_ν. Hence, we arrive at a contradiction to (12.28). Further, since $\lambda \in \sigma(A)$ is also an isolated point of $\sigma(A)$, there is $\varepsilon > 0$ such that

$$U_\varepsilon(\lambda) \cap \sigma(A) = \{\lambda\} .$$

Hence,

$$P_\lambda := \left(\chi_{\{\lambda\}}\big|_{\sigma(A)}\right)(A)$$

is the orthogonal projection onto $\ker(A - \lambda)$, i.e.,

$$\mathrm{Ran}\left(\chi_{U_\varepsilon(\lambda)}\big|_{\sigma(A)}\right)(A)$$

is finite dimensional.$\lightning$ Therefore, it follows that (12.27) is true. $\square$

12.5.4 Relative Compactness

Definition 12.5.19 (Relatively compact operators). Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space and $A : D(A) \to X$ a densely-defined, linear and closed operator in X. A linear operator $B : D(B) \to X$ is called compact relative to A, or A-compact if $D(B) \supset D(A)$ and for every sequence $f_1, f_2, \dots$ in $D(A)$ such that for some $C > 0$

$$\|f_\nu\| + \|Af_\nu\| \leqslant C$$

for every $\nu \in \mathbb{N}^*$, it follows that $Bf_1, Bf_2, \dots$ has a convergent subsequence.

Theorem 12.5.20 (A criterion for relative compactness of operators I). Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X. Further, let $B : D(B) \to X$ be a linear operator in X such that $D(B) \supset D(A)$. Then B is compact relative to A if and only if $B \circ (A + i)^{-1}$ is a compact linear operator on X.

Proof. "$\Rightarrow$: In the following, we assume that B is compact relative to A. If $f_1, f_2, \dots$ is a bounded sequence in X, then the corresponding sequence $(A + i)^{-1}f_1, (A + i)^{-1}f_2, \dots$ is bounded, too. Further,

$$
\begin{aligned}
&\|(A+i)^{-1}f_\nu\| + \|A(A+i)^{-1}f_\nu\| \\
&= \|(A+i)^{-1}f_\nu\| + \|(A+i-i)(A+i)^{-1}f_\nu\|
\end{aligned}
$$

$$= \|(A+i)^{-1}f_\nu\| + \|f_\nu - i(A+i)^{-1}f_\nu\|$$
$$\leqslant \|f_\nu\| + 2\|(A+i)^{-1}f_\nu\| \ ,$$

for every $\nu \in \mathbb{N}^*$. Hence there is $C > 0$ such that

$$\|(A+i)^{-1}f_\nu\| + \|A(A+i)^{-1}f_\nu\| \leqslant C \ ,$$

for every $\nu \in \mathbb{N}^*$. Since B is compact relative to A, there is a convergent subsequence of the sequence $B \circ (A+i)^{-1}f_1, B \circ (A+i)^{-1}f_2, \dots$. Since the sequence $f_1, f_2, \dots$ is arbitrary otherwise, this implies that $B \circ (A+i)^{-1}$ is compact.
"$\Leftarrow$:" In the following, we assume that $B \circ (A+i)^{-1}$ is a compact linear operator on X. For the proof, let $f_1, f_2, \dots$ be a sequence in $D(A)$ such that for some $C > 0$

$$\|f_\nu\| + \|Af_\nu\| \leqslant C \ ,$$

for every $\nu \in \mathbb{N}^*$. Since A is in particular self-adjoint, it follows for every $f \in D(A)$ that

$$\|(A+i)f\|^2 = \langle (A+i)f|(A+i)f\rangle = \|Af\|^2 - i\,\langle f|Af\rangle + i\,\langle Af|f\rangle + \|f\|^2$$
$$= \|Af\|^2 + \|f\|^2$$

and hence that

$$\|(A+i)f\| = \sqrt{\|Af\|^2 + \|f\|^2} \leqslant \|f\| + \|Af\| \ .$$

We conclude that

$$\|(A+i)f_\nu\| \leqslant C \ ,$$

for every $\nu \in \mathbb{N}^*$. Hence, $(A+i)f_1, (A+i)f_2, \dots$ is a bounded sequence. Further, since $B \circ (A+i)^{-1}$ is a compact linear operator on X, it follows that there is a convergent subsequence of

$$B \circ (A+i)^{-1}(A+i)f_1 = Bf_1 \ , \ B \circ (A+i)^{-1}(A+i)f_2 = Bf_2 \ , \ \dots$$

Since the sequence $f_1, f_2, \dots$ is arbitrary otherwise, this implies that B is relative compact to A. □

Corollary 12.5.21 (A criterion for relative compactness of operators II). Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X. Further, let $B : D(B) \to X$ be a linear operator in X such that $D(B) \supset D(A)$. Then B is compact relative to A if and only if $B \circ (A-\lambda)^{-1}$ is a compact linear operator on X, for some $\lambda \in \rho(A)$.

Proof. From the first resolvent formula, it follows that

$$B(A-\lambda)^{-1} - B(A-\mu)^{-1} = (\lambda - \mu)\, B(A-\lambda)^{-1}(A-\mu)^{-1} \ ,$$

for every $\lambda, \mu \in \rho(A)$. Hence it follows that

$$B(A+i)^{-1} = B(A-\lambda)^{-1} - (\lambda + i)\, B(A-\lambda)^{-1}(A+i)^{-1}$$

and that

$$B(A-\mu)^{-1} = B(A+i)^{-1} + (\mu+i)\,B(A+i)^{-1}(A-\mu)^{-1} \ ,$$

for every $\lambda \in \rho(A)$. Since the compact linear operators on X form a closed two-sided *-ideal in $L(X,X)$, we conclude that $B(A+i)^{-1}$ is a compact linear operator on X if and only if $B(A-\lambda)^{-1}$ is a compact linear operator on X for some $\lambda \in \rho(A)$. $\square$

Theorem 12.5.22. Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and closed operator in X and $B : D(B) \to X$ a linear, A-compact operator in X. Then

a)
$$\|Bf\| \leqslant C(\|f\| + \|Af\|) \leqslant C'(\|f\| + \|(A+B)f\|) \ ,$$
for every $f \in D(A)$ and some $C, C' > 0$,

b) B is $(A+B)$-compact,

c) if, in addition, B is closable, then for each $\varepsilon > 0$, there is $K \geqslant 0$ such that
$$\|Bf\| \leqslant \varepsilon\|Af\| + K\|f\|$$
for every $f \in D(A)$.

Proof. "a)": If it is not true that

$$\|Bf\| \leqslant C(\|f\| + \|Af\|)$$

for every $f \in D(A)$ and some $C > 0$, then there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

$$\|Bf_\nu\| > \nu(\|f_\nu\| + \|Af_\nu\|)$$

for every $\nu \in \mathbb{N}^*$. In particular, this implies that $f_\nu \neq 0$ and hence that

$$\|Bg_\nu\| > \nu \ , \tag{12.29}$$

where

$$g_\nu := (\|f_\nu\| + \|Af_\nu\|)^{-1} f_\nu$$

for every $\nu \in \mathbb{N}^*$. We note that

$$\|g_\nu\| + \|Ag_\nu\| = 1$$

for every $\nu \in \mathbb{N}^*$. Therefore, since B is A-compact, there is a convergent subsequence to $Bg_1, Bg_2, \dots$ which is in contradiction to (12.29). Hence there is $C > 0$ such that

$$\|Bf\| \leqslant C(\|f\| + \|Af\|)$$

for every $f \in D(A)$. If it is not true that

$$C(\|f\| + \|Af\|) \leqslant C'(\|f\| + \|(A+B)f\|)$$

for every $f \in D(A)$ and some $C' > 0$, then there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that

$$\|f_\nu\| + \|Af_\nu\| > \nu(\|f_\nu\| + \|(A+B)f_\nu\|)$$

for every $\nu \in \mathbb{N}^*$. In particular, this implies that $f_\nu \neq 0$ and hence that

$$(\,\|g_\nu\|\,,\, \|(A+B)g_\nu\| \leqslant)\;\; \|g_\nu\| + \|(A+B)g_\nu\| < \frac{1}{\nu}\,, \tag{12.30}$$

where again

$$g_\nu := (\|f_\nu\| + \|Af_\nu\|)^{-1} f_\nu$$

for every $\nu \in \mathbb{N}^*$. We note again that

$$\|g_\nu\| + \|Ag_\nu\| = 1 \tag{12.31}$$

for every $\nu \in \mathbb{N}^*$. Therefore, since B is A-compact, there is a convergent subsequence to $Bg_1, Bg_2, \dots$, i.e., there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that the sequence $Bg_{\nu_1}, Bg_{\nu_2}, \dots$ is convergent to some $\zeta \in X$. As a consequence of (12.30), $Ag_{\nu_1}, Ag_{\nu_2}, \dots$ is convergent to $-\zeta$. Since, as a consequence of (12.30), $g_{\nu_1}, g_{\nu_2}, \dots$ is a null-sequence and A is closed, we conclude that $\zeta = 0$. From (12.31), we arrive at the contradiction $0 = 1$.$\lightning$
"b)": Let $f_1, f_2, \dots$ be a sequence in $D(A)$ satisfying

$$\|f_\nu\| + \|(A+B)f_\nu\| \leqslant C$$

for every $\nu \in \mathbb{N}^*$ and some $C > 0$. According to a), there are $C_1, C_2 > 0$

$$\|Bf_\nu\| \leqslant C_1(\|f_\nu\| + \|Af_\nu\|) \leqslant C_2(\|f_\nu\| + \|(A+B)f_\nu\|) \leqslant C_2 C$$

for every $\nu \in \mathbb{N}^*$. Hence, it follows that

$$\|f_\nu\| + \|Af_\nu\| \leqslant \frac{C_2 C}{C_1}$$

every $\nu \in \mathbb{N}^*$. Since B is A-compact, $Bf_1, Bf_2, \dots$ has a convergent subsequence. As a consequence, B is $(A+B)$-compact.
"c)": If it is not true that for each $\varepsilon > 0$, there is $K \geqslant 0$ such that

$$\|Bf\| \leqslant \varepsilon\|Af\| + K\|f\|$$

for every $f \in D(A)$, there is $\varepsilon > 0$ such that for every $\nu \in \mathbb{N}^*$ there is $f_\nu \in D(A)$ satisfying

$$\|Bf_\nu\| > \varepsilon\|Af_\nu\| + \nu\|f_\nu\|\,.$$

In particular, this implies that $f_\nu \neq 0$ and hence that

$$\|Bg_\nu\| > \varepsilon\|Ag_\nu\| + \nu\|g_\nu\| \ \ (\geqslant \varepsilon\|Ag_\nu\|\,,\,\nu\|g_\nu\|\,)\ , \tag{12.32}$$

where

$$g_\nu := (\|Af_\nu\| + \|f_\nu\|)^{-1} f_\nu$$

for every $\nu \in \mathbb{N}^*$. We note that

$$\|g_\nu\| + \|Ag_\nu\| = 1$$

for every $\nu \in \mathbb{N}^*$. As a consequence of a), $Bg_1, Bg_2, \dots$ is bounded. Hence it follows from (12.32) that $g_1, g_2, \dots$ is a null-sequence and therefore that

$$\lim_{\nu\to\infty} \|Ag_\nu\| = 1\ .$$

Since B is A-compact, there is a a convergent subsequence to $Bg_1, Bg_2, \dots$, i.e., there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that the sequence $Bg_{\nu_1}, Bg_{\nu_2}, \dots$ is convergent to some $\zeta \in X$. Since B is closable, $\zeta = 0$, but

$$\|\zeta\| = \lim_{\mu\to\infty} \|Bg_{\nu_\mu}\| \geqslant \varepsilon \lim_{\mu\to\infty} \|Ag_{\nu_\mu}\| = \varepsilon\ .\lightning$$

□

Theorem 12.5.23. Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $B : D(B) \to X$ a linear, symmetric and A-compact operator in X. Then

a) $A + B$ is self-adjoint, and

b) $\sigma_e(A + B) = \sigma_e(A)$.

Proof. "a)": Since B is A-compact and closable, for each $\varepsilon > 0$ and from Theorem 12.5.22) c), it follows the existence of $K \geqslant 0$ such that

$$\|Bf\| \leqslant \varepsilon\|Af\| + K\|f\|$$

for every $f \in D(A)$. As a consequence,

$$\|Bf\|^2 \leqslant \varepsilon^2\|Af\|^2 + K^2\|f\|^2 + 2\|f\|\|Af\| \leqslant 2\varepsilon^2\|Af\|^2 + 2K^2\|f\|^2$$

for every $f \in D(A)$. Hence it follows from the Rellich-Kato theorem, Theorem 12.4.11, that $A + B$ is essentially self-adjoint such that

$$\overline{A + B} = A + \bar{B} = A + B\ .$$

"b)": If $\lambda \in \sigma_e(A)$, then there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that $\|f_\nu\| = 1$

for every $\nu \in \mathbb{N}^*$, $f_1, f_2, \dots$ is weakly convergent to 0, and $\lim_{\nu\to\infty}(A-\lambda)f_\nu = 0$. Hence,

$$\|f_\nu\| + \|Af_\nu\| = 1 + \|(A-\lambda)f_\nu + \lambda f_\nu\| \leqslant 1 + |\lambda| + \|(A-\lambda)f_\nu\| \leqslant C$$

for every $\nu \in \mathbb{N}^*$ and some $C > 0$. Therefore, since B is A-compact, there is a convergent subsequence to $Bf_1, Bf_2, \dots$, i.e., there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that the sequence $Bf_{\nu_1}, Bf_{\nu_2}, \dots$ is convergent to some $\zeta \in X$. Thus,

$$\langle f|\zeta\rangle = \langle f|\lim_{\mu\to\infty} Bf_{\nu_\mu}\rangle = \lim_{\mu\to\infty}\langle f|Bf_{\nu_\mu}\rangle = \lim_{\mu\to\infty}\langle Bf|f_{\nu_\mu}\rangle = 0$$

for every $f \in D(A)$. Since $D(A)$ is dense in X, the latter implies that $\zeta = 0$. Hence, we conclude that

$$\lim_{\mu\to\infty}(A+B-\lambda)f_{\nu_\mu} = 0$$

and therefore that $\lambda \in \sigma_e(A+B)$. If $\lambda \in \sigma_e(A+B)$, then there is a sequence $f_1, f_2, \dots$ in $D(A)$ such that $\|f_\nu\| = 1$ for every $\nu \in \mathbb{N}^*$, $f_1, f_2, \dots$ is weakly convergent to 0, and $\lim_{\nu\to\infty}(A+B-\lambda)f_\nu = 0$. Hence,

$$\|f_\nu\| + \|(A+B)f_\nu\| = 1 + \|(A+B-\lambda)f_\nu + \lambda f_\nu\| \leqslant 1 + \lambda + \|(A+B-\lambda)f_\nu\| \leqslant C$$

for every $\nu \in \mathbb{N}^*$ and some $C > 0$. Therefore, since as a consequence of Theorem 12.5.22, $-B$ is $A+B$-compact, there is a convergent subsequence to $-Bf_1, -Bf_2, \dots$, i.e., there is a strictly monotonically increasing sequence $\nu_1, \nu_2, \dots$ in $\mathbb{N}^*$ such that the sequence $-Bf_{\nu_1}, -Bf_{\nu_2}, \dots$ is convergent to some $\zeta \in X$. Thus,

$$\langle f|\zeta\rangle = -\langle f|\lim_{\mu\to\infty} Bf_{\nu_\mu}\rangle = -\lim_{\mu\to\infty}\langle f|Bf_{\nu_\mu}\rangle = -\lim_{\mu\to\infty}\langle Bf|f_{\nu_\mu}\rangle = 0$$

for every $f \in D(A)$. Since $D(A)$ is dense in X, the latter implies that $\zeta = 0$. Hence, we conclude that

$$\lim_{\mu\to\infty}(A-\lambda)f_{\nu_\mu} = 0$$

and therefore that $\lambda \in \sigma_e(A)$. □

Theorem 12.5.24. Let $(X, \langle\,|\,\rangle)$ be a non-trivial Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $B : D(B) \to X$, $C : D(C) \to X$ linear, symmetric operators in X such that $D(B) \supset D(A)$ and

$$\|Bf\|^2 \leqslant a^2\|Af\|^2 + b^2\|f\|^2$$

for some $a, b \in [0, \infty)$ satisfying $a < 1$ and such that C is A-compact. Then

a) $A + B$ is self-adjoint,

b) C is $A+B$-compact, and

c) $A+B+C$ is self-adjoint and $\sigma_e(A+B+C) = \sigma_e(A+B)$.

Proof. "a)": It follows from the Rellich-Kato theorem, Theorem 12.4.11, that $A+B$ is essentially self-adjoint such that

$$\overline{A+B} = A + \bar{B} = A + B \ .$$

"b)": We note that

$$\|Af\| \leqslant \|(A+B)f\| + \|Bf\| \leqslant \|(A+B)f\| + [\, a^2\|Af\|^2 + b^2\|f\|^2\,]^{1/2}$$
$$\leqslant \|(A+B)f\| + a\|Af\| + b\|f\|$$

and hence that

$$\|Af\| \leqslant \frac{1}{1-a}\,\|(A+B)f\| + \frac{b}{1-a}\,\|f\|$$

for every $f \in D(A)$. Therefore if $f_1, f_2, \dots$ is a sequence in $D(A)$ satisfying

$$\|f_\nu\| + \|(A+B)f_\nu\| \leqslant K$$

for some $K > 0$, then

$$\|f_\nu\| + \|Af_\nu\| \leqslant \frac{1}{1-a}\,\|(A+B)f_\nu\| + \frac{1-a+b}{1-a}\,\|f_\nu\|$$
$$\leqslant K \max\left\{\frac{1}{1-a}, \frac{1-a+b}{1-a}\right\}$$

for every $\nu \in \mathbb{N}^*$. Since C is A-compact, the latter implies the existence of a convergent subsequence to $Cf_1, Cf_2, \dots$. Hence C is $A+B$-compact.
"c)": The statement is a consequence of a), b) and Theorem 12.5.22. □

Theorem 12.5.25. (**Classical Arzela-Ascoli theorem**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, K a non-empty compact subset of a normed vector space with norm $|\ |$ and $f_1, f_2, \dots$ a bounded sequence in $(C(K,\mathbb{K}), \|\ \|_\infty)$ that equicontinuous, i.e., such that for every $\varepsilon > 0$ there is a $\delta > 0$ such that for all $x, y \in K$ satisfying $|x-y| < \delta$, it follows that

$$|f_\nu(x) - f_\nu(y)| < \varepsilon$$

for all $\nu \in \mathbb{N}^*$. Then there is a convergent subsequence to $f_1, f_2, \dots$.

Proof. In the first step, we show that there is countable dense subset S of K. For the proof, let $\nu \in \mathbb{N}^*$. Then the family $(U_{1/\nu}(x))_{x\in K}$ is an open covering of K. Since K is compact, there is a non-empty finite subset S_ν of K such that $(U_{1/\nu}(x))_{x\in S_\nu}$ is an open covering of K. In particular,

$$S := \bigcup_{\nu\in\mathbb{N}^*} S_\nu$$

is countable and dense in K. For the proof of the latter, let $x \in K$ and $\nu \in \mathbb{N}^*$. Since $(U_{1/\nu}(x))_{x \in S_\nu}$ is an open covering of K, there is $x_\nu \in S_\nu \subset S$ such that $x \in U_{1/\nu}(x_\nu)$. If $\varepsilon > 0$ and $\nu_0 \in \mathbb{N}^*$ is such $(1/\nu_0) < \varepsilon$, then it follows that

$$|x_\nu - x| < \frac{1}{\nu} \leqslant \frac{1}{\nu_0} < \varepsilon$$

for every $\nu \in \mathbb{N}^*$ such that $\nu \geqslant \nu_0$ and hence that

$$\lim_{\nu \to \infty} |x_\nu - x| = 0 \ .$$

In the second step, we show the existence of a subsequence of $f_1, f_2, \dots$ that converges pointwise on $S = \{x_1, x_2, \dots\}$. For this, we use the standard diagonal argument. For every $k \in \mathbb{N}^*$, the corresponding sequence $f_1(x_k), f_2(x_k), \dots$ is bounded. Hence according to the Bolzano-Weierstrass theorem for the real numbers, there is an infinite subset $\mathbb{N}_1$ of $\mathbb{N}^*$, along with a strictly increasing bijection $\nu_1 : \mathbb{N}^* \to \mathbb{N}_1$ such that

$$f_{\nu_1(1)}(x_1), f_{\nu_1(2)}(x_1), \dots$$

is convergent. We note that

$$\nu_1(k) \geqslant k$$

for every $k \in \mathbb{N}^*$. Continuing this reasoning sucessively, we arrive at a sequence $\mathbb{N}_1, \mathbb{N}_2, \dots$ of infinite subsets of $\mathbb{N}^*$ such that

$$\mathbb{N}^* \supset \mathbb{N}_1 \supset \mathbb{N}_2 \supset \dots$$

along with strictly increasing bijections $\nu_k : \mathbb{N}^* \to \mathbb{N}_k$, where $k \in \mathbb{N}^*$, such that

$$f_{\nu_k(1)}(x_l), f_{\nu_k(2)}(x_l), \dots$$

is convergent for every $l \in \mathbb{N}^*$ satisfying $l \leqslant k$. In particular,

$$\nu_{l+1}(k) \geqslant \nu_l(k) \tag{12.33}$$

for all $l, k \in \mathbb{N}^*$. The latter implies that

$$\nu_{k+1}(k+1) > \nu_{k+1}(k) \geqslant \nu_k(k)$$

for every $k \in \mathbb{N}^*$ and hence that the sequence $\nu_1(1), \nu_2(2), \dots$ is strictly increasing. Also, (12.24) implies that

$$\nu_{l+k}(l+k) \geqslant \nu_l(l+k) > \nu_l(k) \tag{12.34}$$

for all $l, k \in \mathbb{N}^*$. We claim that

$$f_{\nu_1(1)}(x_l), f_{\nu_2(2)}(x_l), \dots$$

is convergent for every $l \in \mathbb{N}^*$. For the proof, let $\varepsilon > 0$ and $l \in \mathbb{N}^*$. Since, in particular,

$$f_{\nu_l(1)}(x_l), f_{\nu_l(2)}(x_l), \dots$$

is a Cauchy-sequence in $\mathbb{K}$, there is $N \in \mathbb{N}^*$ such that

$$|f_{\nu_l(k)}(x_l) - f_{\nu_l(k')}(x_l)| < \varepsilon$$

for all $k, k' \in \mathbb{N}^*$ satisfying $k \geqslant N$ and $k' \geqslant N$. Hence it follows by (12.34) that

$$|f_{\nu_{l+k}(l+k)}(x_l) - f_{\nu_{l+k'}}(l+k')(x_l)| < \varepsilon$$

for all $k, k' \in \mathbb{N}^*$ satisfying $k \geqslant N$ and $k' \geqslant N$. As a consequence,

$$f_{\nu_1(1)}(x_l), f_{\nu_2(2)}(x_l), \dots$$

is a Cauchy-sequence in $\mathbb{K}$ and hence convergent. In the last step, we show that the sequence $g_1, g_2, \dots$, defined by $g_\mu := f_{\nu_\mu(\mu)}$ for every $\mu \in \mathbb{N}^*$ is convergent. For the proof, let $\varepsilon > 0$ and $\delta > 0$ such that for all $x, y \in K$ satisfying $|x - y| < \delta$, it follows that

$$|\, g_\nu(x) - g_\nu(y)| < \frac{\varepsilon}{3}$$

for all $\nu \in \mathbb{N}^*$. Further, let $\nu_0 \in \mathbb{N}^*$ be such $(1/\nu_0) < \delta$. Then $(U_{1/\nu_0}(x))_{x \in S_{\nu_0}}$ is an open covering of K. Since $g_1(y), g_2(y), \dots$ is convergent for every $y \in S_{\nu_0}$, there is $N \in \mathbb{N}^*$ such that for $\nu, \mu \in \mathbb{N}^*$ satisfying $\nu \geqslant N$ and $\mu \geqslant N$, it follows that

$$|\, g_\mu(y) - g_\nu(y)| < \frac{\varepsilon}{3}$$

for every $y \in S_{\nu_0}$. If $x \in K$, there is $y \in S_{\nu_0}$ such that $x \in U_{1/\nu_0}(y) \subset U_\delta(y)$. Hence it follows for $\nu, \mu \in \mathbb{N}^*$ satisfying $\nu \geqslant N$ and $\mu \geqslant N$ that

$$|\, g_\mu(x) - g_\nu(x)| \leqslant |\, g_\mu(x) - g_\mu(y)| + |\, g_\mu(y) - g_\nu(y)| + |\, g_\nu(y) - g_\nu(x)| < \varepsilon \ .$$

Hence $g_1, g_2, \dots$ is a Cauchy-sequence in $(C(K, \mathbb{K}), \|\ \|_\infty)$ and therefore convergent to an element of $C(K, \mathbb{K})$. □

12.6 Spectral Theorems for Densely-Defined, Linear and Self-adjoint Operators in Complex Hilbert Spaces.

Definition 12.6.1. (**Spectral Families**) Let $X, \langle\,|\,\rangle$ be a complex Hilbert space. A map

$$E : \mathbb{R} \to L(X, X)$$

is called a *spectral family* if:

(i) For every $\lambda \in \mathbb{R}$, E_λ is an orthogonal projection, i.e., E_λ is self-adjoint such that

$$E_\lambda^2 = E_\lambda \ ,$$

(ii) for all $\lambda, \mu \in \mathbb{R}$, satisfying $\lambda \leqslant \mu$, it follows that

$$E_\lambda \leqslant E_\mu \ ,$$

i.e.,

$$\langle f|E_\lambda f\rangle \leqslant \langle f|E_\mu f\rangle$$

for every $f \in X$,

(iii) for every $f \in X$

$$\lim_{\lambda\to-\infty} E_\lambda f = 0 \ , \ \lim_{\lambda\to\infty} E_\lambda f = f \ ,$$

(iv) for every $f \in X$

$$E_\lambda f = \lim_{\mu\to\lambda+} E_\mu f \ .$$

For every $f \in X$, we call the Lebesgue-Stieltjes measure that is generated by the monotonically increasing function

$$(\mathbb{R} \to \mathbb{R}, \lambda \mapsto \langle f|E_\lambda f\rangle) \ ,$$

the Lebesgue-Stieltjes measure corresponding to E and f.

Theorem 12.6.2. (**Spectral Theorems for Densely-Defined, Linear and Self-adjoint Operators in Complex Hilbert Spaces, Version I**) Let $X, \langle\,|\,\rangle$ be a complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X. Then there is a *unique spectral family*

$$E : \mathbb{R} \to L(X, X)$$

with the following properties:

(i) For every $f \in X$, $f \in D(A)$ if and only if $(\text{id}_\mathbb{R})^2$ is integrable with respect ψ_f,

(ii) for every $f \in D(A)$

$$\langle f|Af\rangle = \int_\mathbb{R} \text{id}_\mathbb{R}\, d\psi_f \ ,$$

where ψ_f is the Lebesgue-Stieltjes measure that is generated by monotonically increasing function

$$(\mathbb{R} \to \mathbb{R}, \lambda \mapsto \langle f|E_\lambda f\rangle) \ .$$

In addition, if $f \in D(A)$, then

$$\|Af\| = \left(\int_{\mathbb{R}} \mathrm{id}_{\mathbb{R}}^2 \, d\psi_f \right)^{1/2} .$$

In the following, this spectral family is called the spectral family corresponding to A and for every $f \in X$, the corresponding ψ_f is called the spectral measure that is associated with A and f.

Theorem 12.6.3. (**Universally Measurable Functions**) Let S be a non-empty subset of $\mathbb{R}$. Then

(i) $U_{\mathbb{C}}(S)$,

consisting of all elements of $f \in B(S, \mathbb{C})$ such that $\hat{f} : \mathbb{R} \to \mathbb{C}$, defined for every $x \in \mathbb{R}$ by

$$\hat{f}(x) := \begin{cases} f(x) & \text{if } x \in S \\ 0 & \text{if } x \in \mathbb{R} \setminus S \end{cases} ,$$

is measurable with respect to every measure induced by an additive, monotone and regular interval function,

and equipped with pointwise addition, scalar multiplication, multiplication and the norm $\| \, \|_\infty$,

is a $\mathbb{C}^*$-subalgebra of $(B(S, \mathbb{C}), +, ., \cdot, \| \, \|_\infty)$

(ii) $V_{\mathbb{C}}(S)$,

consisting of all elements of $f \in B(S, \mathbb{C})$ for which there is a sequence $f_1, f_2, \dots$ of elements of $C(S, \mathbb{C})$ such that for every $x \in S$

$$\lim_{\nu \to \infty} f_\nu(x) = f(x) ,$$

and equipped with pointwise addition, scalar multiplication and multiplication,

is an involutive subalgebra of $(U_{\mathbb{C}}(S), +, ., \cdot)$ that contains $C(S, \mathbb{C})$ as well as all restrictions of complex-valued step functions on $\mathbb{R}$ to S.

(iii) $U^s_{\mathbb{C}}(S)$,

consisting of all elements of $B(S, \mathbb{C})$ for which there is a sequence $s_1, s_2, \dots$ of complex-valued step functions on $\mathbb{R}$ such that

$$\lim_{\nu \to \infty} s_\nu(x) = f(x) ,$$

for all $x \in S$,

is an involutive subalgebra of $(U_{\mathbb{C}}(S), +, \, . \, , \cdot \,)$ that contains $V_{\mathbb{C}}(S)$.

Theorem 12.6.4. (**Spectral Theorems for Densely-Defined, Linear and Self-adjoint Operators in Complex Hilbert Spaces, Version II**) Let $X, \langle \, | \, \rangle$ be a complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X, with spectrum $\sigma(A) (\subset \mathbb{R})$. Further, let $E : \mathbb{R} \to L(X, X)$ be the spectral family corresponding to A and, for every $f \in X$, ψ_f be the spectral measure corresponding to A and f. Then there is a *unique continuous *-homomorphism*

$$\Psi : (\,\overline{U^s_{\mathbb{C}}(\sigma(A))}, +, \, . \, , \cdot \, , {}^*, \| \, \|_\infty) \to (L(X, X), +, \, . \, , \circ \, , {}^*, \| \, \|)$$

of $\mathbb{C}^*$-algebras such that

(i)
$$\Psi(1_{\sigma(A)}) = \mathrm{id}_X \ , \ \Psi\left(\frac{\mathrm{id}_{\sigma(A)} - i}{\mathrm{id}_{\sigma(A)} + i}\right) = (A - i) \circ (A + i)^{-1} \ .$$

(ii) If $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$, $f_1, f_2, \dots$ a bounded sequence in $\overline{U^s_{\mathbb{C}}(\sigma(A))}$ that is everywhere on $\sigma(A)$ pointwise convergent to f, then for every $f \in X$

$$\lim_{\nu \to \infty} \Psi(f_\nu) f = \Psi(f) f \ .$$

This *-homomorphism has the following additional properties:

(iii) If $\lambda \in \sigma(A)$ is an eigenvalue of A, then for every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$ and every $f \in \ker(A - \lambda)$
$$\Psi(f) f = f(\lambda) . f \ .$$

(iv) For every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$ and $f \in X$

$$\langle f | \Psi(f) f \rangle = \int_{\sigma(A)} f \, d\psi_f \ .$$

(v) If $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$ is real-valued and positive, then $\Psi(f)$ is too positive, i.e.,

$$\langle f | \Psi(f) f \rangle \geqslant 0 \ ,$$

for every $f \in X$.

(vi) For every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$

$$\| \Psi(f) \| \leqslant \| f \|_\infty \ .$$

(vii) If $C \in L(X, X)$ is such that $A \circ C \supset C \circ A$, then

$$[\Psi(f), C] = 0 \ ,$$

for every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

(viii)
$$E = (\mathbb{R} \to L(X, X), \lambda \mapsto \Psi(\chi_{(-\infty,\lambda]}|_{\sigma(A)})) \ .$$

Remark 12.6.5. The operator
$$(A - i) \circ (A + i)^{-1}$$
is called the Cayley transform of A.

Remark 12.6.6. In future, we will use instead of
$$\Psi(f) \ ,$$
the notation
$$f(A) \ ,$$
for every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

Theorem 12.6.7. (**Maximal Multiplication Operators**) Let $n \in \mathbb{N}^*$, φ and additive, monotone and regular interval function on $\mathbb{R}^n$, M a φ-measurable subset of $\mathbb{R}^n$ such that $L^2_{\mathbb{C}}(M)$ is non-trival, h a complex-valued function that is a.e. defined on M and φ-measurable. We define the maximal multiplication operator with h,
$$T_h : D(T_h) \to L^2_{\mathbb{C}}(M, \varphi) \ ,$$
by
$$D(T_h) := \{f \in L^2_{\mathbb{C}}(M, \varphi) : h \cdot f \in L^2_{\mathbb{C}}(M, \varphi)\}$$
and
$$T_h f := h \cdot f \ ,$$
for every $f \in D(T_h)$. Then,

(i) T_h is a densely-defined, linear operator in $L^2_{\mathbb{C}}(M, \varphi)$,

(ii) $(T_h)^* = T_{h^*}$,

(iii) the following statements are equivalent
  a) T_h is continuous,
  b) $h \in L^\infty_{\mathbb{C}}(M, \varphi)$,
  c) $D(T_h) = L^2_{\mathbb{C}}(M, \varphi)$.

  If one these statements is true,
$$\|T_h\| = \|h\|_\infty \ ,$$

(iv) the following statements are equivalent
  a) T_h is injective,
  b) $h^{-1}(\{0\})$ is a set of φ-measure 0,

c) $\mathrm{Ran}(h)$ is dense in $L^2_{\mathbb{C}}(M,\varphi)$.

If one these statement is true, the inverse operator $(T_h)^{-1}$ is defined, and

$$(T_h)^{-1} = T_{\frac{1}{h}} \ ,$$

where

$$\frac{1}{h} : M \to \mathbb{C}$$

is defined by

$$\frac{1}{h}(x) := \begin{cases} \frac{1}{h(x)} & \text{if } h(x) \neq 0 \\ 0 & \text{if } h(x) = 0 \end{cases} ,$$

(v) the following statements are equivalent

a) T_h is surjective,

b) there is $c > 0$ such that $|h|^{-1}((-c,c))$ is a set of φ-measure 0,

c) T_h is bijective.

If one these statement is true, the inverse operator $(T_h)^{-1}$ is defined on the whole of $L^2_{\mathbb{C}}(M,\varphi)$ and is continuous.

Theorem 12.6.8. (**Spectrum, Spectral Family and Spectral Measures of a Maximal Multiplication Operator**) Let $n \in \mathbb{N}^*$, φ and additive, monotone and regular interval function on $\mathbb{R}^n$, M a φ-measurable subset of $\mathbb{R}^n$ such that $L^2_{\mathbb{C}}(M)$ is non-trivial, h a real-valued function that is a.e. defined on M and φ-measurable. As a consequence, the maximal multiplication operator with h

$$T_h : D(T_h) \to L^2_{\mathbb{C}}(M,\varphi) \ ,$$

defined by

$$D(T_h) := \{f \in L^2_{\mathbb{C}}(M,\varphi) : h \cdot f \in L^2_{\mathbb{C}}(M,\varphi)\}$$

and

$$T_h f := h \cdot f \ ,$$

for every $f \in D(T_h)$, is densely-defined, linear and self-adjoint. Then

(i) the spectrum $\sigma(T_h)$ and the point spectrum $\sigma_p(T_h)$ of T_h are given by

$$\sigma(T_h) = \{\lambda \in \mathbb{R} : \text{For every } c > 0, \\ h^{-1}(U_c(\lambda)) \text{ is no set of } \varphi\text{-measure } 0\} \ ,$$
$$\sigma_p(T_h) = \{\lambda \in \mathbb{R} : h^{-1}(\{\lambda\}) \text{ is no set of } \varphi\text{-measure } 0\} \ ,$$

(ii) the spectral family $E : \mathbb{R} \to L(L^2_{\mathbb{C}}(M,\varphi), L^2_{\mathbb{C}}(M,\varphi))$ corresponding to T_h is given by

$$E(\lambda) = T_{\chi_{h^{-1}((-\infty,\lambda])}|_M} \ ,$$

and for every $f \in L^2_{\mathbb{C}}(M, \varphi)$, the corresponding spectral measure is given by the interval function $\psi_f : \gamma^1(\mathbb{R}) \to \mathbb{R}$, defined by

$$\psi_f(I) := \int_{\mathbb{R}^n} \chi_{_{h^{-1}(I)}} \cdot |\hat{f}|^2 \cdot d\varphi$$

for every interval $I \in \gamma^1(\mathbb{R})$.

Corollary 12.6.9 (Functional Calculus associated with a Maximal Multiplication Operator). Let n, φ, M, h, T_h as in the previous Theorem. Then

$$f(T_h) = T_{f \circ h} \ ,$$

for every $f \in U^s_{\mathbb{C}}(\sigma(T_h))$.

12.7 Calculation of the Free Propagator for Quantum Mechanics

Theorem 12.7.1. Let $n \in \mathbb{N}^*$, $t \in \mathbb{R}^*$ and $\bar{H}_0$ the free Hamiltonian of quantum mechanics, then

$$e^{-i\,\frac{t}{\hbar}\bar{H}_0} g = \left(\pi i \, \frac{4\varepsilon_0 t}{\hbar}\right)^{-n/2} \cdot \left(e^{i\frac{\hbar}{4\varepsilon_0 t} \cdot |\ |^2} * g\right) \ ,$$

for every $f \in L^1_{\mathbb{C}}(\mathbb{R}^n) \cap L^2_{\mathbb{C}}(\mathbb{R}^n)$, and

$$e^{-i\,\frac{t}{\hbar}\bar{H}_0} g = \lim_{\nu \to \infty} \left(\pi i \, \frac{4\varepsilon_0 t}{\hbar}\right)^{-n/2} \cdot \left[e^{i\frac{\hbar}{4\varepsilon_0 t} \cdot |\ |^2} * (\chi_{_{[-\nu,\nu]^n}} g)\right] \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, almost everywhere pointwise on $\mathbb{R}^n$, where

$$\varepsilon_0 := \frac{\hbar^2 \kappa^2}{2m} \ .$$

Proof. First, we recall some information from Section **??**. For this purpose, let $\alpha > 0$. Then

$$\hat{H}_0 : C_0^\infty(\mathbb{R}^n, \mathbb{C}) \to L^2_{\mathbb{C}}(\mathbb{R}^n) \ ,$$

defined for every $f \in C_0^\infty(\mathbb{R}^n, \mathbb{C})$ by

$$\hat{H}_0 f := -\varepsilon_0 . \sum_{k=1}^{n} \frac{\partial^2 f}{\partial u_k^2} \ ,$$

is a densely-defined, linear, positive symmetric and essentially self-adjoint operator in $L^2_{\mathbb{C}}(\mathbb{R}^n)$, whose closure $\bar{H}_0$ has the spectrum

$$\sigma(\bar{H}_0) = [0, \infty) \ .$$

Further, for every bounded and universally measurable function $f : [0, \infty) \to \mathbb{C}$:

$$f(\bar{H}_0) = F_2^{-1} \circ T_{[f \circ (\varepsilon_0 .|\ |^2)]} \circ F_2 \ ,$$

where $T_{f \circ (\varepsilon_0 .|\ |^2)}$ is the maximal multiplication operator with the function $f \circ (\varepsilon_0 .|\ |^2)$, defined by

$$T_{f \circ (\varepsilon_0 .|\ |^2)} g := [f \circ (\varepsilon_0 .|\ |^2)] \cdot g \ ,$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. In particular,

$$e^{-\frac{1}{\varepsilon} . \bar{H}_0} e^{-i \frac{t}{\hbar} \bar{H}_0} g = e^{-\left(\frac{1}{\varepsilon} + i \frac{t}{\hbar}\right) \bar{H}_0} g = e^{-\sigma_\varepsilon \bar{H}_0} g = F_2^{-1} \exp(-\varepsilon_0 \, \sigma_\varepsilon \, |\ |^2) F_2 g \ .$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where

$$\sigma_\varepsilon := \frac{1}{\varepsilon} + i \, \frac{t}{\hbar} \ ,$$

where $\varepsilon > 0$ has the dimension of an energy. By application of the spectral theorem for densely-defined, linear and self-adjoint operators, Theorem 12.6.4, the latter implies that

$$e^{-i \frac{t}{\hbar} \bar{H}_0} g = \lim_{\varepsilon \to \infty} F_2^{-1} \exp(- \, \varepsilon_0 \, \sigma_\varepsilon \, |\ |^2) F_2 g \ .$$

Further, we note that, for every $\sigma \in (0, \infty) \times \mathbb{R}$ and according to Corollary 12.9.24

$$(2\sigma)^{n/2} . F_2 e^{-\sigma . |\ |^2} = e^{-|\ |^2/(4\sigma)} \ .$$

In particular for

$$\sigma = \frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} \ ,$$

it follows that

$$(2 \, \varepsilon_0 \, \sigma_\varepsilon)^{-n/2} \, F_2 \, e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |\ |^2} = e^{- \, \varepsilon_0 \, \sigma_\varepsilon |\ |^2} \ .$$

Hence

$$\begin{aligned} e^{-\left(\frac{1}{\varepsilon} + i \frac{t}{\hbar}\right) \bar{H}_0} g &= (2 \, \varepsilon_0 \, \sigma_\varepsilon)^{-n/2} \, F_2^{-1} [(F_2 \, e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |\ |^2}) \cdot F_2 g] \\ &= (2 \, \varepsilon_0 \, \sigma_\varepsilon)^{-n/2} \, F_2 \{ [(F_2 \, e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |\ |^2}) \cdot F_2 g] \circ (-\mathrm{id}_{\mathbb{R}^n}) \} \\ &= (4\pi \, \varepsilon_0 \, \sigma_\varepsilon)^{-n/2} \, e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |\ |^2} * g \ . \end{aligned}$$

and

$$e^{-i \frac{t}{\hbar} \bar{H}_0} g = \lim_{\varepsilon \to \infty} (4\pi \, \varepsilon_0 \, \sigma_\varepsilon)^{-n/2} \, e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |\ |^2} * g \ . \tag{12.35}$$

In particular, if $g \in L^1_{\mathbb{C}}(\mathbb{R}^n) \cap L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $t \neq 0$, for every $u \in \mathbb{R}^n$

$$\left[e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |\ |^2} * g \right](u) = \int_{\mathbb{R}} e^{-\frac{1}{4 \, \varepsilon_0 \, \sigma_\varepsilon} . |u - \mathrm{id}_{\mathbb{R}^n}|^2} g \, dv^n$$

$$= \int_{\mathbb{R}} e^{-\frac{1}{4\left(\frac{\varepsilon_0}{\varepsilon} + i\,\frac{\varepsilon_0 t}{\hbar}\right)} \cdot |u - \mathrm{id}_{\mathbb{R}^n}|^2} g\, dv^n$$

and

$$\left(e^{-\frac{1}{4\left(\frac{\varepsilon_0}{\varepsilon} + i\,\frac{\varepsilon_0 t}{\hbar}\right)} \cdot |u - \mathrm{id}_{\mathbb{R}^n}|^2} g \right)_{\varepsilon \in \mathbb{N}^*}$$

is a sequence of integrable function that is everywhere pointwise convergent to

$$e^{i\,\frac{\hbar}{4\varepsilon_0 t} \cdot |u - \mathrm{id}_{\mathbb{R}^n}|^2} g \ ,$$

and whose members are dominated by the integrable function $|g|$. Hence it follows from Lebesgue's dominated convergence theorem and for every $u \in \mathbb{R}^n$ that

$$\lim_{\varepsilon \to \infty} \left(e^{-\frac{1}{4\,\varepsilon_0\,\sigma_\varepsilon} \cdot |\ |^2} * g \right)(u) = \left(e^{i\,\frac{\hbar}{4\varepsilon_0 t} \cdot |\ |^2} * g \right)(u) \ .$$

As a consequence, (12.35) implies that

$$e^{-i\,\frac{t}{\hbar}\,\bar{H}_0} g = \left(\pi i\, \frac{4\varepsilon_0 t}{\hbar} \right)^{-n/2} \cdot \left(e^{i\,\frac{\hbar}{4\varepsilon_0 t} \cdot |\ |^2} * g \right) \ ,$$

for every $t \in \mathbb{R}^*$ and $g \in L^1_{\mathbb{C}}(\mathbb{R}^n) \cap L^2_{\mathbb{C}}(\mathbb{R}^n)$. Finally, the latter implies for $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$ and $t \in \mathbb{R}^*$ that

$$(e^{-i\,\frac{t}{\hbar}\,\bar{H}_0} g)(u) = \lim_{\nu \to \infty} \left(\pi i\, \frac{4\varepsilon_0 t}{\hbar} \right)^{-n/2} \cdot \left[e^{i\,\frac{\hbar}{4\varepsilon_0 t} \cdot |\ |^2} * (\chi_{[-\nu,\nu]^n}\, g) \right](u) \ ,$$

for almost all $u \in \mathbb{R}^n$. □

Corollary 12.7.2. Let $n \in \mathbb{N}^*$, $t > 0$, $z \in \mathbb{R} \times (-\infty, 0)$ and $\bar{H}_0$ the free Hamiltonian of quantum mechanics, then

$$e^{-i\,(t/\hbar)\,z\bar{H}_0} f = \left(\pi i\, 4\, \frac{\varepsilon_0 t}{\hbar}\, z \right)^{-n/2} e^{i\,|\ |^2 / \left(4\,\frac{\varepsilon_0 t}{\hbar}\, z\right)} * f \ ,$$

for every $f \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where

$$\varepsilon_0 := \frac{\hbar^2 \kappa^2}{2m} \ .$$

Proof. According to the proof of Theorem 12.7.1, for every bounded and universally measurable function $f : [0, \infty) \to \mathbb{C}$:

$$f(\bar{H}_0) = F_2^{-1} \circ T_{[f \circ (\varepsilon_0 . |\ |^2)]} \circ F_2 \ ,$$

where $T_{f \circ (\varepsilon_0 . |\ |^2)}$ is the maximal multiplication operator with the function $f \circ (\varepsilon_0 . |\ |^2)$, defined by

$$T_{f \circ (\varepsilon_0 . |\ |^2)} g := [f \circ (\varepsilon_0 . |\ |^2)] \cdot g \ ,$$

for every $g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. In particular, for $t > 0$, $z \in \mathbb{R} \times (-\infty, 0)$

$$e^{-i\,(t/\hbar)\,z\bar{H}_0} g = F_2^{-1} \exp[-i\,(\varepsilon_0 t/\hbar)\,z.|\ |^2] F_2 g = F_2^{-1} \exp[-|\ |^2/(4\sigma)] F_2 g \ ,$$

where

$$\sigma := -\frac{i}{4\,(\varepsilon_0 t/\hbar)\,z} = -\frac{iz^*}{4\,(\varepsilon_0 t/\hbar)\,|z|^2} \in (0,\infty) \times \mathbb{R} \ .$$

Further, since according to Corollary 12.9.24

$$(2\sigma)^{n/2}.F_2 e^{-\sigma.|\ |^2} = e^{-|\ |^2/(4\sigma)} \ ,$$

we have that

$$\begin{aligned}
& e^{-i\,(t/\hbar)\,z\bar{H}_0} g = (2\sigma)^{n/2}.F_2^{-1}[(F_2 e^{-\sigma.|\ |^2}) \cdot (F_2 g)] \\
& = (2\sigma)^{n/2}.F_2\{[(F_2 e^{-\sigma.|\ |^2}) \cdot (F_2 g)] \circ (-\mathrm{id}_{\mathbb{R}^n})\} \\
& = (2\pi)^{-n/2}\,(2\sigma)^{n/2}.F_1\{[(F_2 e^{-\sigma.|\ |^2}) \cdot (F_2 g)] \circ (-\mathrm{id}_{\mathbb{R}^n})\} \\
& = (\sigma/\pi)^{n/2}\,e^{-\sigma.|\ |^2} * g = [\pi i\,4\,(\varepsilon_0 t/\hbar)\,z]^{-n/2}\,e^{i\,|\ |^2/[4\,(\varepsilon_0 t/\hbar)\,z]} * g \ .
\end{aligned}$$

□

12.8 Solutions of Systems of Ordinary Differential Equations with Asymptotically Constant Coefficients

The following results, on the asymptotic of the solutions of systems of ordinary differential equations with asymptotically constant coefficients, was first proved by Dunkel in [14] (compare also [27, 6, 20]). To the experience of the author, these result are not widely known in physics. Similar results to Corollary 12.8.2 are well-known in the physics, but under the much stronger assumption that the coefficients of the systems are analytic.

Theorem 12.8.1. Let $n \in \mathbb{N} \setminus \{0\}$, $a \in \mathbb{R}$, $I := [a, \infty)$ and $I_0 := (a, \infty)$. In addition let A_0 be a diagonalizable complex $n \times n$ matrix and $e'_1, \dots, e'_n$ be a basis of $\mathbb{C}^n$ consisting of eigenvectors of A_0. Further, for each $j \in \{1, \cdots, n\}$, let λ_j be the eigenvalue corresponding to e'_j and P_j be the matrix representing the projection of $\mathbb{C}^n$ onto $\mathbb{C}.e'_j$ with respect to the canonical basis of $\mathbb{C}^n$. Finally, let A_1 be a continuous map from I into the complex $n \times n$ matrices $M(n \times n, \mathbb{C})$ such that A_{1jk} is Lebesgue integrable for each $j, k \in 1, ..., n$.

Then there is a C^1 map $R : I_0 \to M(n \times n, \mathbb{C})$ with $\lim_{t\to\infty} R_{jk}(t) = 0$ for each $j, k \in 1, \dots, n$ and such that $u : I_0 \to M(n \times n, \mathbb{C})$ defined by

$$u(t) := \sum_{j=1}^{n} \exp(\lambda_j t) \cdot (E + R(t)) \cdot P_j \tag{12.36}$$

for all $t \in I_0$ (where E is the $n \times n$ unit matrix), maps into the invertible $n \times n$ matrices and satisfies

$$u'(t) = (A_0 + A_1(t)) \cdot u(t) \tag{12.37}$$

for all $t \in I_0$.

This theorem has the following

Corollary 12.8.2. Let $n \in \mathbb{N} \setminus \{0\}$; $a, t_0 \in \mathbb{R}$ with $a < t_0$; $\mu \in \mathbb{N}$; $\alpha_\mu := 1$ for $\mu = 0$ and $\alpha_\mu := \mu$ for $\mu \neq 0$. In addition, let A_0 be a diagonalizable complex $n \times n$ matrix and $e'_1, \dots, e'_n$ be a basis of $\mathbb{C}^n$ consisting of eigenvectors of A_0. Further, for each $j \in \{1, \cdots, n\}$, let λ_j be the eigenvalue corresponding to e'_j and P_j be the matrix representing the projection of $\mathbb{C}^n$ onto $\mathbb{C}.e'_j$ with respect to the canonical basis of $\mathbb{C}^n$. Finally, let A_1 be a continuous map from (a, t_0) into the complex $n \times n$ matrices $M(n \times n, \mathbb{C})$, for which there is a number $c \in (a, t_0)$ such that the restriction of A_{1jk} to $[c, t_0)$ is Lebesgue integrable for each $j, k \in 1, ..., n$.

Then there is a C^1 map $R : (a, t_0) \to M(n \times n, \mathbb{C})$ with $\lim_{t \to 0} R_{jk}(t) = 0$ for each $j, k \in 1, \dots, n$ and such that $u : (a, t_0) \to M(n \times n, \mathbb{C})$ defined by

$$u(t) := \begin{cases} \sum_{j=1}^n (t_0 - t)^{-\lambda_j} \cdot (E + R(t)) \cdot P_j \text{ for } \mu = 0 \\ \sum_{j=1}^n \exp(\lambda_j (t_0 - t)^{-\mu}) \cdot (E + R(t)) \cdot P_j \text{ for } \mu \neq 0 \end{cases} , \tag{12.38}$$

for all $t \in (a, t_0)$ (where E is the $n \times n$ unit matrix), maps into the invertible $n \times n$ matrices and satisfies

$$u'(t) = \left(\frac{\alpha_\mu}{(t_0 - t)^{\mu+1}} A_0 + A_1(t) \right) \cdot u(t) \tag{12.39}$$

for each $t \in (a, t_0)$.

12.9 Miscellaneous

12.9.1 Operator Theory

Reduction of Operators

Theorem 12.9.1 (Commuting Self-Adjoint Operators). Let $(X, \langle \, | \, \rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ and $B : D(B) \to X$ densely-defined, linear and self-adjoint operators in X, with corresponding spectra $\sigma(A)$ and $\sigma(B)$, respectively, and E^A and E^B the spectral families that are associated with A and B, respectively. We say that B and A commute, if

$$\left[E^B_s, E^A_t \right] = 0 \ ,$$

for all $s, t \in \mathbb{R}$. Finally, let $U_A := (A - i)(A + i)^{-1}$ and $U_B := (B - i)(B + i)^{-1}$ be the Cayley transforms of A and B, respectively.

(i) If in addition $B \in L(X,X)$, then the following statements are equivalent.

a)
$$[g(B), f(A)] = 0 \ ,$$
for all $g \in \overline{U^s_{\mathbb{C}}(\sigma(B))}$ and $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

b) A und B commute.

c) $[B, U_A] = 0$.

d) $[B, e^{itA}] = 0$, for all $t \in \mathbb{R}$.

e) $A \circ B \supset B \circ A$.

(ii) The following statements are equivalent.

a)
$$[g(B), f(A)] = 0 \ ,$$
for all $g \in \overline{U^s_{\mathbb{C}}(\sigma(B))}$ and $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$.

b) A and B commute.

c) $[e^{isB}, e^{itA}] = 0$, for all $s, t \in \mathbb{R}$.

d) $[U_B, U_A] = 0$.

Proof. "Part (i)": In addition, let $B \in L(X,X)$.
"Part a) $\Rightarrow$ Part b)": Obvious.
"Part b) $\Rightarrow$ Part c)": Since A and B commute, it follows for $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that $\alpha < \beta$ and $\gamma < \delta$ that

$$[E^B_\delta - E^B_\gamma, E^A_\beta - E^A_\alpha] = \left[\left(\chi_{(\gamma,\delta]}\big|_{\sigma(B)}\right)(B), \left(\chi_{(\alpha,\beta]}\big|_{\sigma(A)}\right)(A)\right] = 0 \ . \quad (12.40)$$

Further, if $f : \mathbb{R} \to \mathbb{R}$ is a bounded continuous function and $s_\nu : \mathbb{R} \to \mathbb{R}$ is defined by

$$s_\nu := \sum_{\mu \in \{-2^{2\nu}, -2^{2\nu}+1, \dots, 2^{2\nu}-1\}} \inf\{f(\lambda) : \lambda \in (2^{-\nu} \cdot \mu, 2^{-\nu} \cdot (\mu+1)]\} \cdot \chi_{(2^{-\nu}\cdot\mu, 2^{-\nu}\cdot(\mu+1)]} \ ,$$

for every $\nu \in \mathbb{N}^*$, then $(s_\nu)_{\nu \in \mathbb{N}^*}$ is a uniformly bounded sequence of step functions that everywhere on $\mathbb{R}$ pointwise convergent to f and hence it follows from the spectral theorem, Theorem 12.6.4, that

$$\begin{aligned} &\left(f\big|_{\sigma(A)}\right)(A) = s - \lim_{\nu\to\infty} \left(s_\nu\big|_{\sigma(A)}\right)(A) \\ &= s - \lim_{\nu\to\infty} \sum_{\mu \in \{-2^{2\nu}, -2^{2\nu}+1, \dots, 2^{2\nu}-1\}} \inf\{f(\lambda) : \lambda \in (2^{-\nu} \cdot \mu, 2^{-\nu} \cdot (\mu+1)]\} \\ &\quad \cdot \left(\chi_{(2^{-\nu}\cdot\mu, 2^{-\nu}\cdot(\mu+1)]}\big|_{\sigma(A)}\right)(A) \ , \end{aligned}$$

$$\left(f\big|_{\sigma(B)}\right)(B) = s - \lim_{\nu\to\infty}\left(s_\nu\big|_{\sigma(B)}\right)(B)$$
$$= s - \lim_{\nu\to\infty}\sum_{\mu\in\{-2^{2\nu},-2^{2\nu}+1,\dots,2^{2\nu}-1\}} \inf\{f(\lambda):\lambda\in(2^{-\nu}\cdot\mu,2^{-\nu}\cdot(\mu+1)]\}$$
$$\cdot\left(\chi_{(2^{-\nu}\cdot\mu,2^{-\nu}\cdot(\mu+1)]}\big|_{\sigma(B)}\right)(B)\ .$$

From (12.40) and the latter, we conclude that

$$\left[\left(g\big|_{\sigma(B)}\right)(B),\left(f\big|_{\sigma(A)}\right)(A)\right] = 0\ ,$$

for all real-valued bounded continuous functions f and g on $\mathbb{R}$ and hence also that

$$\left[\left(g\big|_{\sigma(B)}\right)(B),\left(f\big|_{\sigma(A)}\right)(A)\right] = 0\ , \tag{12.41}$$

for all complex-valued bounded continuous functions f and g on $\mathbb{R}$. Further, since $B\in L(X,X)$, $\sigma(B)\subset\mathbb{R}$ is in particular compact. Hence there is $\nu_0\in\mathbb{N}^*$ such that $\sigma(B)\subset[-\nu_0,\nu_0]$. From (12.41), it follows that

$$[B,U_A] = \left[\mathrm{id}_{\sigma(B)}(B),\frac{\mathrm{id}_{\sigma(A)}-i}{\mathrm{id}_{\sigma(A)}+i}(A)\right] = 0\ .$$

"Part c) $\Rightarrow$ Part d)": Since $[B,U_A]=0$, it follows for $f\in D(A)$ that

$$\begin{aligned} B\circ(A-i)f &= B\circ(A-i)\circ(A+i)^{-1}(A+i)f \\ &= (A-i)\circ(A+i)^{-1}B\,(A+i)f \\ &= (A+i-2i)\circ(A+i)^{-1}B\,(A+i)f \\ &= B(A+i)f-2i(A+i)^{-1}B\,(A+i)f \end{aligned}$$

Hence,

$$Bf = (A+i)^{-1}B\,(A+i)f\in D(A)$$

and

$$(A+i)Bf = B\,(A+i)f$$

as well as

$$ABf = BAf\ .$$

Hence, it follows that

$$A\circ B\supset B\circ A$$

and from the spectral theorem, Theorem 12.6.4, that

$$[B,f(A)] = 0\ ,$$

for every $f\in\overline{U^s_{\mathbb{C}}(\sigma(A))}$.
"Part d) $\Rightarrow$ Part e)": If $[B,e^{itA}]=0$, for all $t\in\mathbb{R}$, we conclude as follows. If $f\in D(A)$, then $(\mathbb{R}\to X,t\mapsto e^{itA}f)$ is differentiable at $t=0$, with derivative iAf.

Therefore, since $B \in L(X, X)$, also $(\mathbb{R} \to X, t \mapsto Be^{itA}f) = (\mathbb{R} \to X, t \mapsto e^{itA}Bf)$ is differentiable at $t = 0$. Hence, $Bf \in D(A)$ and $BiAf = iABf$, implying that $BAf = ABf$. As a consequence, $A \circ B \supset B \circ A$.
"Part e) $\Rightarrow$ Part a)": If $A \circ B \supset B \circ A$, it follows from the spectral theorem, Theorem 12.6.4 that

$$[B, f(A)] = 0 \ ,$$

for $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$. From the latter and again from the spectral theorem, Theorem 12.6.4, it follows that

$$[g(B), f(A)] = 0 \ ,$$

for all $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}, g \in \overline{U^s_{\mathbb{C}}(\sigma(B))}$.
"Part (ii)": "Part a) $\Rightarrow$ Part b)": Obvious.
"Part b) $\Rightarrow$ Part c)": If A and B commute, it follows as in the proof of (i) "Part b) $\Rightarrow$ Part c)" that

$$\left[\left(g\big|_{\sigma(B)}\right)(B), \left(f\big|_{\sigma(A)}\right)(A)\right] = 0 \ ,$$

for all complex-valued bounded continuous functions f and g on $\mathbb{R}$ and hence in particular that $[e^{isB}, e^{itA}] = 0$, for all $s, t \in \mathbb{R}$.
"Part c) $\Rightarrow$ Part d)": Since $[e^{isB}, e^{itA}] = 0$, for all $s, t \in \mathbb{R}$, it follows for $s \in \mathbb{R}$, that

$$[\sin(sB), e^{itA}] = [\cos(sB), e^{itA}] = 0 \ ,$$

for all $t \in \mathbb{R}$ and hence from Part (i) that

$$[\sin(sB), U_A] = [\cos(sB), U_A] = 0 \ .$$

The latter implies also that

$$[\exp(isB), U_A] = 0 \ ,$$

for every $s \in \mathbb{R}$. Finally, from the latter and Part (i), we conclude that

$$[U_B, U_A] = 0 \ .$$

"Part d) $\Rightarrow$ Part a)": If $[U_B, U_A] = 0$, it follows as in the proof of (i) "Part c) $\Rightarrow$ Part d)" that

$$U_B \circ A \supset A \circ U_B \ ,$$

and hence from the spectral theorem, Theorem 12.6.4, that

$$[U_B, f(A)] = 0 \ ,$$

for $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$ and hence, again as in the proof of (i) "Part c) $\Rightarrow$ Part d)," that

$$B \circ f(A) \supset f(A) \circ B \ ,$$

and again from the spectral theorem, Theorem 12.6.4, that

$$[g(B), f(A)] = 0 \ ,$$

for all $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}, g \in \overline{U^s_{\mathbb{C}}(\sigma(B))}$. ☐

Lemma 12.9.2 (Reduction of Operators I). Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $(\phi \neq)\, \sigma(A)\, (\subset \mathbb{R})$ the spectrum of A, $P \in L(X, X)$ a non-trivial orthogonal projection that commutes with A and $Y := \operatorname{Ran} P$ the non-trivial and closed projection space corresponding to P. Then the following is true.

(i) By $A_P := (D(A) \cap Y \to Y, f \mapsto Af)$, there is defined a densely-defined, linear and self-adjoint Operator in Y. The spectrum $\sigma(A_P)$ of A_P is contained in $\sigma(A)$.

(ii) For every $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$,

$$f\big|_{\sigma(A_P)} \in \overline{U^s_{\mathbb{C}}\,(\sigma(A_P))} \text{ and } \big(f\big|_{\sigma(A_P)}\big)(A_p) = (Y \to Y, g \mapsto f(A)g)\ .$$

Proof. In the following, let $U : \mathbb{R} \to L(X, X)$ be the strongly continuous one-parameter unitary group that is generated by A.
"Part (i)": Since A and P commute, it follows that $U(t)$ leaves Y invariant, for every $t \in \mathbb{R}$ and hence that $U_P := (\mathbb{R} \to L(Y, Y), t \mapsto (Y \to Y, g \mapsto U(t)g))$ is well-defined. Further, the properties of U imply that U_P is a strongly continuous one-parameter unitary group, whose infinitesimal generator is given by $A_P := (D(A) \cap Y \to Y, f \mapsto Af)$. In the following, let $\sigma(A_P)$ be the non-empty real spectrum of A_P. For $\lambda \in \sigma(A_P)$, it follows that $A_P - \lambda$ is not bijective and hence also that $A - \lambda$ is not bijective, implying that $\lambda \in \sigma(A)$. Hence $\sigma(A_P) \subset \sigma(A)$.
"Part (ii)": From the definition of $U^s_{\mathbb{C}}(\sigma(A)), U^s_{\mathbb{C}}\,(\sigma(A_P))$ and the fact that $\sigma(A_p) \subset \sigma(A)$, it follows for $f \in U^s_{\mathbb{C}}(\sigma(A))$ that $f\big|_{\sigma(A_P)} \in U^s_{\mathbb{C}}(\sigma(A_P))$. Further, for $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$, there is a sequence $f_1, f_2, \dots$ of elements of $U^s_{\mathbb{C}}(\sigma(A))$ that converges uniformly on $\sigma(A)$ to f. Hence the sequence $f_1\big|_{\sigma(A_P)}, f_2\big|_{\sigma(A_P)}, \dots$ of elements of $U^s_{\mathbb{C}}(\sigma(A_P))$ converges uniformly on $\sigma(A_P)$ to $f\big|_{\sigma(A_P)}$, implying that $f\big|_{\sigma(A_P)} \in \overline{U^s_{\mathbb{C}}(\sigma(A_P))}$. Further, let $E : \mathbb{R} \to L(X, X)$ be the spectral family corresponding to A, and for every $g \in X$, let ψ_g be the spectral measure corresponding to A and g. Since A and P commute, it follows that $E(\lambda)$ leaves Y invariant, for every $\lambda \in \mathbb{R}$. The properties of E imply that $E_P : \mathbb{R} \to L(Y, Y)$ is a spectral family, where for every $\lambda \in \mathbb{R}$ the map $E_p(\lambda)$ is defined as the restriction in domain and in image to Y. From the spectral theorem, Theorem 12.6.2, it follows for every $g \in Y$ that $g \in D(A_P)$ if and only if $\mathrm{id}^2_{\mathbb{R}}$ is integrable with respect to ψ_g; for every $g \in D(A_P)$ the function $\mathrm{id}_{\mathbb{R}}$ is integrable with respect to ψ_g and $\langle g|A_P g\rangle = \int_{\mathbb{R}} \mathrm{id}_{\mathbb{R}}\, d\psi_g$. Hence it follows from Part (i) and from Theorem 12.6.2 that spectral family that corresponds to A_P coincides with E_P as well as that $\mathbb{R} \setminus \sigma(A_P)$ is a ψ_g zero set, for every $g \in Y$. From the spectral theorem, Theorem 12.6.4, we conclude for $f \in \overline{U^s_{\mathbb{C}}(\sigma(A))}$ and every $g \in Y$ that

$$\langle g|\big(f\big|_{\sigma(A_P)}\big)(A_P)g\rangle = \int_{\mathbb{R}} \widehat{f\big|_{\sigma(A_P)}}\, d\psi_g = \int_{\mathbb{R}} \hat{f}\, d\psi_g = \langle g|f(A)g\rangle\ \ ,$$

where for every $f : D \to \mathbb{C}$, defined on a subset $D \subset \mathbb{R}^n$, $n \in \mathbb{N}^*$, we define $\hat{f} : \mathbb{R}^n \to \mathbb{C}$ by $\hat{f}(\lambda) := f(\lambda)$, for every $\lambda \in D$ and $\hat{f}(\lambda) := 0$, for every $\lambda \in \mathbb{R}^n \backslash D$. Using the polarization identity, valid for every linear map $B : D(B) \to X$, defined on a subspace $D(B)$ of X,

$$\begin{aligned}\langle h|Bk\rangle = &\frac{1}{4}\left(\langle h+k|B(k+h)\rangle - \langle h-k|B(k-h)\rangle\right) \\ &+ \frac{1}{4i}\left(\langle h+ik|B(k+ih)\rangle - \langle h-ik|B(k-ih)\rangle\right) \ ,\end{aligned}$$

for $h, k \in D(B)$, it follows that

$$\langle g|\big(f\big|_{\sigma(A_P)}\big)(A_P)h\rangle = \langle g|f(A)h\rangle \ ,$$

for $g, h \in Y$. Further, since A and P commute, $f(A)$ is leaving Y invariant. Hence, we conclude that

$$\big(f\big|_{\sigma(A_P)}\big)(A_P) = (Y \to Y, g \mapsto f(A)g) \ .$$

□

Lemma 12.9.3 (Reduction of Operators II). Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and symmetric operator in X, $(P_j)_{j\in\mathbb{N}}$ a sequence of orthogonal projections with pairwise orthogonal projection spaces and such that

$$s - \lim_{n\to\infty} \sum_{j=0}^{n} P_j = \mathrm{id}_X \ .$$

Furthermore, for every $j \in \mathbb{N}$ let D_j be a dense subspace of $\mathrm{Ran} P_j$ with $D_j \subset D(A)$, $A\,(D_j) \subset \mathrm{Ran}\, P_j$ and such that densely-defined, linear and symmetric operator $A_j := (D_j \to \mathrm{Ran}\, P_j, f \mapsto Af)$ in $\mathrm{Ran}\, P_j$ is essentially self-adjoint. Then

(i) A is essentially self-adjoint,

(ii) $\bar{A} \circ P_j \supset P_j \circ \bar{A}$, for every $j \in \mathbb{N}$.

Proof. Since for every $j \in \mathbb{N}$, D_j $(\subset D(A))$ is dense in $\mathrm{Ran}\, P_j$ and

$$s - \lim_{N\to\infty} \sum_{j=0}^{N} P_j = \mathrm{id}_X \ ,$$

it follows that the subspace $D\,(A_c) := \mathcal{L}\left(\bigcup_{j\in\mathbb{N}} D_j\right)$ of $D(A)$ is dense in X and hence that $A_c := A\big|_{D(A_c)}$ is a densely-defined, linear and symmetric operator in X. Further, for every $f \in [\mathrm{Ran}\,(A_c \pm i.\mathrm{id}_X)]^{\perp}$ and $j \in \mathbb{N}$ follows that $P_j f \in \left[\mathrm{Ran}\left(A_j \pm i.\mathrm{id}_{\mathrm{Ran}\, P_j}\right)\right]^{\perp}$ and hence, since $A_j^* = \bar{A}_j^*$, A_j is essentially self-adjoint and from properties of the Cayley transform and related results on self-adjoint extensions of densely-defined, linear and symmetric operators, that $P_j f = 0$. Since $j \in \mathbb{N}$ is arbitrary otherwise and since $s - \lim_{N \to \infty} \sum_{j=0}^{N} P_j = \mathrm{id}_X$, this implies that $f = 0$. Since f is arbitary otherwise, and since $A_c^* = \bar{A}_c^*$, it follows, from properties of the Cayley transform and related results on self-adjoint extensions of densely-defined, linear and symmetric operators, the essential self-adjointness of A_c and since $\bar{A}_c \subset \bar{A}$ that $\bar{A}_c = \bar{A}$ and hence also the essential self-adjointness of A. Further, for every $j \in \mathbb{N}$ follows that $A_c \circ P_j \supset P_j \circ A_c$, implying that $\bar{A}_c \circ P_j \supset P_j \circ \bar{A}_c$, and hence, since $\bar{A}_c = \bar{A}$, that $\bar{A} \circ P_j \supset P_j \circ \bar{A}$. □

Corollary 12.9.4. Under the assumptions of Lemma 12.9.3, it follows that

$$\bar{A}|_{D(\bar{A}\,) \cap \mathrm{Ran}(P_j)} = \bar{A}_j \ , \tag{12.42}$$

for every $j \in \mathbb{N}$, where $\bar{A}_j$ denotes the closure of A_j in $\mathrm{Ran}(P_j)$.

Proof. According to Lemma 12.9.2, $\bar{A}|_{D(\bar{A}\,) \cap \mathrm{Ran}(P_j)}$ is a densely-defined, linear and self-adjoint operator in $\mathrm{Ran}(P_j)$. Also, $\bar{A}|_{D(\bar{A}\,) \cap \mathrm{Ran}(P_j)}$ is an extension of A_j. Since, according to the assumptions, A_j is a densely-defined, linear, symmetric and essentially self-adjoint operator in $\mathrm{Ran}(P_j)$, this implies that (12.42) is true. □

A decomposition of an operator as in Lemma 12.9.3 induces a decomposition of the spectrum of that operator.

Theorem 12.9.5 (Reduction of Operators III). Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $(\phi \neq)\, \sigma(A)\ (\subset \mathbb{R})$ the spectrum of A. In addition, let $(P_n)_{n \in \mathbb{N}}$ be a sequence of orthogonal projections with pairwise orthogonal projection spaces that commute with A. According to Lemma 12.9.2, for every $n \in \mathbb{N}$ by $A_n := (D(A) \cap \mathrm{Ran}\, P_n \to \mathrm{Ran}\, P_n, f \mapsto Af)$, there is defined a densely-defined, linear and self-adjoint operator in $\mathrm{Ran}\, P_n$. Finally, let $\sigma(A_n), \sigma_p(A_n)$ be the spectrum of A_n and the point spectrum, i.e., the set of all eigenvalues, of A_n, respectively. We note that $\sigma(A_n) = \phi$, if $\mathrm{Ran}\, P_n = \{0\}$. Then

$$\sigma_p(A) = \bigcup_{n \in \mathbb{N}} \sigma_p(A_n) \ , \ \sigma(A) = \overline{\bigcup_{n \in \mathbb{N}} \sigma(A_n)} \ .$$

Proof. First, we note that obviously $\sigma_p(A_n) \subset \sigma_p(A)$, for every $n \in \mathbb{N}$ and hence that $\bigcup_{n \in \mathbb{N}} \sigma_p(A_n) \subset \sigma_p(A)$. Since $s - \lim_{N \to \infty} \sum_{n=0}^{N} P_n = \mathrm{id}_X$, it follows for $\lambda \in \sigma_p(A)$, $f \in \ker(A - \lambda) \setminus \{0\}$ the existence of $n_0 \in \mathbb{N}$ such that $P_{n_0} f \neq 0$ and hence, since $A_{n_0} P_{n_0} f = A P_{n_0} f = P_{n_0} A f = \lambda P_{n_0} f$, that $\lambda \in \sigma_p(A_{n_0})$ as well as $\lambda \in \bigcup_{n \in \mathbb{N}} \sigma_p(A_n)$. Therefore, we conclude that $\sigma_p(A) = \bigcup_{n \in \mathbb{N}} \sigma_p(A_n)$. Further, if $n \in \mathbb{N}$ and $\lambda \in \sigma(A_n)$, then there is according to Theorem 12.5.3 (ii) a sequence $f_1, f_2, \dots$ of unit vectors in $D(A_n)$ such that

$$0 = \lim_{\nu \to \infty} (A_n - \lambda) f_\nu = \lim_{\nu \to \infty} (A - \lambda) f_\nu \ .$$

Hence, it follows from Theorem 12.5.3 (ii) that $\lambda \in \sigma(A)$. Therefore, we conclude that $\sigma(A_n) \subset \sigma(A)$ for every $n \in \mathbb{N}$ and hence that $\bigcup_{n\in\mathbb{N}} \sigma(A_n) \subset \sigma(A)$ as well as that

$$\overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)} \subset \sigma(A) \ ,$$

since $\sigma(A)$ is in particular a closed subset of $\mathbb{R}$, Finally, it follows that

$$\sigma(A) \setminus \overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)} = \phi$$

and hence that

$$\overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)} = \sigma(A) \ .$$

Otherwise, there is $\lambda \in \sigma(A) \setminus \overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)}$ and follows the existence of

$$d := \min\left\{|\mu - \lambda| : \mu \in \overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)}\right\}$$

as well as that $d > 0$, where we use that, since X is non-trivial and $s - \lim_{N\to\infty} \sum_{n=0}^{N} P_n = \text{id}_X$, there is $n \in \mathbb{N}$ such hat $\text{Ran}\, P_n$ is non-trivial and hence that $\overline{\bigcup_{n\in\mathbb{N}} \sigma(A_n)}$ is non-empty. Therefore, from the spectral theorem Theorem 12.6.4, it follows that

$$\|(A_n - \lambda)^{-1}\| \leqslant \frac{1}{d} \ ,$$

for $n \in \mathbb{N}$ such that $\text{Ran}\, P_n$ is non-trivial. Further, for $f \in X$ and $N, N' \in \mathbb{N}$, we conclude that

$$\begin{aligned}
&= \left\|\sum_{n=0}^{N}(A_n - \lambda)^{-1}P_n f - \sum_{n=0}^{N'}(A_n - \lambda)^{-1}P_n f\right\|^2 = \left\|\sum_{n=m+1}^{M}(A_n - \lambda)^{-1}P_n f\right\|^2 \\
&= \sum_{n=m+1}^{M}\ \sum_{n'=m+1}^{M} \langle (A_n - \lambda)^{-1}P_n f | (A_{n'} - \lambda)^{-1}P_{n'} f\rangle \\
&= \sum_{n=m+1}^{M} \|(A_n - \lambda)^{-1}P_n f\|^2 \leqslant \frac{1}{d^2} \cdot \left\|\sum_{n=m+1}^{M} P_n f\right\| \\
&= \frac{1}{d^2}\left\|\sum_{n=0}^{N} P_n f - \sum_{n=0}^{N'} P_n f\right\|^2 \ ,
\end{aligned}$$

where $m := \min\{N, N'\}\, , M := \max\{N, N'\}$. Since

$$\lim_{N\to\infty} \sum_{n=0}^{N} P_n f = f \ ,$$

it follows that
$$\left(\sum_{n=0}^{N}(A_n-\lambda)^{-1}P_n f\right)_{N\in\mathbb{N}}$$
is a Cauchy sequence in X and hence convergent to some $g_f \in X$,
$$\lim_{N\to\infty}\sum_{n=0}^{N}(A_n-\lambda)^{-1}P_n f = g_f\ ,$$
since X is complete. Since
$$\lim_{N\to\infty}(A-\lambda)\sum_{n=0}^{N}(A_n-\lambda)^{-1}P_n f = \lim_{N\to\infty}\sum_{n=0}^{N}P_n f = f\ ,$$
and $A-\lambda$ is closed, we conclude hat $(g_f, f) \in G(A-\lambda)$ and hence that $g_f \in D(A)$ and $(A-\lambda)g_f = f$. Hence $A-\lambda$ is surjective. Finally, since
$$\lambda \in \sigma(A) \setminus \overline{\bigcup_{n\in\mathbb{N}}\sigma(A_n)} \subset \sigma(A)\setminus\sigma_p(A)\ ,$$
$A-\lambda$ is also injective and hence bijective. As a consequence, we arrive at the contradiction that $\lambda \notin \sigma(A)$.↯ □

Lemma 12.9.6 (Reduction of Operators IV). Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, $P_0, P_1, \dots$ be a sequence of orthogonal projections on X with pairwise orthogonal projection spaces and such that
$$\lim_{n\to\infty}\sum_{j=0}^{n}P_j f = f\ , \tag{12.43}$$
for every $f \in X$. Further, for each $j \in \mathbb{N}$, let $A_j : D_j \to \text{Ran}(P_j)$ be a densely-defined, linear, symmetric and essentially self-adjoint operator in $\text{Ran}(P_j)$. We define the subspace $D \leqslant X$ by
$$D := \left\{\sum_{j=0}^{n} f_j :\ n \in \mathbb{N} \text{ and } f_j \in D_j, \text{ for every } j \in \{1,\dots,n\}\right\}\ ,$$
and $A : D \to X$ by
$$A\sum_{j=0}^{n} f_j := \sum_{j=0}^{n} A_j f_j\ ,$$
where $n \in \mathbb{N}$ and $f_j \in D_j$, for every $j \in \{0,\dots,n\}$. Then A is a densely-defined, linear, symmetric and essentially self-adjoint operator in X, whose closure $\bar{A}$ commutes strongly with every P_j, $j \in \mathbb{N}$, i.e.,
$$\bar{A}\circ P_j \supset P_j \circ \bar{A} \tag{12.44}$$
holds for each $j \in \mathbb{N}$.

Proof. First, we note that if

$$\sum_{j=0}^{n} f_j = \sum_{j=0}^{m} g_j \ ,$$

where $n, m \in \mathbb{N}$ and $f_j \in D_j$, for every $j \in \{0, \dots, n\}$, $g_j \in D_j$, for every $j \in \{0, \dots, m\}$, it follows from the pairwise orthogonality of $\mathrm{Ran}(P_0), \mathrm{Ran}(P_1), \dots$, that

$$\begin{cases} f_j = g_j \text{ for } j = 0, \dots n \text{ and } g_j = 0 \text{ for } j = n+1, \dots m & \text{if } m \geqslant n \\ f_j = g_j \text{ for } j = 0, \dots m \text{ and } f_j = 0 \text{ for } j = m+1, \dots n & \text{if } m < n \end{cases}$$

and hence also that

$$\begin{cases} A_j f_j = A_j g_j \text{ for } j = 0, \dots n \text{ and } A_j g_j = 0 \text{ for } j = n+1, \dots m & \text{if } m \geqslant n \\ A_j f_j = A_j g_j \text{ for } j = 0, \dots m \text{ and } A_j f_j = 0 \text{ for } j = m+1, \dots n & \text{if } m < n \end{cases} .$$

As a consequence, A is well-defined. Further, for $f \in X$, since D_j is dense in $\mathrm{Ran}(P_j)$, there is f_j such that

$$\|P_j f - f_j\| \leqslant 2^{-(j+2)} \varepsilon \ ,$$

for every $j \in \mathbb{N}$, where $\varepsilon > 0$. Hence

$$\begin{aligned} \left\| \sum_{j=0}^{n} f_j - f \right\| &= \left\| \sum_{j=0}^{n} (f_j - P_j f) + \sum_{j=0}^{n} P_j f - f \right\| \\ &\leqslant \left\| \sum_{j=0}^{n} (f_j - P_j f) \right\| + \left\| \sum_{j=0}^{n} P_j f - f \right\| \\ &\leqslant \frac{\varepsilon}{2} + \left\| \sum_{j=0}^{n} P_j f - f \right\| \ . \end{aligned}$$

Hence, as consequence of (12.43), there is $n_0 \in \mathbb{N}$, such that

$$\left\| \sum_{j=0}^{n} f_j - f \right\| \leqslant \varepsilon \ ,$$

for $n \in \mathbb{N}$ such that $n \geqslant n_0$. This implies that D is dense in X. Also, A is linear. Summarizing the previous, A is a densely-defined, linear operator in X. In addition, A is symmetric, since if $n, m \in \mathbb{N}$ and $f_j \in D_j$, for every $j \in \{0, \dots, n\}$, $g_j \in D_j$, for every $j \in \{0, \dots, m\}$, then

$$\langle \sum_{j=0}^{n} f_j | A \sum_{k=0}^{m} g_k \rangle = \langle \sum_{j=0}^{n} f_j | \sum_{k=0}^{m} A_k g_k \rangle = \sum_{j=0}^{n} \sum_{k=0}^{m} \langle f_j | A_k g_k \rangle$$

$$
\begin{aligned}
&= \sum_{j=0}^{n} \langle f_j | A_j g_j \rangle = \sum_{j=0}^{n} \langle A_j f_j | g_j \rangle \\
&= \sum_{j=0}^{n} \sum_{k=0}^{m} \langle A_j f_j | g_k \rangle = \langle\, A \sum_{j=0}^{n} f_j | \sum_{k=0}^{m} g_k \,\rangle \ .
\end{aligned}
$$

From the characterization of essential self-adjointness in Theorem 12.4.9, it follows for every $j \in \mathbb{N}$ that $\mathrm{Ran}(A_j - i)$ and $\mathrm{Ran}(A_j + i)$ are dense in $\mathrm{Ran}(P_j)$. Hence for $g \in X$, $\varepsilon > 0$, $j \in \mathbb{N}$, there is $f_j \in D_j$ such that

$$
\|(A_j \underset{(-)}{+} i) f_j - P_j g\|^2 \leqslant 2^{-(j+1)} \, \frac{\varepsilon^2}{4} \ .
$$

Hence,

$$
\begin{aligned}
&\left\| (A \underset{(-)}{+} i) \sum_{j=0}^{n} f_j - \sum_{j=0}^{n} P_j g \right\|^2 = \left\| \sum_{j=0}^{n} [(A_j \underset{(-)}{+} i) f_j - P_j g] \right\|^2 \\
&= \sum_{j=0}^{n} \|(A_j \underset{(-)}{+} i) f_j - P_j g\|^2 \leqslant \sum_{j=0}^{n} 2^{-(j+1)} \, \frac{\varepsilon^2}{4} \leqslant \frac{\varepsilon^2}{4} \ .
\end{aligned}
$$

If

$$
\left\| \sum_{j=0}^{n} P_j g - g \right\|^2 \leqslant \frac{\varepsilon^2}{4} \ ,
$$

this implies that

$$
\left\| (A \underset{(-)}{+} i) \sum_{j=0}^{n} f_j - g \right\|^2 \leqslant \varepsilon^2 \ .
$$

Hence, $\mathrm{Ran}(A \underset{(-)}{+} i)$ is dense in X and, according to the characterization of essential self-adjointness in Theorem 12.4.9, A is essentially self-adjoint. We note that for every $k \in \mathbb{N}$, if $k \in \{0, \dots, n\}$, then

$$
P_k A \sum_{j=0}^{n} f_j = P_k \sum_{j=0}^{n} A_j f_j = A_k f_k = \sum_{j=0}^{n} A_k P_k f_j = A \sum_{j=0}^{n} P_k f_j = A P_k \sum_{j=0}^{n} f_j \ ,
$$

and if $k \notin \{0, \dots, n\}$, then

$$
P_k A \sum_{j=0}^{n} f_j = P_k \sum_{j=0}^{n} A_j f_j = 0 = \sum_{j=0}^{n} A_k P_k f_j = A \sum_{j=0}^{n} P_k f_j = A P_k \sum_{j=0}^{n} f_j \ ,
$$

where $n \in \mathbb{N}$ and $f_j \in D_j$, for every $j \in \{0, \dots, n\}$. Hence for every $j \in \mathbb{N}$, $f \in D$, we have that

$$
P_j A f = A P_j f \ .
$$

Further, for $f \in D(\bar{A})$, there is a sequence $f_1, f_2, \ldots$ in D such that

$$\lim_{\nu \to \infty} f_\nu = f \text{ and } \lim_{\nu \to \infty} A f_\nu = \bar{A} f \ .$$

Then, for $j \in \mathbb{N}$,

$$\lim_{\nu \to \infty} P_j f_\nu = P_j f \text{ and } \lim_{\nu \to \infty} P_j A f_\nu = \lim_{\nu \to \infty} A P_j f_\nu = P_j \bar{A} f \ .$$

Hence, $P_j f \in D(\bar{A})$ and $\bar{A} P_j f = P_j \bar{A} f$, and it follows that $\bar{A} \circ P_j \supset P_j \circ \bar{A}$. □

Calculation of the Functional Calculus

Lemma 12.9.7 (A Relation Between the Functional Calculus of an Operator and the Generated Strongly Continuous One-Parameter Unitary Group). Let $(X, \langle \,|\, \rangle)$ be a non-trivial complex Hilbert space, $U : \mathbb{R} \to L(X, X)$ a strongly continuous one-parameter unitary group, with, (hence densely-defined, linear and self-adjoint), infinitesimal generator $A : D(A) \to X$. In addition, let $\sigma(A) \subset \mathbb{R}$ be the non-empty spectrum of A. Hence,

$$U(t) = \exp(it.\mathrm{id}_{\sigma(A)})(A) \ ,$$

for every $t \in \mathbb{R}$. Then,

$$\left(F_1(f)\big|_{\sigma(A)} \right)(A) = \int_{\mathbb{R}} f(t).U(-t) \, dt \ ,$$

for every $f \in L^1_{\mathbb{C}}(\mathbb{R})$, where we use weak integration.

Proof. In the following, let $F_0 : \mathscr{S}_{\mathbb{C}}(\mathbb{R}) \to \mathscr{S}_{\mathbb{C}}(\mathbb{R})$ be the linear isomorphism, defined for every $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R})$ by

$$[F_0(f)](v) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ivu} f(u) \, du \ ,$$

for every $v \in \mathbb{R}$. Then, $F_0^{-1} : \mathscr{S}_{\mathbb{C}}(\mathbb{R}) \to \mathscr{S}_{\mathbb{C}}(\mathbb{R})$ is given by

$$[F_0^{-1}(f)](u) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{iuv} f(v) \, dv \ ,$$

for every $u \in \mathbb{R}$. In first step, we show for $f \in C_0^\infty(\mathbb{R}, \mathbb{C})$ that

$$\langle g_1 | \left(F_0^{-1}(f)\big|_{\sigma(A)} \right)(A) g_2 \rangle = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(t) \cdot \langle g_1 | U(t) g_2 \rangle \ dt \ , \tag{12.45}$$

for all $g_1, g_2 \in X$. For the proof, let $f \in C_0^\infty(\mathbb{R}, \mathbb{C})$. Since f has a compact support, there is $N \in \mathbb{N}^*$ such that $\mathrm{supp}(f) \subset [-N, N)$. Hence for $\lambda \in \mathbb{R}$,

$$\left(\sum_{k=0}^{2N\nu - 1} \left(e^{i\lambda \, \mathrm{id}_{\mathbb{R}}} f \right) \left(-N + \frac{k}{v} \right) \cdot \chi_{[-N + \frac{k}{\nu}, -N + \frac{k+1}{\nu})} \right)_{\nu \in \mathbb{N}^*}$$

is a sequence of integrable functions whose members are dominated by the integrable function

$$\left(\sup_{t \in \text{supp}(f)} |f(t)| \right) \cdot \chi_{[-N,N]}$$

that is pointwise on $\mathbb{R}$ convergent to $e^{i\lambda \, \text{id}_{\mathbb{R}}} f$, since the latter function is in particular continuous. Hence it follows from Lebesgue's dominated convergence theorem that

$$[F_0^{-1}(f)](\lambda) = \lim_{\nu \to \infty} \frac{(2\pi)^{-1/2}}{\nu} \sum_{k=0}^{2N\nu-1} \left(e^{i\lambda \, \text{id}_{\mathbb{R}}} f\right)\left(-N + \frac{k}{v}\right) \ .$$

We note that by the same reasoning, it follows that

$$\int_{\mathbb{R}} g(t)\, dt = \lim_{\nu \to \infty} \frac{1}{\nu} \sum_{k=0}^{2N\nu-1} g\left(-N + \frac{k}{v}\right) \ ,$$

for every $g \in C_0(\mathbb{R}, \mathbb{C})$. Further,

$$\left(\frac{(2\pi)^{-1/2}}{\nu} \sum_{k=0}^{2N\nu-1} f\left(-N + \frac{k}{v}\right) e^{i\left(-N+\frac{k}{\nu}\right)\text{id}_{\mathbb{R}}} \Big|_{\sigma(A)} \right)_{\nu \in \mathbb{N}^*}$$

is a sequence of bounded continuous functions on $\sigma(A)$ that is pointwise convergent to $F_0^{-1}(f)\big|_{\sigma(A)}$ and is uniformly bounded, e.g., by

$$\frac{2N}{\sqrt{2\pi}} \left(\sup_{t \in \text{supp}(f)} |f(t)| \right) \ .$$

Hence it follows from Theorem 12.6.4 that

$$\left(F_0^{-1}(f)\big|_{\sigma(A)}\right)(A) = s - \lim_{\nu \to \infty} \frac{(2\pi)^{-1/2}}{\nu} \cdot \sum_{k=0}^{2N\nu-1} (f.U)\left(-N + \frac{k}{\nu}\right)$$

and hence also that

$$\begin{aligned} &\langle g_1 | \left(F_0^{-1}(f)\big|_{\sigma(A)}\right)(A) g_2 \rangle \\ &= \lim_{\nu \to \infty} \frac{(2\pi)^{-1/2}}{\nu} \cdot \sum_{k=0}^{2N\nu-1} (f \cdot \langle g_1 | U g_2 \rangle)\big(-N + \frac{k}{\nu}\big) \\ &= (2\pi)^{-1/2} \int_{\mathbb{R}} f(t) \cdot \langle g_1 | U(t) g_2 \rangle \ dt \ , \end{aligned}$$

for all $g_1, g_2 \in X$. The latter implies that

$$\left(F_0^{-1}(f)\big|_{\sigma(A)}\right)(A) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(t).\, U(t)\, dt \ .$$

For the second step, let $g_1, g_2 \in X$ und $f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R})$. In addition, let $\varphi \in C^\infty(\mathbb{R}, \mathbb{R})$ be an auxiliary function, defined by

$$\varphi(t) := \begin{cases} 0 & \text{if } t \leqslant 0 \\ e^{-\frac{1}{t}} & \text{if } t > 0 \end{cases} .$$

Then $\operatorname{Ran}\varphi \subset [0,1)$ and $\lim_{t\to\infty}\varphi(t) = 1$. We define for $\nu \in \mathbb{N}^*$ the auxiliary function $\varphi_\nu \in C_0^\infty(\mathbb{R}, \mathbb{R})$ by

$$\varphi_\nu(t) := \varphi(\nu \cdot (\nu^2 - t^2)) ,$$

for every $t \in \mathbb{R}$. We note that $\operatorname{supp}(\varphi_\nu) \subset [-\nu, \nu]$, $\operatorname{Ran}\varphi_\nu \subset [0,1)$ and everywhere pointwise

$$\lim_{\nu\to\infty} \varphi_\nu = \chi_{_\mathbb{R}} .$$

Hence $(\langle g_1 | U g_2 \rangle \, \varphi_\nu f)_{\nu\in\mathbb{N}^*}$ is a sequence of integrable functions whose members are dominated by the Lebesgue integrable function $\|g_1\| \|g_2\| |f|$. Thus it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\nu\to\infty} (2\pi)^{-1/2} \int_{\mathbb{R}} \langle g_1 | U(t) g_2 \rangle \, \varphi_\nu(t) f(t) \, dt = (2\pi)^{-1/2} \int_{\mathbb{R}} \langle g_1 | U(t) g_2 \rangle \, f(t) \, dt . \tag{12.46}$$

Further, $\left(F_0^{-1}(\varphi_\nu f)\right)_{\nu\in\mathbb{N}^*} \in (\mathscr{S}_{\mathbb{C}}(\mathbb{R}))^{\mathbb{N}^*}$ is a sequence that is uniformly bounded by $(2\pi)^{-1/2}\|f\|_1$ and that is everywhere pointwise convergent to $F_0^{-1} f \in \mathscr{S}_{\mathbb{C}}(\mathbb{R})$, since for every $\lambda \in \mathbb{R}$, $\left(e^{i\lambda\, \mathrm{id}_{\mathbb{R}}} \varphi_\nu f\right)_{\nu\in\mathbb{N}^*}$ is a sequence of integrable functions whose members are dominated by the integrable function $|f|$ and that is everywhere convergent to $e^{i\lambda\, \mathrm{id}_{\mathbb{R}}} f$, according to Lebesgue's dominated convergence theorem implying that

$$\lim_{\nu\to\infty} \int_{\mathbb{R}} e^{i\lambda\, t} \varphi_\nu(t) f(t) \, dt = \int_{\mathbb{R}} e^{i\lambda\, t} f(t) \, dt .$$

Hence it follows from Theorem 12.6.4 that

$$s - \lim_{\nu\to\infty} \left(F_0^{-1}(\varphi_\nu f)\big|_{\sigma(A)} \right)(A) = \left(F_0^{-1}(f)\big|_{\sigma(A)} \right)(A)$$

and hence also that

$$\lim_{\nu\to\infty} \langle g_1 | \left(F_0^{-1}(\varphi_\nu f)\big|_{\sigma(A)} \right)(A) g_2 \rangle = \langle g_1 | \left(F_0^{-1}(f)\big|_{\sigma(A)} \right)(A) g_2 \rangle . \tag{12.47}$$

From (12.45), (12.46) and (12.47), it follows that

$$\langle g_1 | \left(F_0^{-1}(f)\big|_{\sigma(A)} \right)(A) g_2 \rangle = (2\pi)^{-1/2} \int_{\mathbb{R}} \langle g_1 | U(t) g_2 \rangle \, f(t) \, dt .$$

Finally, since F_0 bijective, we conclude that

$$\langle g_1 | \left(f|_{\sigma(A)} \right)(A) g_2 \rangle = (2\pi)^{-1/2} \int_{\mathbb{R}} (F_0(f))(t) \, \langle g_1 | U(t) g_2 \rangle \, dt$$

as well as that

$$\begin{aligned}
&\langle g_1| \big(F_1(f)|_{\sigma(A)}\big)(A)g_2\rangle = (2\pi)^{1/2} \langle g_1| \big(F_0(f)|_{\sigma(A)}\big)(A)g_2\rangle \\
&= \int_{\mathbb{R}} (F_0(F_0 f))(t) \langle g_1|U(t)g_2\rangle \, dt = \int_{\mathbb{R}} (F_0(F_0 f))(-t) \langle g_1|U(-t)g_2\rangle \, dt \\
&= \int_{\mathbb{R}} f(t) \langle g_1|U(-t)g_2\rangle \, dt \, . \qquad (12.48)
\end{aligned}$$

Further, since $\mathscr{S}_{\mathbb{C}}(\mathbb{R})$ is dense in $L^1_{\mathbb{C}}(\mathbb{R})$, for $f \in L^1_{\mathbb{C}}(\mathbb{R})$, there is a sequence $(f_\nu)_{\nu\in\mathbb{N}}$ in $\mathscr{S}_{\mathbb{C}}(\mathbb{R})$ that converges in $L^1_{\mathbb{C}}(\mathbb{R})$ to f. Then $f \cdot \langle g_1|[U \circ (-\mathrm{id}_{\mathbb{R}})]g_2\rangle$ is integrable, since $\langle g_1|[U \circ (-\mathrm{id}_{\mathbb{R}})]g_2\rangle$ is bounded continuous. Further,

$$\begin{aligned}
&\left| \int_{\mathbb{R}} f_\nu(t) \langle g_1|[U(-t)]g_2\rangle \, dt - \int_{\mathbb{R}} f(t) \langle g_1|U(-t)]g_2\rangle \, dt \right| \\
&\leqslant \int_{\mathbb{R}} |f_\nu(t) - f(t)| \cdot |\langle g_1|[U(-t)]g_2\rangle| \, dt \leqslant \|g_1\| \, \|g_2\| \, \|f_\nu - f\|_1
\end{aligned}$$

and hence

$$\lim_{\nu\to\infty} \int_{\mathbb{R}} f_\nu(t) \langle g_1|[U(-t)]g_2\rangle \, dt = \int_{\mathbb{R}} f(t) \langle g_1|U(-t)]g_2\rangle \, dt \, .$$

Also, since $F_1 : L^1_{\mathbb{C}}(\mathbb{R}) \to (C_\infty(\mathbb{R}, \mathbb{C}), \| \, \|_\infty)$ is continuous, the sequence $(F_1(f_\nu))_{\nu\in\mathbb{N}}$ converges uniformly on $\mathbb{R}$ to $F_1(f)$. Thus, the sequence $(F_1(f_\nu)|_{\sigma(A)})_{\nu\in\mathbb{N}}$ is a uniformly bounded sequence of universally measurable functions that is everywhere pointwise convergent on $\sigma(A)$ to $F_1(f)|_{\sigma(A)}$. Thus, from Theorem 12.6.4, it follows that

$$s - \lim_{\nu\to\infty} (F_1(f_\nu)|_{\sigma(A)})(A) = (F_1(f)|_{\sigma(A)})(A) \, .$$

Hence, it follows from (12.48) that

$$\langle g_1| \big(F_1(f)|_{\sigma(A)}\big)(A)g_2\rangle = \int_{\mathbb{R}} f(t) \langle g_1|U(-t)g_2\rangle \, dt \, .$$

□

Theorem 12.9.8 (A Relation between the Resolvent of an Operator and its Spectral Projections). Let $(X, \langle \, | \, \rangle)$ be a non-trivial complex Hilbert space, $A : D(A) \to X$ a densely-defined, linear and self-adjoint operator in X and $\sigma(A)$ the (non-empty and real) spectrum of A, $R : \mathbb{C} \setminus \sigma(A) \to L(X, X), \lambda \mapsto (A - \lambda)^{-1}$ the resolvent of A and $U : \mathbb{R} \to L(X, X)$ the strongly continuous one-parameter unitary group that is generated by A, given by $U(t) = e^{itA}$, for every $t \in \mathbb{R}$. Further, for every $f : \mathbb{R} \to \mathbb{C}$, $a : \mathbb{R} \to L(X, X)$, we define $fa := (\mathbb{R} \to L(X, X), t \mapsto f(t)a(t))$. Finally, let $\alpha, \beta \in \mathbb{R}$, such that $\alpha < \beta$. Then, the following is true.

(i) For $\lambda \in \mathbb{R} \times \mathbb{R}^*$ and $f \in X$:

$$R(\lambda)f = \begin{cases} i\int_{-\infty}^{0} \exp(-i\lambda t)U(t)f\,dt & \text{if } \mathrm{Im}(\lambda) > 0 \\ -i\int_{0}^{\infty} \exp(-i\lambda t)U(t)f\,dt & \text{if } \mathrm{Im}(\lambda) < 0 \ . \end{cases}$$

(ii) For $\varepsilon \in (0, \infty)$, $f \in X$:

$$\begin{aligned} &\frac{1}{2\pi i}\int_{\alpha}^{\beta} [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]f\,d\lambda \\ &= \frac{1}{\pi}\left[\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)} - \alpha\right)\right) - \arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)} - \beta\right)\right)\right](A)f \ . \end{aligned}$$

Proof. "Part (i)": We note that

$$R(\lambda) = \frac{1}{\mathrm{id}_{\sigma(A)} - \lambda}(A) \ , \tag{12.49}$$

for $\lambda \in \mathbb{C}\backslash\sigma(A)$. For the proof, we note that for $\lambda \in \mathbb{C}\backslash\sigma(A)$ such that $\mathrm{Im}(\lambda) \neq 0$, the function $1/\left(\mathrm{id}_{\mathbb{R}} - \lambda\right)$ is bounded continuous, and if $\mathrm{Im}(\lambda) = 0$, then

$$\frac{1}{\mathrm{id}_{\sigma(A)} - \lambda} = \widehat{\left.\frac{1}{\mathrm{id}_{\mathbb{R}} - \lambda}\right|_{\mathbb{R}\backslash[\lambda-(\varepsilon/2),\lambda+(\varepsilon/2)]}}\Bigg|_{\sigma(A)} \ ,$$

where the hat denotes the extension of a function to a function that is constant of value 0 outside the domain of the former function, and $\varepsilon > 0$ is such that $(\lambda - \varepsilon, \lambda + \varepsilon) \subset \mathbb{R} \setminus \sigma(A)$. Hence it follows from integration theory that

$$\frac{1}{\mathrm{id}_{\sigma(A)} - \lambda} \in U^s_{\mathbb{C}}(\sigma(A)) \ .$$

Further,

$$\begin{aligned} &\frac{1}{\mathrm{id}_{\sigma(A)} - \lambda}(A)(A - \lambda) \\ &= \frac{1}{\mathrm{id}_{\sigma(A)} - \lambda}(A)\left[\left(\frac{1}{i} - \lambda\right)U_A + \frac{1}{i} + \lambda\right][(U_A - 1)\restriction_{D(A)}]^{-1} \\ &= \frac{1}{\mathrm{id}_{\sigma(A)} - \lambda}(A)\,\frac{2}{i}\,\frac{\mathrm{id}_{\sigma(A)} - \lambda}{\mathrm{id}_{\sigma(A)} + i}(A)[(U_A - 1)\restriction_{D(A)}]^{-1} \\ &= (U_A - 1)[(U_A - 1)\restriction_{D(A)}]^{-1} = \iota_{D(A)\hookrightarrow X} \ , \end{aligned}$$

where U_A denotes the Cayley transform of A. Since $A - \lambda$ is bijective, the latter implies (12.49). Further, for $\lambda \in \mathbb{R} \times (0, \infty)$, it follows that

$$F_1[\exp\left(i\lambda\,\mathrm{id}_{\mathbb{R}}\right) \cdot \chi_{[0,\infty)}] = (-i) \cdot \frac{1}{\mathrm{id}_{\mathbb{R}} - \lambda} \ . \tag{12.50}$$

For the proof, we note that for every $k \in \mathbb{R}$

$$\big(\exp(i\,(\lambda - k)\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{[0,\nu]}\big)_{\nu \in \mathbb{N}^*}$$

is a sequence of integrable functions whose members are dominated by the integrable function $\exp(-\mathrm{Im}(\lambda)\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{[0,\infty)}$ that is everywhere pointwise on $\mathbb{R}$ convergent to

$$\exp(i\,(\lambda - k)\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{[0,\infty)}$$

and whose corresponding sequence of integrals is given by

$$\left(\frac{1}{i\,(\lambda - k)}\,[\exp(i\,(\lambda - k)\,\nu) - 1]\right)_{\nu \in \mathbb{N}^*} .$$

Hence, it follows from Lebesgue's dominated convergence theorem that

$$\exp(i\,(\lambda - k)\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{[0,\infty)}$$

is integrable as well as that

$$\int_{\mathbb{R}} \exp(i\,(\lambda - k)\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{[0,\infty)}\,dv^1 = \lim_{\nu \to \infty} \int_{\mathbb{R}} \exp(i\,(\lambda - k)\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{[0,\nu]}\,dv^1$$
$$= -\frac{1}{i\,(\lambda - k)} = -i\,\frac{1}{k - \lambda}$$

and therefore also (12.50). The relation (12.50) and Lebesgue's change of variable formula also imply that

$$F_1[\exp(i\lambda\,\mathrm{id}_{\mathbb{R}}) \cdot \chi_{(-\infty,0]}] = i \cdot \frac{1}{\mathrm{id}_{\mathbb{R}} - \lambda}, \tag{12.51}$$

for every $\lambda \in \mathbb{R} \times (-\infty, 0)$. According to Lemma 12.9.7,

$$\left(F_1(f)\big|_{\sigma(A)}\right)(A) = \int_{\mathbb{R}} f(t).U(-t)\,dt\ ,$$

for every $f \in L^1_{\mathbb{C}}(\mathbb{R})$. Hence it follows for every $\lambda \in \mathbb{R} \times (0, \infty)$ that

$$-i(A - \lambda)^{-1} = \int_0^{\infty} \exp(i\lambda\,t) \cdot U(-t)\,dt$$

and for every $\lambda \in \mathbb{R} \times (-\infty, 0)$ that

$$i(A - \lambda)^{-1} = \int_{-\infty}^{0} \exp(i\lambda\,t) \cdot U(-t)\,dt\ .$$

"Part (ii)": For the proof, let $\varepsilon > 0$ and $f, g \in X$. It follows from Part (i) and for every $\lambda \in \mathbb{R}$ that

$$\frac{1}{2\pi i}\,\langle f|[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]g\rangle = \frac{1}{2\pi} \int_{\mathbb{R}} \exp(i\lambda\,t - \varepsilon|t|)\,\langle f|U(-t)g\rangle\,dt\ . \tag{12.52}$$

Further, according to integration theory, the function

$$\overline{((\alpha,\beta)\times\mathbb{R},(\lambda,t)\mapsto \widehat{\exp}(i\lambda t-\varepsilon\cdot|t|)\,\langle f|U(-t)g\rangle)}$$

is v^2-measurable and dominated by the, according to Tonelli's theorem, v^2-integrable function

$$\|f\|\cdot\|g\|\cdot\left(\mathbb{R}^2\to\mathbb{R},(\lambda,t)\mapsto\chi_{(\alpha,\beta)}(\lambda)\cdot\exp(-\varepsilon\,|t|)\right)\ .$$

Hence it follows from Lebesgue's dominated convergence theorem the v^2-summability of the former function and from Fubini's theorem and (12.52) the v^1-summability of

$$\left(\mathbb{R}\to\mathbb{C},\lambda\mapsto\chi_{(\alpha,\beta)}(\lambda)\cdot\langle f|[R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon)]g\rangle\right)$$

as well as that

$$\begin{aligned}&\frac{1}{2\pi i}\int_\alpha^\beta\langle f|[R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon)]g\rangle\ d\lambda\\&=\frac{1}{2\pi}\int_{(\alpha,\beta)\times\mathbb{R}}\exp(i\lambda t-\varepsilon|t|)\,\langle f|U(-t)g\rangle\ d\lambda\,dt\ .\end{aligned}$$

Further, it follows from Lebesgue's change of variable formula and from Fubini's theorem that

$$\begin{aligned}&\frac{1}{2\pi i}\int_\alpha^\beta\langle f|[R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon)]g\rangle\ d\lambda\\&=\frac{1}{2\pi}\int_{\mathbb{R}}\left[\int_\alpha^\beta\exp(i\lambda t)\,d\lambda\right]\exp(-\varepsilon|t|)\,\langle f|U(-t)g\rangle\ dt\ .\end{aligned}\tag{12.53}$$

We note that (12.50) and (12.51) imply that

$$F_1\exp(-\varepsilon|\ |)=\frac{2\varepsilon}{\mathrm{id}_{\mathbb{R}}^2+\varepsilon^2}\ .$$

Since $\exp(-\varepsilon|\ |)\in\mathcal{L}^2_{\mathbb{C}}(\mathbb{R}),1/(\mathrm{id}_{\mathbb{R}}^2+\varepsilon^2)\in\mathcal{L}^1_{\mathbb{C}}(\mathbb{R})$, it follows that

$$\int_{\mathbb{R}}\exp(it\,\mathrm{id}_{\mathbb{R}})\cdot\frac{\varepsilon/\pi}{\mathrm{id}_{\mathbb{R}}^2+\varepsilon^2}\,dv^1=\exp(-\varepsilon|\ |)\ .\tag{12.54}$$

Further, from $1/(\mathrm{id}_{\mathbb{R}}^2+\varepsilon^2),\chi_{(\alpha,\beta)}\in\mathcal{L}^1_{\mathbb{C}}(\mathbb{R})\cap\mathcal{L}^2_{\mathbb{C}}(\mathbb{R})$ and as a consequence of

$$f*g=F_1[(F_2^{-1}f)\cdot(F_2^{-1}g)]\ ,$$

for all $f,g\in L^2_{\mathbb{C}}(\mathbb{R}^n)$, where $*$ denotes the convolution product, we conclude that

$$\chi_{(\alpha,\beta)}*\frac{\varepsilon/\pi}{\mathrm{id}_{\mathbb{R}}^2+\varepsilon^2}=\frac{1}{2\pi}\,F_1[(F_1\chi_{(\alpha,\beta)})\cdot(F_1\exp(-\varepsilon|\ |))]\tag{12.55}$$

$$= \frac{1}{\pi}\left[\arctan\left(\frac{1}{\varepsilon}\,(\mathrm{id}_{\mathbb{R}}-\alpha)\right)-\arctan\left(\frac{1}{\varepsilon}\,(\mathrm{id}_{\mathbb{R}}-\beta)\right)\right] .$$

Hence, it follows from Lemma 12.9.7, (12.54) and (12.55) that

$$\begin{aligned}
&\frac{1}{2\pi i}\int_{\alpha}^{\beta}\langle f|\left[R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon)\right]g\rangle\,d\lambda \\
&=\langle f|\frac{1}{\pi}\left[\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)}-\alpha\right)\right)-\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)}-\beta\right)\right)\right](A)g\rangle \ ,
\end{aligned}$$

for all $f, g \in X$. □

Remark 12.9.9. We note that it follows from the spectral theorem, Theorem 12.6.4, that

$$\begin{aligned}
&s-\lim_{\varepsilon\to 0}\frac{1}{\pi}\left[\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)}-\alpha\right)\right)-\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)}-\beta\right)\right)\right](A) \\
&=\frac{1}{2}\left[\left(\chi_{(\alpha,\beta)}\big|_{\sigma(A)}\right)(A)+\left(\chi_{[\alpha,\beta]}\big|_{\sigma(A)}\right)(A)\right] .
\end{aligned}$$

Remark 12.9.10. We note that since for all $f, g \in X$, the corresponding function $(\mathbb{C}\backslash\sigma(A), \lambda \mapsto \langle g|R(\lambda)f\rangle)$ is holomorphic, Theorem 12.9.8 (ii) opens the path to the calculation of the spectral projections of A by contour integration. In particular, if A is positive, i.e., the spectrum $\sigma(A)$ of A is part of the interval $[0,\infty)$, using that the covering $pr := (\mathbb{C}\to\mathbb{C}, \mu\mapsto -\mu^2)$ of $\mathbb{C}$ maps the open right half-plane, $(0,\infty)\times\mathbb{R}$, biholomorphically onto the simply connected slized plane $\mathbb{C}\setminus[0,\infty)$, it follows for $\alpha,\beta\in\mathbb{R}$, such that $\alpha<\beta$ and $\varepsilon>0$ that

$$\begin{aligned}
&\frac{1}{\pi i}\left[\int_{C_\nu(\varepsilon)}\mu\,\langle g|R(-\mu^2)f\rangle\,d\mu-\int_{D_\nu(\varepsilon)}\mu\,\langle g|R(-\mu^2)f\rangle\,d\mu\right] \\
&=\frac{1}{\pi}\,\langle g|\left[\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)}-\alpha\right)\right)-\arctan\left(\frac{1}{\varepsilon}\left(\mathrm{id}_{\sigma(A)}-\beta\right)\right)\right](A)f\rangle \ ,
\end{aligned}$$

where $C_\nu(\varepsilon)$ is a contour from the point $\sqrt{-\beta-i\varepsilon}$ to the point $\sqrt{-\alpha-i\varepsilon}$ in the open 4th quadrant $(0,\infty)\times(-\infty,0)$ and $D_\nu(\varepsilon)$ is a contour from the point $\sqrt{-\beta+i\varepsilon}$ to the point $\sqrt{-\alpha+i\varepsilon}$ in the open 1st quadrant $(0,\infty)^2$.

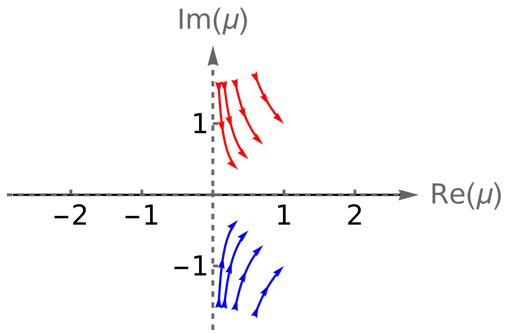


Fig. 12.1: Ranges of the paths $([-2,0] \to \mathbb{C}, \tau \mapsto \sqrt{\tau - \varepsilon\, i})$ (blue) and $([-2,0] \to \mathbb{C}, \tau \mapsto \sqrt{\tau + \varepsilon\, i})$ (red), respectively, corresponding to $\alpha = 0$ and $\beta = 2$, for $\varepsilon = 0.25, 0.5, 1, 2$, inside the covering space. The arrows indicate the orientation of the paths. For decreasing ε, the ranges approach $-i\,[0, \sqrt{\beta}\,]$ and $i\,[0, \sqrt{\beta}\,]$, respectively. The inverse image $pr^{-1}([0,\infty))$ of the interval $[0,\infty)$ that is containing the spectrum of A is given by the (dashed) imaginary axis.

Corollary 12.9.11 (A Relation Between the Resolvent of an Operator and the Generated Strongly Continuous One-Parameter Unitary Group). Under the assumptions of Theorem 12.9.8, the following is true. For every $f, g \in X$, $\lambda_2 \in \mathbb{R}^*$,

$$\langle g|R(\cdot + i\lambda_2)f\rangle \in L^2_{\mathbb{C}}(\mathbb{R}) \cap C_\infty(\mathbb{R}, \mathbb{C}) \ .$$

Further, if $\lambda_2 < 0$, then for almost all $t > 0$

$$\lim_{\nu \to \infty} -\frac{1}{2\pi i} \int_{C_\nu(\lambda_2)} \exp(it\lambda)\, \langle g|R(\lambda)f\rangle \, d\lambda = \langle g|U(t)f\rangle \ \ ,$$

and, if $\lambda_2 > 0$, then for almost all $t < 0$

$$\lim_{\nu \to \infty} \frac{1}{2\pi i} \int_{C_\nu(\lambda_2)} \exp(it\lambda)\, \langle g|R(\lambda)f\rangle \, d\lambda = \langle g|U(t)f\rangle \ \ ,$$

where, for every $\nu \in \mathbb{N}$ and $\lambda_2 < 0$, $C_\nu(\lambda_2)$ is a contour from the point $-\nu + i\lambda_2$ to the point $\nu + i\lambda_2$ in the open lower half-plane, $\mathbb{R} \times (-\infty, 0)$, and, for every $\nu \in \mathbb{N}$ and $\lambda_2 > 0$, $C_\nu(\lambda_2)$ is a contour from the point $-\nu + i\lambda_2$ to the point $\nu + i\lambda_2$ in the open upper half-plane, $\mathbb{R} \times (0, \infty)$, respectively.

Proof. According to Theorem 12.9.8 (i), for $\lambda = \lambda_1 + i\lambda_2 \in \mathbb{R} \times \mathbb{R}^*$, where $\lambda_1 \in \mathbb{R}$, $\lambda_2 \in \mathbb{R}^*$ and $f, g \in X$:

$$\begin{aligned} &\langle g|R(\lambda_1 + i\lambda_2)f\rangle \\ &= i \begin{cases} \int_{\mathbb{R}} \exp(-i\lambda_1 t)\, \chi_{(-\infty,0)}(t) \exp(\lambda_2 t)\, \langle g|U(t)f\rangle \, dt & \text{if } \lambda_2 > 0 \\ -\int_{\mathbb{R}} \exp(-i\lambda_1 t)\, \chi_{(0,\infty)}(t) \exp(\lambda_2 t)\, \langle g|U(t)f\rangle \, dt & \text{if } \lambda_2 < 0 \ . \end{cases} \end{aligned}$$

Since

$$\begin{cases} \chi_{(-\infty,0)} \exp(\lambda_2 . \mathrm{id}_{\mathbb{R}})\, \langle g|Uf\rangle \in L^1_{\mathbb{C}}(\mathbb{R}) \cap L^2_{\mathbb{C}}(\mathbb{R}) & \text{if } \lambda_2 > 0 \\ \chi_{(0,\infty)} \exp(\lambda_2 . \mathrm{id}_{\mathbb{R}})\, \langle g|Uf\rangle \in L^1_{\mathbb{C}}(\mathbb{R}) \cap L^2_{\mathbb{C}}(\mathbb{R}) & \text{if } \lambda_2 < 0 \end{cases} ,$$

this implies that

$$\langle g|R(\cdot + i\lambda_2)f\rangle = i\sqrt{2\pi}\begin{cases} F_2\left[\chi_{(-\infty,0)}\exp(\lambda_2.\mathrm{id}_{\mathbb{R}})\,\langle g|Uf\rangle\right] & \text{if } \lambda_2 > 0 \\ F_2\left[-\chi_{(0,\infty)}\exp(\lambda_2.\mathrm{id}_{\mathbb{R}})\,\langle g|Uf\rangle\right] & \text{if } \lambda_2 < 0 \end{cases}$$

and hence that

$$\langle g|R(\cdot + i\lambda_2)f\rangle \in L^2_{\mathbb{C}}(\mathbb{R}) \cap C_\infty(\mathbb{R},\mathbb{C})$$

as well as that

$$\frac{1}{i\sqrt{2\pi}}\,F_2^{-1}\,\langle g|R(\cdot + i\lambda_2)f\rangle = \begin{cases} \chi_{(-\infty,0)}\exp(\lambda_2.\mathrm{id}_{\mathbb{R}})\,\langle g|Uf\rangle & \text{if } \lambda_2 > 0 \\ -\chi_{(0,\infty)}\exp(\lambda_2.\mathrm{id}_{\mathbb{R}})\,\langle g|Uf\rangle & \text{if } \lambda_2 < 0 \end{cases} .$$

As a consequence, if $\lambda_2 > 0$, then

$$\lim_{\nu\to\infty}\Bigg\|\left(\begin{array}{c}\mathbb{R}\to\mathbb{C} \\ t\mapsto \frac{1}{2\pi i}\int_{-\nu}^{\nu}\exp(it\lambda_1)\,\langle g|R(\lambda_1+i\lambda_2)f\rangle\,d\lambda_1\end{array}\right) - \chi_{(-\infty,0)}\exp(\lambda_2.\mathrm{id}_{\mathbb{R}})\,\langle g|Uf\rangle\Bigg\|_2 = 0 ,$$

and if $\lambda_2 < 0$, then

$$\lim_{\nu\to\infty}\Bigg\|\left(\begin{array}{c}\mathbb{R}\to\mathbb{C} \\ t\mapsto -\frac{1}{2\pi i}\int_{-\nu}^{\nu}\exp(it\lambda_1)\,\langle g|R(\lambda_1+i\lambda_2)f\rangle\,d\lambda_1\end{array}\right) - \chi_{(0,\infty)}\exp(\lambda_2.\mathrm{id}_{\mathbb{R}})\,\langle g|Uf\rangle\Bigg\|_2 = 0 .$$

As a consequence, if $\lambda_2 > 0$, it follows for almost all $t < 0$ that

$$\lim_{\nu\to\infty}\frac{1}{2\pi i}\int_{-\nu}^{\nu}\exp(it(\lambda_1+i\lambda_2))\,\langle g|R(\lambda_1+i\lambda_2)f\rangle\,d\lambda_1 = \langle g|U(t)f\rangle \ ,$$

and if $\lambda_2 < 0$, it follows for almost all $t > 0$ that

$$\lim_{\nu\to\infty} -\frac{1}{2\pi i}\int_{-\nu}^{\nu}\exp(it(\lambda_1+i\lambda_2))\,\langle g|R(\lambda_1+i\lambda_2)f\rangle\,d\lambda_1 = \langle g|U(t)f\rangle \ .$$

$\square$

Remark 12.9.12. We note that since for all $f, g \in X$, the corresponding function $(\mathbb{C}\backslash\sigma(A), \lambda \mapsto \langle g|R(\lambda)f\rangle)$ is holomorphic, Corollary 12.9.11 opens the path to the calculation of the one-parameter unitary group U that is generated by A by contour integration. In particular, if A is positive, i.e., the spectrum $\sigma(A)$ of A is part of the interval $[0,\infty)$, using that the covering $pr := (\mathbb{C}\to\mathbb{C}, \mu \mapsto -\mu^2)$ of $\mathbb{C}$ maps the open right half-plane, $(0,\infty)\times\mathbb{R}$, biholomorphically onto the simply connected slized plane $\mathbb{C}\setminus[0,\infty)$, it follows that

(i) if $\lambda_2 < 0$, then for almost all $t > 0$

$$\lim_{\nu\to\infty} -\frac{1}{\pi i}\int_{C_\nu(\lambda_2)} \exp(-it\mu^2)\,\mu\,\langle g|R(-\mu^2)f\rangle\; d\mu = \langle g|U(t)f\rangle\ \ ,$$

(ii) and, if $\lambda_2 > 0$, then for almost all $t < 0$

$$\lim_{\nu\to\infty} \frac{1}{\pi i}\int_{C_\nu(\lambda_2)} \exp(-it\mu^2)\,\mu\,\langle g|R(-\mu^2)f\rangle\; d\mu = \langle g|U(t)f\rangle\ \ ,$$

where $C_\nu(\lambda_2)$ is a contour from the point $\sqrt{-\nu-\lambda_2\, i}$ to the point $\sqrt{\nu-\lambda_2\, i}$ in the open right half-plane, $(0,\infty)\times\mathbb{R}$.

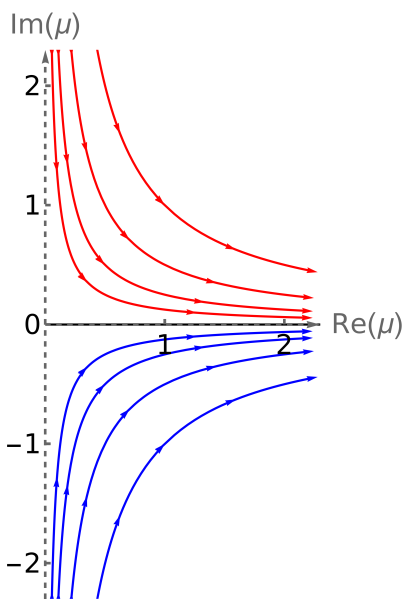


Fig. 12.2: Ranges of the paths $([-5,5]\to\mathbb{C}, \nu\mapsto\sqrt{\nu-\lambda_2\, i}\,)$ for $\lambda_2 = 0.25, 0.5, 1, 2$ (blue), and for $\lambda_2 = -2, -1, -0.5, -0.25$ (red), respectively, inside the covering space. The arrows indicate the orientation of the paths. For decreasing $|\lambda_2|$, the ranges approach $[0,\infty)\cup i\,(-\infty,0]$ and $[0,\infty)\cup i\,[0,\infty)$, respectively. The inverse image $pr^{-1}([0,\infty))$ of the interval $[0,\infty)$ that is containing the spectrum of A is given by the (dashed) imaginary axis.

Friedrichs Mollifiers

Lemma 12.9.13 (Friedrichs mollifiers). Let $n\in\mathbb{N}^*$, Ω be a non-empty open subset of $\mathbb{R}^n$ and $h\in C_0^\infty(\mathbb{R}^n)$ be positive with a support contained in $B_1(0)$ as well as such that $h(x)=h(-x)$ for all $x\in\mathbb{R}^n$ and $\|h\|_1 = 1$. For instance,

$$h(x) := \begin{cases} C\exp\left(-\frac{1}{1-|x|^2}\right) & \text{if } |x|<1 \\ 0 & \text{if } |x|\geqslant 1 \end{cases}$$

for every $x \in \mathbb{R}^n$, where

$$C := \left[\int_{U_1(0)} \exp\left(- \frac{1}{1 - |\ |^2} \right) dv^n \right]^{-1} .$$

In addition, define for every $\nu \in \mathbb{N}^*$ the corresponding $h_\nu \in C_0^\infty(\mathbb{R}^n)$ by

$$h_\nu(x) := \nu^n h(\nu x)$$

for all $x \in \mathbb{R}^n$. Finally, define for every $\nu \in \mathbb{N}^*$ and every $f \in L^2_{\mathbb{C}}(\Omega)$

$$H_\nu f := (\, h_\nu * \hat{f}\,)\big|_\Omega \ ,$$

where

$$\hat{f}(x) := \begin{cases} f(x) & \text{if } x \in \Omega \\ 0 & \text{if } x \in \mathbb{R}^n \backslash \Omega \end{cases}$$

and '$*$' denotes the convolution product. Then

(i) for every $\nu \in \mathbb{N}^*$ the corresponding H_ν defines a bounded self-adjoint linear operator on $L^2_{\mathbb{C}}(\Omega)$ with operator norm $\|H_\nu\| \leqslant 1$,

(ii)
$$\text{s}-\lim_{\nu \to \infty} H_\nu = \text{id}_{L^2_{\mathbb{C}}(\Omega)} \ .$$

Proof. '(i)': For this, let $\nu \in \mathbb{N}^*$. Moreover, define $K_\nu \in C^\infty(\bar{\Omega}^{\,2})$ by

$$K_\nu(x, y) := h_\nu(x - y)$$

for all $x, y \in \Omega$. Then K_ν is in particular measurable and such that $K_\nu(x, \cdot), K_\nu(\cdot, y) \in L^1(\Omega)$ and

$$\|K_\nu(x, \cdot)\|_1 \leqslant 1 \ , \ \|K_\nu(\cdot, y)\|_1 \leqslant 1$$

for all $x, y \in \Omega$. Hence to K_ν there is associated a bounded linear integral operator $\text{Int}(K_\nu) = H_\nu$ on $L^2_{\mathbb{C}}(\Omega)$ with operator norm equal or smaller than 1. Finally, this operator is self-adjoint since it follows from the assumptions on K that $K^*(y - x) = K(x - y)$ for all $x, y \in \Omega$.

'(ii)': For $\nu \in \mathbb{N}^*$ and $f \in C_0(\Omega, \mathbb{C})$, it follows that

$$\text{supp}(h_\nu * \hat{f} - \hat{f}\,) \subset \text{supp}(f) + B_1(0)$$

and

$$|h_\nu * \hat{f} - \hat{f}|(x) \leqslant \int_{\mathbb{R}^n} |\hat{f}(x - \text{id}_{\mathbb{R}^n}) - \hat{f}(x)|\, h_\nu \, dv^n$$

for all $x \in \mathbb{R}^n$. Since $\hat{f}$ is in particular uniformly continuous, it follows for every $\varepsilon > 0$ the existence of $\delta > 0$ such that for all $x \in \mathbb{R}^n, y \in U_\delta(0)$

$$|\hat{f}(x - y) - \hat{f}(x)| \leqslant [v^n(\text{supp}(f) + B_1(0))]^{-1/2} \, \varepsilon^{1/2} \ .$$

As a consequence, for all $\nu \in \mathbb{N}^*$ such that $\nu > 1/\delta$

$$\|h_\nu * \hat{f} - \hat{f}\|_2 \leqslant \varepsilon$$

holds. Hence it follows for every $f \in C_0(\Omega, \mathbb{C})$ that

$$\lim_{\nu \to \infty} \|H_\nu f - f\|_2 = 0 \ .$$

Since $C_0(\Omega, \mathbb{C})$ is dense in $L^2_{\mathbb{C}}(\Omega)$ and $H_1, H_2, \dots$ is in particular uniformly bounded, this implies also that

$$\text{s}-\lim_{\nu \to \infty} H_\nu = \text{id}_{L^2_{\mathbb{C}}(\Omega)} \ .$$

□

Trotter Product Formulas

This Section uses methods from the theory of strongly continuous semigroups which are not discussed in this book. For this theory, we refer to specialized literature listed below. The class of generators of such semigroups is considerably larger than the class of linear self-adjoint operators in Hilbert spaces. As a consequence, applications extend to the field of partial differential equations, including non-linear equations, in particular see [7], [15], [18], [33], [5], [28], [19].

Theorem 12.9.14. (**Definition and properties of the exponential function**) Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and $(X, \| \ \|)$ a $\mathbb{K}$-Banach space. Then we define the exponential function $\exp : L(X, X) \to L(X, X)$ by

$$\exp(A) := \sum_{k=0}^{\infty} \frac{1}{k!} \, . \, A^k$$

where $A^0 := \text{id}_X$ and $A^{k+1} := A \circ A^k$ for all $k \in \mathbb{N}$. Note that this series is absolutely convergent since $\|A^k\| \leqslant \|A\|^k$ for all $k \in \mathbb{N}$.

(i) The map $u_A : \mathbb{K} \to L(X, X)$, defined by

$$u_A(t) := \exp(t.A)$$

for every $t \in \mathbb{K}$, is differentiable with derivative

$$u'_A(t) = A \circ u_A(t)$$

for all $t \in \mathbb{K}$.

(ii) For all $A, B \in L(X, X)$ satisfying $A \circ B = B \circ A$

$$\exp(A + B) = \exp(A) \circ \exp(B) \ . \tag{12.56}$$

(iii) For all $A \in L(X,X)$ satisfying $\|A\| \leqslant 1$, $n \in \mathbb{N}$ and $f \in X$,

$$\left\| \exp\left(n.(A - \mathrm{id}_X)\right) f - A^n f \right\| \leqslant \sqrt{n} \cdot \|(A - \mathrm{id}_X) f\| \ . \tag{12.57}$$

Proof. '(i)': For this, let $A \in L(X,X)$. Then it follows for $t \in \mathbb{K}$, $h \in \mathbb{K}^*$, by using the bilinearity and continuity of the composition map on $((L(X,X))^2$, that

$$\begin{aligned}
&\left\| \frac{1}{h} . \left[\exp((t+h).A) - \exp(t.A) \right] - A \circ \exp(t.A) \right\| \\
&= \left\| \sum_{k=2}^{\infty} \frac{1}{k!} \left[\frac{(t+h)^k - t^k}{h} - k t^{k-1} \right] . A^k \right\| \\
&= \lim_{n \to \infty} \left\| \sum_{k=2}^{n} \frac{1}{k!} \left[\frac{(t+h)^k - t^k}{h} - k t^{k-1} \right] . A^k \right\| \ .
\end{aligned} \tag{12.58}$$

Further, for any $n \in \mathbb{N}, n \geqslant 2$:

$$\left\| \sum_{k=2}^{n} \frac{1}{k!} \left[\frac{(t+h)^k - t^k}{h} - k t^{k-1} \right] . A^k \right\| \leqslant \sum_{k=2}^{n} \frac{1}{k!} \left| \frac{(t+h)^k - t^k}{h} - k t^{k-1} \right| \|A\|^k \ , \tag{12.59}$$

and for any $k \in \mathbb{N}, k \geqslant 2$:

$$\begin{aligned}
&\left| \frac{(t+h)^k - t^k}{h} - k t^{k-1} \right| = \left| \frac{t+h-t}{h} \cdot \left[\sum_{l=0}^{k-1} (t+h)^l \cdot t^{k-(l+1)} \right] - k t^{k-1} \right| \\
&= \left| \sum_{l=1}^{k-1} \left[(t+h)^l \cdot t^{k-(l+1)} - t^{k-1} \right] \right| = \left| \sum_{l=1}^{k-1} t^{k-(l+1)} \left[(t+h)^l - t^l \right] \right| \\
&= \left| \sum_{l=1}^{k-1} \sum_{m=0}^{l-1} (t+h)^m \cdot t^{k-(m+2)} \right| \cdot |h| \leqslant |h| \cdot \sum_{l=1}^{k-1} \sum_{m=0}^{l-1} (\,|t| + |h|\,)^{k-2} \\
&= \frac{|h|}{2} \cdot k(k-1) \cdot (\,|t| + |h|\,)^{k-2} \ .
\end{aligned}$$

Inserting the last into (12.59) gives

$$\begin{aligned}
&\left\| \sum_{k=2}^{n} \frac{1}{k!} \left[\frac{(t+h)^k - t^k}{h} - k t^{k-1} \right] . A^k \right\| \leqslant \frac{|h|}{2} \sum_{k=2}^{n} \frac{1}{(k-2)!} \cdot (\,|t| + |h|\,)^{k-2} \|A\|^k \\
&\leqslant \frac{|h| \cdot \|A\|^2}{2} \exp\left((|t| + |h|) \cdot \|A\| \right) \ .
\end{aligned}$$

Finally, inserting the last into (12.58) gives

$$\left\| \frac{1}{h} . \left[\exp((t+h).A) - \exp(t.A) \right] - A \circ \exp(t.A) \right\|$$

$$\leqslant \frac{|h| \cdot \|A\|^2}{2} \exp\big((|t| + |h|) \cdot \|A\|\big)$$

and hence

$$\lim_{h \to 0, h \neq 0} \left\| \frac{1}{h} . \left[\exp((t+h).A) - \exp(t.A) \right] - A \circ \exp(t.A) \right\| = 0 \; .$$

'(ii)': For this, let $A, B \in L(X, X)$ be such that $A \circ B = B \circ A$ and $t \in \mathbb{K}, h \in \mathbb{K}^*$. Then

$$\begin{aligned}
&\Big\| \frac{1}{h} . \big(u_A(t+h) \circ u_B(t+h) \\
&\quad - u_A(t) \circ u_B(t)\big) - \big(u_A'(t) \circ u_B(t) + u_A(t) \circ u_B'(t)\big) \Big\| \\
&= \Big\| \left[\frac{1}{h} . \big(u_A(t+h) - u_A(t)\big) - u_A'(t) \right] \circ u_B(t) \\
&\quad + u_A(t) \circ \left[\frac{1}{h} . \big(u_B(t+h) - u_B(t)\big) - u_B'(t) \right] \\
&\quad + \frac{1}{h} . \big(u_A(t+h) - u_A(t)\big) \circ \big(u_B(t+h) - u_B(t)\big) \Big\| \\
&\leqslant \left\| \left[\frac{1}{h} . \big(u_A(t+h) - u_A(t)\big) - u_A'(t) \right] \right\| \cdot \|u_B(t)\| \\
&\quad + \|u_A(t)\| \cdot \left\| \left[\frac{1}{h} . \big(u_B(t+h) - u_B(t)\big) - u_B'(t) \right] \right\| \\
&\quad + \left\| \frac{1}{h} . \big(u_A(t+h) - u_A(t)\big) \right\| \cdot \left\| \big(u_B(t+h) - u_B(t)\big) \right\| \; .
\end{aligned}$$

Hence it follows by (i) the differentiability of $g_{A,B} : \mathbb{K} \to L(X, X)$ defined by $h_{A,B}(t) := u_{A+B}(t) - u_A(t) \circ u_B(t)$ for every $t \in \mathbb{K}$ and

$$\begin{aligned}
h_{A,B}'(t) &= (A+B) \circ u_{A+B}(t) - A \circ u_A(t) \circ u_B(t) - u_A(t) \circ B \circ u_B(t) \\
&= (A+B) \circ u_{A+B}(t) - A \circ u_A(t) \circ u_B(t) - B \circ u_A(t) \circ u_B(t) \\
&= (A+B) \circ h_{A,B}(t)
\end{aligned}$$

for all $t \in \mathbb{K}$ where the bilinearity and continuity of the composition map on $(L(X, X))^2$ has been used as well as that $A \circ B = B \circ A$ by assumption. Hence it follows by $h_{A,B}(0) = u_{A+B}(0) - u_A(0) \circ u_B(0) = 0$ along with Theorem 3.2.9 and Theorem 3.2.5 of [7] that

$$\|h_{A,B}(t)\| \leqslant \|A+B\| \cdot \int_0^t \| h_{A,B}(s)\| \, ds$$

for all $t \in [0, \infty)$. As a consequence, it follows for $\varepsilon > 0$ that

$$\|h_{A,B}(t)\| < \varepsilon \, e^{\, t\|A+B\|} \tag{12.60}$$

for all $t \in [0, \infty)$. Because otherwise there is $t_0 \in (0, \infty)$ such that

$$\|h_{A,B}(t_0)\| \geqslant \varepsilon \, e^{\,t_0 \|A+B\|}$$

and such that (12.60) is valid for all $t \in [0, t_0)$. Then

$$\|h_{A,B}(t_0)\| \leqslant \|A+B\| \cdot \int_0^{t_0} \| \, h_{A,B}(s)\| \, ds \leqslant \|A+B\| \cdot \int_0^{t_0} \varepsilon \, e^{\,t\|A+B\|} \, ds$$
$$= \varepsilon \cdot \left(e^{\,t_0\|A+B\|} - 1\right) < \varepsilon \cdot e^{\,t_0\|A+B\|} \ \lightning$$

From (12.60) it follows that $h_{A,B}(t) = 0$ for all $t \geqslant 0$ and hence (12.56).
'(iii)': For this, let $A \in L(X, X)$ be such that $\|A\| \leqslant 1$, $n \in \mathbb{N}$ and $f \in X$. Then

$$\left\| \exp\left(n.(A - \mathrm{id_X})\right) f - A^n f \right\| = e^{-n} \cdot \| \exp(n.A) f - e^n . \, A^n f \|$$
$$= e^{-n} \cdot \lim_{m \to \infty} \left\| \sum_{k=0}^{m} \frac{n^k}{k!} (A^k - A^n) f \right\| \ . \tag{12.61}$$

Further, it follows for $m \in \mathbb{N}$ by using the Cauchy-Schwarz inequality for the Euclidean scalar product on $\mathbb{R}^{m+1}$:

$$\left\| \sum_{k=0}^{m} \frac{n^k}{k!} (A^k - A^n) f \right\| \leqslant \sum_{k=0}^{m} \frac{n^k}{k!} \, \|(A^k - A^n) f\| \leqslant \sum_{k=0}^{m} \frac{n^k}{k!} \, \left\|(A^{|k-n|} - \mathrm{id_X}) f\right\|$$
$$= \sum_{k=0}^{m} \frac{n^k}{k!} \left\| \sum_{l=0}^{|k-n|-1} A^l \circ (A - \mathrm{id_X}) f \right\| \leqslant \|(A - \mathrm{id_X}) f\| \cdot \sum_{k=0}^{m} |k-n| \, \frac{n^k}{k!}$$
$$\leqslant \|(A - \mathrm{id_X}) f\| \cdot \left(\sum_{k=0}^{m} (k-n)^2 \, \frac{n^k}{k!} \right)^{1/2} \cdot \left(\sum_{k=0}^{m} \frac{n^k}{k!} \right)^{1/2} \tag{12.62}$$
$$\leqslant \|(A - \mathrm{id_X}) f\| \cdot e^{n/2} \cdot \left(\sum_{k=0}^{\infty} (k-n)^2 \, \frac{n^k}{k!} \right)^{1/2}$$
$$= \|(A - \mathrm{id_X}) f\| \cdot e^{n/2} \cdot \left(\sum_{k=0}^{\infty} \left[k(k-1) - (2n-1)k + n^2 \right] \frac{n^k}{k!} \right)^{1/2}$$
$$= \|(A - \mathrm{id_X}) f\| \cdot e^{n/2} \cdot \left(\left[n^2 - (2n-1)n + n^2 \right] e^n \right)^{1/2} \tag{12.63}$$
$$= \sqrt{n} \, e^n \, \|(A - \mathrm{id_X}) f\| \ .$$

Finally, (12.57) follows from (12.61) and (12.62). ☐

Lemma 12.9.15. Let $(X, \langle \, | \, \rangle)$ be a non-trivial complex Hilbert space, A a semi-bounded densely-defined, linear and self-adjoint operator in X, with lower bound γ, implying that spectrum $\sigma(A)$ of A is contained in $[\gamma, \infty)$. Further, let $z \in \mathbb{R} \times (-\infty, 0]$. Then, $T : [0, \infty) \to L(X, X)$, defined by

$$T(t) := e^{-itzA} \ ,$$

for every $t \geqslant 0$ is a strongly continuous semigroup, i.e, such that $T(0) = \mathrm{id}_X$, $T(t+s) = T(t)T(s)$, for all $t, s \in [0,\infty)$ and such that $([0,\infty) \to X, t \mapsto T(t)f)$ is continuous for every $f \in X$, with corresponding generator izA. Further, $\|T(t)\| \leqslant e^{y\gamma t}$, for every $t \geqslant 0$, where $y := \mathrm{Im}(z)$, i.e., T is a quasi-contraction as well as a contraction if A is positive.

Proof. For the case that $z = 0$, the statement of the lemma is obviously true. In the following, we consider the remaining case that $z \neq 0$. Then it follows from the functional calculus for A that T is a strongly continuous semigroup as well as that

$$\|T(t)\| \leqslant \|\, e^{-itz\,\mathrm{id}_{\sigma(A)}}\|_\infty = \|\, e^{ty\,\mathrm{id}_{\sigma(A)}}\|_\infty \leqslant e^{y\gamma t} \ ,$$

for every $t \geqslant 0$, where $y := \mathrm{Im}(z)$. In the following, let

$$U_A = \frac{\mathrm{id}_{\sigma(A)} - i\,\mathbb{1}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) = \mathrm{id}_X + \frac{2}{i}\,(A+i)^{-1}$$

be the Cayley transform of A. Then,

$$U_A - \mathrm{id}_X = \frac{2}{i}\,\frac{1}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) \ , \ U_A + \mathrm{id}_X = \frac{2\,\mathrm{id}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) \ .$$

We claim that

$$\lim_{t\to 0+} \frac{1}{t}\,(e^{-itzA} - \mathrm{id}_X)(U_A - \mathrm{id}_X)g = -z\,(U_A + \mathrm{id}_X)g \ , \tag{12.64}$$

for every $g \in X$. For the proof, let $g \in X$ and $t_1, t_2, \dots$ a sequence in $(0,\infty)$ that is convergent to 0. We note that

$$\frac{1}{t_\nu}\,(e^{-it_\nu zA} - \mathrm{id}_X)(U_A - \mathrm{id}_X) = \frac{2}{i}\,\frac{\frac{1}{t_\nu}[e^{-it_\nu z\,\mathrm{id}_{\sigma(A)}} - \mathbb{1}_{\sigma(A)}]}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) \ ,$$

for every $\nu \in \mathbb{N}^*$. Since for every $\lambda \in \mathbb{R}$, the function $(\mathbb{R} \to \mathbb{C}, t \mapsto \exp(-iz\lambda t))$ is differentiable with derivative $(\mathbb{R} \to \mathbb{C}, t \mapsto -i\lambda z\exp(-iz\lambda t))$, we have that

$$\lim_{\nu\to\infty} \frac{2}{i}\,\frac{\frac{1}{t_\nu}[e^{-it_\nu z\,\mathrm{id}_{\sigma(A)}} - \mathbb{1}_{\sigma(A)}]}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}} = -z\,\frac{2\,\mathrm{id}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}$$

everywhere pointwise on $\sigma(A)$. Further, for $\lambda \geqslant \gamma$,

$$\frac{1}{t_\nu}\,|\,e^{-it_\nu z\lambda} - 1\,| = \frac{1}{t_\nu}\,|\,i\lambda z\int_0^{t_\nu} e^{-iz\lambda t}\,dt\,| \leqslant \frac{|\lambda|\cdot|z|}{t_\nu}\int_0^{t_\nu} |e^{-iz\lambda t}|\,dt$$
$$= \frac{|\lambda|\cdot|z|}{t_\nu}\int_0^{t_\nu} e^{\mathrm{Im(z)}\lambda t}\,dt \leqslant |\lambda|\cdot|z|\,e^{-C\,\mathrm{Im(z)}|\mu|} \ ,$$

where $C \geqslant 0$ is such that $|t_\nu| \leqslant C$, for every $\nu \in \mathbb{N}^*$. Hence,

$$\|\frac{2}{i}\,\frac{\frac{1}{t_\nu}[e^{-it_\nu z\,\mathrm{id}_{\sigma(A)}} - \mathbb{1}_{\sigma(A)}]}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}\|_\infty \leqslant 2\,|z|\,e^{-C\,\mathrm{Im(z)}|\mu|}\cdot\|\frac{\mathrm{id}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}\|_\infty \ ,$$

and it follows from the spectral theorem, Theorem 12.6.4, the validity of (12.64), for every $g \in X$. Since $U_A - \mathrm{id}_X$ is injective with $\mathrm{Ran}(U_A - \mathrm{id}_X) = D(A)$ and since

$$A = \frac{1}{i}\,(U_A + \mathrm{id}_X)[(U_A - \mathrm{id}_X)\restriction_{D(A)}]^{-1} \ ,$$

it follows that

$$\lim_{t\to 0+} \frac{1}{t}\,(e^{-itzA} f - f) = -izAf \ ,$$

for every $f \in D(A)$ and hence that the generator of T is an extension of izA. Further, we note that

$$\begin{aligned}\mathrm{Re}\,\langle f|izAf\rangle &= \mathrm{Re}\,\langle f|(ix-y)Af\rangle = \mathrm{Re}(ix\,\langle f|Af\rangle - y\,\langle f|Af\rangle) \\ &= -y\,\langle f|Af\rangle \geqslant -y\gamma\|f\|^2 \ ,\end{aligned}$$

for every $f \in D(A)$, where $x = \mathrm{Re}(z), y = \mathrm{Im}(z) \leqslant 0$, and hence that izA is quasi-accretive with bound $-y\gamma$. Further, we note that

$$izA - \lambda = iz \cdot \left(A + \frac{y}{|z|^2}\,\lambda + i\,\frac{x}{|z|^2}\,\lambda\right) .$$

We consider cases. If $x = 0$, then $y < 0$ and $izA - \lambda$ is bijective for every $\lambda < \min\{-\frac{|z|^2}{y}\,\gamma, -y\gamma\}$. If $x \neq 0$, then $izA - \lambda$ is bijective for every $\lambda < -y\gamma$. Hence, it follows from the Lumer-Phillips theorem, e.g., see Theorem 4.2.6 in [7], that izA is the generator of a strongly continuous semigroup. Finally, since generators of strongly continuous semigroups have no proper extensions, e.g., see Theorem 4.1.1 (vii) in [7], it follows that izA is the generator of T. □

Employing the same methods as in the proof Lemma 12.9.15, we can show the strong complex analyticity of the exponential function for semi-bounded densely-defined, linear and self-adjoint operators in complex Hilbert spaces.

Corollary 12.9.16. Let $(X, \langle\,|\,\rangle)$ be a non-trivial complex Hilbert space, A a semi-bounded densely-defined, linear and self-adjoint operator in X, with lower bound γ, implying that spectrum $\sigma(A)$ of A is contained in $[\gamma, \infty)$. Further, let $\bar{H}_- := \mathbb{R} \times (-\infty, 0]$. Then

$$\lim_{z\to a, z\in \bar{H}_-\setminus\{a\}} \frac{1}{z-a}\left(e^{-izA} - e^{-iaA}\right) f = -ie^{-iaA}Af \ ,$$

for every $f \in D(A)$.

Proof. In the following, let

$$U_A = \frac{\mathrm{id}_{\sigma(A)} - i\,\mathbb{1}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) = \mathrm{id}_X + \frac{2}{i}\,(A+i)^{-1}$$

be the Cayley transform of A. Then,

$$U_A - \mathrm{id}_X = \frac{2}{i}\,\frac{1}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) \ , \ U_A + \mathrm{id}_X = \frac{2\,\mathrm{id}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i\,\mathbb{1}_{\sigma(A)}}(A) \ .$$

We claim that

$$\lim_{z \to 0, z \in \bar{H}_- \setminus \{0\}} \frac{1}{z} \, (e^{-izA} - \mathrm{id}_X)(U_A - \mathrm{id}_X) g = -(U_A + \mathrm{id}_X) g \ , \tag{12.65}$$

for every $g \in X$. For the proof, let $g \in X$ and $z_1, z_2, \dots$ a sequence in $\bar{H}_- \setminus \{0\}$ that is convergent to 0. We note that

$$\frac{1}{z_\nu} \, (e^{-iz_\nu A} - \mathrm{id}_X)(U_A - \mathrm{id}_X) = \frac{2}{i} \, \frac{\frac{1}{z_\nu}[e^{-iz_\nu \, \mathrm{id}_{\sigma(A)}} - \mathbb{1}_{\sigma(A)}]}{\mathrm{id}_{\sigma(A)} + i \, \mathbb{1}_{\sigma(A)}}(A) \ ,$$

for every $\nu \in \mathbb{N}^*$. Further,

$$\left(\frac{2}{iz_\nu} \, \frac{e^{-iz_\nu \, \mathrm{id}_{\sigma(A)}} - \mathbb{1}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i \, \mathbb{1}_{\sigma(A)}} \right)_{\nu \in \mathbb{N}^*}$$

is a sequence in $U^s_{\mathbb{C}}(\sigma(A))$ that is everywhere pointwise convergent to

$$-\frac{2 \, \mathrm{id}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i \, \mathbb{1}_{\sigma(A)}} = - \left[\mathbb{1}_{\sigma(A)} + \frac{\mathrm{id}_{\sigma(A)} - i \, \mathbb{1}_{\sigma(A)}}{\mathrm{id}_{\sigma(A)} + i \, \mathbb{1}_{\sigma(A)}} \right] \in U^s_{\mathbb{C}}(\sigma(A)) \ .$$

That this sequence is in addition uniformly bounded, can be seen as follows. For $\nu \in \mathbb{N}^*$, $\lambda \in \sigma(A)$, we have that

$$\begin{aligned}
&\left| \frac{2}{iz_\nu} \, \frac{e^{-iz_\nu \lambda} - 1}{\lambda + i} \right| = \frac{2}{|z_\nu| \sqrt{1+\lambda^2}} \left| e^{-i\lambda x_\nu} (e^{-\lambda |y_\nu|} - 1) + e^{-i\lambda x_\nu} - 1 \right| \\
&\leqslant \frac{2}{|z_\nu| \sqrt{1+\lambda^2}} \left[|\, e^{-\lambda |y_\nu|} - 1| + 2 \, |\sin(\lambda x_\nu / 2)| \right] \\
&\leqslant \frac{2}{|z_\nu| \sqrt{1+\lambda^2}} \left[\Big| \int_0^{\lambda |y_\nu|} (-e^{-s}) \, ds \, \Big| + |\lambda| \cdot |x_\nu| \right] \\
&\leqslant \frac{2}{|z_\nu| \sqrt{1+\lambda^2}} \left[\Big| \int_0^{\lambda |y_\nu|} e^{K|\gamma|} \, ds \Big| + |\lambda| \cdot |x_\nu| \right] \\
&\leqslant \frac{2 \, |\lambda|}{|z_\nu| \sqrt{1+\lambda^2}} \left[e^{K|\gamma|} \cdot |y_\nu| + |x_\nu| \right] \leqslant 2 \left(e^{K|\gamma|} + 1 \right) \ ,
\end{aligned}$$

where $K := \sup\{|z_\mu| : \mu \in \mathbb{N}^*\}$ and $x_\nu := \mathrm{Re}(z_\nu)$, $y_\nu := \mathrm{Im}(z_\nu) \leqslant 0$. Hence, it follows from the spectral theorem, Theorem 12.6.4, the validity of (12.65), for every $g \in X$. Since $U_A - \mathrm{id}_X$ is injective with $\mathrm{Ran}(U_A - \mathrm{id}_X) = D(A)$ and since

$$A = \frac{1}{i} \, (U_A + \mathrm{id}_X)[(U_A - \mathrm{id}_X) \restriction_{D(A)}]^{-1} \ ,$$

it follows that

$$\lim_{z \to 0, z \in \bar{H}_- \setminus \{0\}} \frac{1}{z} \left(e^{-izA} - \mathrm{id}_X \right) f = -iAf \ ,$$

for every $f \in D(A)$. From the latter, we conclude with the help of the functional calculus for A for $a \in \bar{H}_-$ that

$$\begin{aligned}
&\lim_{z \to a, z \in \bar{H}_- \setminus \{a\}} \frac{1}{z-a}\left(e^{-izA} - e^{-iaA}\right) f \\
&= \lim_{z-a \to 0, z-a \in \bar{H}_- \setminus \{0\}} e^{-iaA}\, \frac{1}{z-a}\left[e^{-i(z-a)A} - \mathrm{id}_X\right] f = -ie^{-iaA} A f \ ,
\end{aligned}$$

for every $f \in D(A)$.

□

Theorem 12.9.17 (Trotter Product Formula for Strongly Continuous Contraction Semigroups). Let $(X, \| \, \|)$ be a non-trivial complex Banach space, A and B generators of strongly continuous contraction semigroups, V and W, respectively, and such that $A+B : D(A) \cap D(B) \to X$ is the generator of a strongly continuous contraction semigroup S. Then

$$s - \lim_{n \to \infty} [\, V(t/n) W(t/n)\,]^n = S(t) \ ,$$

for every $t \in \mathbb{R}$.

Proof. We define $T : [0, \infty) \to L(X, X)$ by

$$T(t) := V(t) W(t) \ ,$$

for every $t \geqslant 0$, Then T is a strongly continuous contraction. In addition, we define the strongly continuous map $K : (0, \infty) \to L(X, X)$ by

$$K(s) := \frac{1}{s}\left[S(s) - T(s)\right] \ ,$$

for every $s > 0$. If $f \in Y := D(A) \cap D(B)$, then

$$\lim_{s \to 0+} \frac{1}{s}\left[S(s) - 1\right] f = -(A+B) f \ ,$$

for $s > 0$

$$\begin{aligned}
&\frac{1}{s}\left[T(s) - 1\right] f = \frac{1}{s}\left(V(s)W(s)f - f\right) \\
&= \frac{1}{s}\left[V(s)(W(s)f - f) + V(s)f - f\right] \\
&= \frac{1}{s}\left[(V(s) - \mathrm{id}_X)\left(W(s)f - f\right) + W(s)f - f + V(s)f - f\right] \\
&= (V(s) - \mathrm{id}_X)\, \frac{1}{s}\left(W(s)f - f\right) + \frac{1}{s}\left(W(s)f - f\right) + \frac{1}{s}\left(V(s)f - f\right) \ ,
\end{aligned}$$

and hence

$$\lim_{s \to 0+} \frac{1}{s}\left[T(s)f - f\right] = -(A+B) f \ .$$

As a result,

$$\lim_{s \to 0+} K(s)f = 0 \; . \tag{12.66}$$

Therefore, the map $((0, \infty) \to X, s \mapsto K(s)f)$ admits an extension to a continuous map on $[0, \infty)$ that vanishes in 0. Hence for every $\varepsilon > 0$, there is $\delta > 0$ such that for every $s \in (0, \delta)$

$$\|K(s)f\| < \varepsilon \; .$$

We note that $\| \;\|_{A+B} : Y \to \mathbb{R}$, defined by

$$\|f\|_{A+B} := \sqrt{\|f\|^2 + \|(A+B)f\|^2} \; ,$$

for every $f \in Y$ defines a norm on Y such that $A + B \in L(Y, X)$ and, since $A + B$ is closed, such that $(Y, \| \;\|_{A+B})$ is a Banach space. Further, since the inclusion $\iota : Y \hookrightarrow X$ is continuous, $B \circ \iota \in L(Y, X)$, for every $B \in L(X, X)$. From (12.66), it follows that the family $(K(s))_{s \in (0,\infty)} \in (L(Y, X))^{\mathbb{N}}$ is pointwise bounded and hence, according to the uniform boundedness principle, uniformly bounded, i.e., there is $C > 0$ such that

$$\|K(s)\|_{Y,X} \leqslant C \; ,$$

for every $s > 0$, where $\| \;\|_{Y,X}$ denotes the operator norm on $L(Y, X)$. Further, if $B \subset Y$ is non-empty and compact, $\varepsilon > 0$ and $\varepsilon_1, \varepsilon_2 > 0$ such that $C\varepsilon_1 + \varepsilon_2 < \varepsilon$, then there are $m \in \mathbb{N}^*$ and $f_1, f_2, \dots, f_m \in Y$ such that

$$B \subset \bigcup_{k=1}^{m} U^Y_{\varepsilon_1}(f_k)$$

and $\delta > 0$ such that for every $k \in \{1, \dots, m\}$

$$\|K(s)f_k\| < \varepsilon_2 \; ,$$

for every $s \in (0, \delta)$. Hence, it follows for $s \in (0, \delta)$, $k \in \{1, \dots, m\}$ and $f \in U^Y_{\varepsilon_1}(f_k)$ that

$$\begin{aligned}\|K(s)f\| &= \|K(s)(f - f_k + f_k)\| \leqslant \|K(s)(f - f_k)\| + \|K(s)f_k\| \\ &\leqslant C\,\|f - f_k\|_{A+B} + \varepsilon_2 < C\varepsilon_1 + \varepsilon_2 < \varepsilon \; .\end{aligned}$$

As a consequence, for every $\varepsilon > 0$, there is $\delta > 0$ such that

$$\|K(s)f\| < \varepsilon \; ,$$

for every $s \in (0, \delta)$ and every $f \in B$. Further, we note that, e.g., see Theorem 6.1.1 in [7], S leaves Y invariant and that $S_Y : [0, \infty) \to L(Y, Y)$, where for every $t \geqslant 0$ the corresponding $S_Y(t)$ denotes the restriction of $S(t)$ in domain and image to Y, is a strongly continuous semigroup. Hence, if $f \in Y$ and $t \geqslant 0$, the latter are both held fixed in the following, then

$$\{S(\tau)f : \tau \in [0, t]\} \; ,$$

is a compact subset of Y, as an image of a compact subset of $\mathbb{R}$ under a continuous map. As a consequence, for $\varepsilon > 0$, there is $\delta > 0$ such that

$$\|K(s)g\| < \varepsilon \ ,$$

for every $s \in (0, \delta)$ and every $g \in \{S(\tau)f : \tau \in [0,t]\}$. In particular, for $n \in \mathbb{N}^*$, there is $\delta_n > 0$ such that

$$\|K(t/n)g\| < \frac{1}{n} \ ,$$

for every $g \in \{S(\tau)f : \tau \in [0,t]\}$, if $n > t/\delta_n$. We note that without loss of generality, we can assume that the sequence $\delta_1, \delta_2, \dots$ is decreasing. Continuing, we observe that

$$\begin{aligned}
&\sum_{j=0}^{n-1} [T(t/n)]^j \, [S(t/n) - T(t/n)] \, [S(t/n)]^{n-1-j} f \\
&= \sum_{j=0}^{n-1} [T(t/n)]^j [S(t/n)]^{n-j} f - \sum_{j=0}^{n-1} [T(t/n)]^{j+1} [S(t/n)]^{n-1-j} f \\
&= \sum_{j=0}^{n-1} [T(t/n)]^j [S(t/n)]^{n-j} f - \sum_{j=0}^{n-1} [T(t/n)]^{j+1} [S(t/n)]^{n-(j+1)} f \\
&= \sum_{j=0}^{n-1} [T(t/n)]^j [S(t/n)]^{n-j} f - \sum_{j=1}^{n} [T(t/n)]^j [S(t/n)]^{n-j} f \\
&= [S(t/n)]^n f - [T(t/n)]^n f = (S(t) - [T(t/n)]^n) f
\end{aligned}$$

and hence if $n > t/\delta_n$ that

$$\begin{aligned}
&\|(S(t) - [T(t/n)]^n) \, f\| \\
&= \left\| \sum_{j=0}^{n-1} [T(t/n)]^j \, [S(t/n) - T(t/n)] \, [S(t/n)]^{n-1-j} f \right\| \\
&\leqslant \sum_{j=0}^{n-1} \| \, [S(t/n) - T(t/n)] \, [S((n-1-j) \, t/n)] f \| \\
&\leqslant n \sup_{\tau \in [0,t]} \| [S(t/n) - T(t/n)] \, S(\tau) f \| = t \sup_{\tau \in [0,t]} \|K(t/n) S(\tau) f\| \leqslant \frac{t}{n} \ ,
\end{aligned}$$

where we used the additivity of S. Hence, it follows that

$$\lim_{n \to \infty} [T(t/n)]^n f = S(t) f \ ,$$

for every $f \in Y$ and since Y is dense in X that

$$s - \lim_{n \to \infty} [T(t/n)]^n = S(t) \ .$$

$\square$

As a consequence, with the help of Stone's theorem and Lemma 12.9.15, we arrive at the following corollaries of the previous theorem.

Corollary 12.9.18 (Trotter Product Formula for Self-Adjoint Operators). Let $(X, \langle \,|\, \rangle)$ be a non-trivial complex Hilbert space, A and B densely-defined, linear and self-adjoint operators in X such that $A + B$ is densely-defined, linear and self-adjoint. Then

$$s - \lim_{n\to\infty} [\, e^{-i\,(t/n)\,A} e^{-i\,(t/n)\,B} \,]^n = e^{-it\,(A+B)} \ ,$$

for every $t \in \mathbb{R}$.

Corollary 12.9.19 (Trotter Product Formulas for Positive Self-Adjoint Operators). Let $(X, \langle \,|\, \rangle)$ be a non-trivial complex Hilbert space, A and B positive densely-defined, linear and self-adjoint operators in X such that $A + B$ is densely-defined, linear and self-adjoint. Further, let $z \in \mathbb{R} \times (-\infty, 0]$. Then

$$s - \lim_{n\to\infty} [\, e^{-i\,(t/n)\,zA} e^{-i\,(t/n)\,zB} \,]^n = e^{-itz\,(A+B)} \ ,$$

for every $t \in [0, \infty)$.

Corollary 12.9.20 (Trotter Product Formulas for Semibounded Self-Adjoint Operators). Let $(X, \langle \,|\, \rangle)$ be a non-trivial complex Hilbert space, A and B semibounded densely-defined, linear and self-adjoint operators in X, with lower bound $\gamma_1 \in \mathbb{R}$ and lower bound $\gamma_2 \in \mathbb{R}$, respectively, and such that $A + B$ is densely-defined, linear and self-adjoint. Further, let $z \in \mathbb{R} \times (-\infty, 0]$. Then

$$s - \lim_{n\to\infty} [\, e^{-i\,(t/n)\,zA} e^{-i\,(t/n)\,zB} \,]^n = e^{-itz\,(A+B)} \ ,$$

for every $t \in [0, \infty)$.

Proof. From Corollary 12.9.19, we obtain for $t \in [0, \infty)$ that

$$s - \lim_{n\to\infty} [\, e^{-i\,(t/n)\,z\,(A-\gamma_1)} e^{-i\,(t/n)\,z\,(B-\gamma_2)}) \,]^n = e^{-itz\,(A+B-(\gamma_1+\gamma_2))} \ .$$

Since,

$$[\, e^{-i\,(t/n)\,z\,(A-\gamma_1)} e^{-i\,(t/n)\,z\,(B-\gamma_2)}) \,]^n = [\, e^{i\,(\gamma_1+\gamma_2)\,(t/n)} e^{-i\,(t/n)\,zA} e^{-i\,(t/n)\,zB} \,]^n$$
$$= e^{i\,(\gamma_1+\gamma_2)\,t} \,[\, e^{-i\,(t/n)\,zA} e^{-i\,(t/n)\,zB} \,]^n$$
$$e^{-itz\,[A+B-(\gamma_1+\gamma_2)]} = e^{i\,(\gamma_1+\gamma_2)\,t}\, e^{-itz\,(A+B)} \ ,$$

it follows that

$$s - \lim_{n\to\infty} [\, e^{-i\,(t/n)\,zA} e^{-i\,(t/n)\,zB} \,]^n = e^{-itz\,(A+B)} \ .$$

□

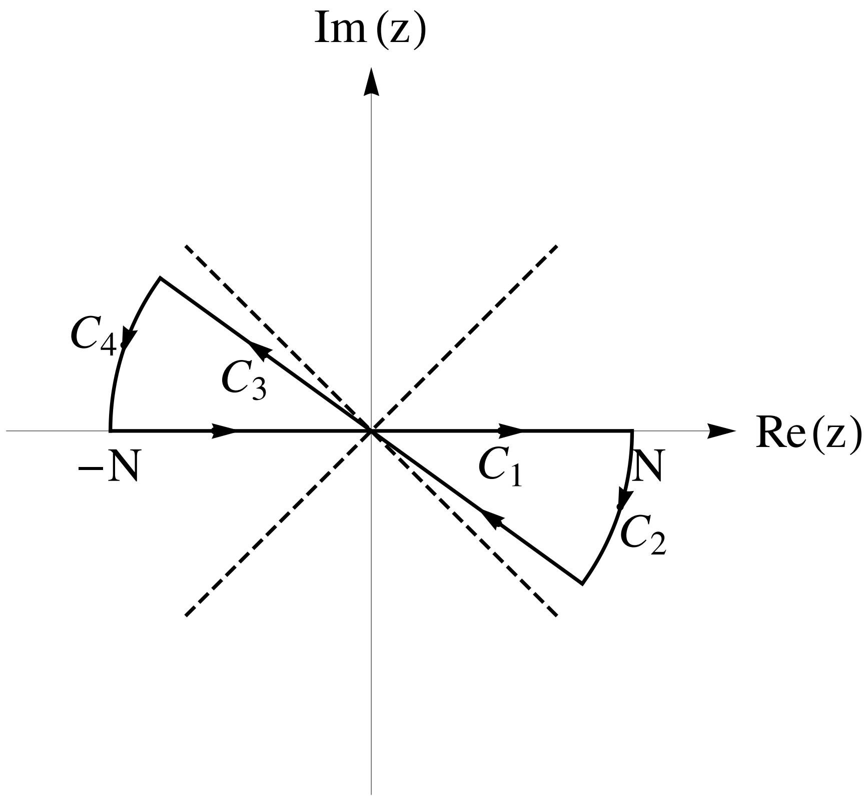


Fig. 12.3: Path for the contour integration in the proof of Lemma 12.9.21, if $\arg(\sigma) \geqslant 0$.

12.9.2 Fourier Integrals

In the following, we show auxiliary results.

Lemma 12.9.21. (**A Gaussian Integral**) Let $\sigma = (\sigma_1, \sigma_2) \in (0, \infty) \times \mathbb{R}$. Then

$$\int_{-\infty}^{\infty} e^{-\sigma x^2} \, dx = \sqrt{\frac{\pi}{\sigma}} \ .$$

Proof. Since $\sigma \in (0, \infty) \times \mathbb{R}$, we note that

$$\arg(\sqrt{\sigma}\,) = \frac{\arg(\sigma)}{2} \ , \ \arg\left(\frac{1}{\sqrt{\sigma}}\right) = -\frac{\arg(\sigma)}{2} \in (-\pi/4, \pi/4) \ .$$

Further, since

$$(\mathbb{C} \to \mathbb{C}, z \mapsto e^{-\sigma z^2})$$

is holomorphic, an application of Cauchy's Integral Theorem gives

$$0 = \int_C e^{-\sigma z^2} \, dz$$

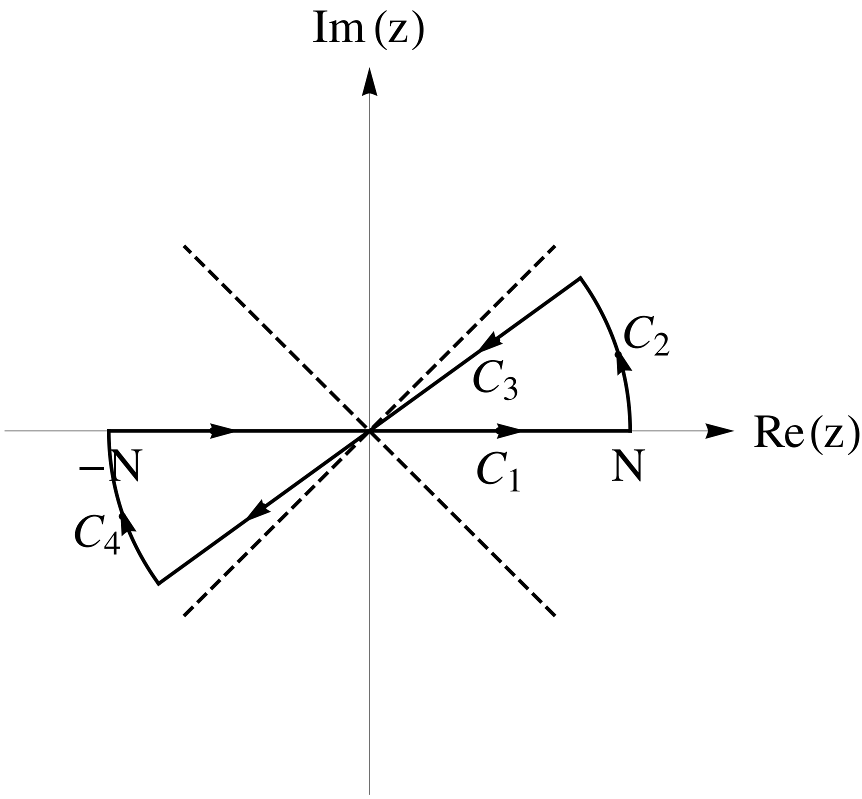


Fig. 12.4: Path for the contour integration in the proof of Theorem 12.9.21, if $\arg(\sigma) < 0$.

$$= \int_{C_1} e^{-\sigma z^2}\, dz + \int_{C_2} e^{-\sigma z^2}\, dz + \int_{C_3} e^{-\sigma z^2}\, dz + \int_{C_4} e^{-\sigma z^2}\, dz \ ,$$

where $N \in \mathbb{N}^*$ and the corresponding the contour C consists of the curves C_1, C_2, C_3, C_4, defined by

$$C_1 := [-N, N] \times \{0\} \ ,$$
$$C_2 := \begin{cases} \{\frac{N}{\sqrt{|\sigma|}} \cdot e^{i\varphi} : \varphi \in [-\frac{\arg(\sigma)}{2}, 0]\} & \text{if } \arg(\sigma) \geqslant 0 \\ \{\frac{N}{\sqrt{|\sigma|}} \cdot e^{i\varphi} : \varphi \in [0, -\frac{\arg(\sigma)}{2}]\} & \text{if } \arg(\sigma) < 0 \end{cases} ,$$
$$C_3 := \left\{ t.\frac{1}{\sqrt{\sigma}} : t \in [-N, N] \right\} \ ,$$
$$C_4 := \begin{cases} \{-\frac{N}{\sqrt{|\sigma|}} \cdot e^{i\varphi} : \varphi \in [-\frac{\arg(\sigma)}{2}, 0]\} & \text{if } \arg(\sigma) \geqslant 0 \\ \{-\frac{N}{\sqrt{|\sigma|}} \cdot e^{i\varphi} : \varphi \in [0, -\frac{\arg(\sigma)}{2}]\} & \text{if } \arg(\sigma) < 0 \end{cases} ,$$

see Fig. 12.9.2. Then,

$$\int_{C_1} e^{-\sigma z^2}\, dz = \int_{-N}^{N} e^{-\sigma x^2}\, dx \ ,$$

$$\int_{C_2} e^{-\sigma z^2}\,dz = i\frac{N}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} e^{-(\sigma/|\sigma|)N^2\cdot e^{2i\varphi}}\,e^{i\varphi}d\varphi$$

$$= i\frac{N}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} e^{-N^2\cdot e^{i(\arg(\sigma)+2\varphi)}}\,e^{i\varphi}d\varphi\ ,$$

$$\int_{C_3} e^{-\sigma z^2}\,dz = -\frac{1}{\sqrt{\sigma}}\int_{-N}^{N} e^{-\sigma\left(t\frac{1}{\sqrt{\sigma}}\right)^2}\,dt = -\frac{1}{\sqrt{\sigma}}\int_{-N}^{N} e^{-t^2}\,dt$$

$$= -\frac{1}{\sqrt{2\sigma}}\int_{-N\sqrt{2}}^{N\sqrt{2}} e^{-x^2/2}\,dx\ ,$$

$$\int_{C_4} e^{-\sigma z^2}\,dz = -i\frac{N}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} e^{-(\sigma/|\sigma|)N^2\cdot e^{2i\varphi}}\,e^{i\varphi}d\varphi$$

$$-\,i\frac{N}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} e^{-N^2\cdot e^{i(\arg(\sigma)+2\varphi)}}\,e^{i\varphi}d\varphi\ .$$

We note that for every

$$\varphi \in \begin{cases}[-\arg(\sigma)/2, 0] & \text{if } \arg(\sigma)\geqslant 0\\ [0, -\arg(\sigma)/2] & \text{if } \arg(\sigma) < 0\end{cases}\ ,$$

it follows that

$$\arg(\sigma)+2\varphi \in \begin{cases}[0, \arg(\sigma)] \subset [0, \pi/2) & \text{if } \arg(\sigma)\geqslant 0\\ [\arg(\sigma), 0] \subset (-\pi/2, 0] & \text{if } \arg(\sigma) < 0\end{cases}$$

and hence that for almost all φ

$$\cos(\arg(\sigma)+2\varphi) > 0\ .$$

Hence

$$\left|\int_{C_2} e^{-\sigma z^2}\,dz\right| = \left|i\frac{N}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} e^{-N^2\cdot e^{i(\arg(\sigma)+2\varphi)}}\,e^{i\varphi}d\varphi\right|\ ,$$

$$\leqslant \frac{1}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} Ne^{-N^2\cdot\cos(\arg(\sigma)+2\varphi)}\,d\varphi\ ,$$

$$\left|\int_{C_4} e^{-\sigma z^2}\,dz\right| = \left|-i\frac{N}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} e^{-N^2\cdot e^{i(\arg(\sigma)+2\varphi)}}\,e^{i\varphi}d\varphi\right|\ ,$$

$$\leqslant \frac{1}{\sqrt{|\sigma|}}\int_{-\arg(\sigma)/2\ (0)}^{0\ (-\arg(\sigma)/2\,)} Ne^{-N^2\cdot\cos(\arg(\sigma)+2\varphi)}\,d\varphi\ ,$$

and it follows from Lebesgue's dominated convergence theorem that

$$\lim_{N\to\infty}\int_{C_2} e^{-\sigma z^2}\,dz = \lim_{N\to\infty}\int_{C_4} e^{-\sigma z^2}\,dz = 0\ .$$

Again, using Lebesgue's dominated convergence theorem, we arrive at

$$\lim_{N\to\infty}\int_{-N}^{N} e^{-\sigma x^2}\,dx = \lim_{N\to\infty}\frac{1}{\sqrt{2\sigma}}\int_{-N\sqrt{2}}^{N\sqrt{2}} e^{-x^2/2}\,dx = \frac{1}{\sqrt{2\sigma}}\int_{-\infty}^{\infty} e^{-x^2/2}\,dx$$
$$= \frac{\sqrt{2\pi}}{\sqrt{2\sigma}} = \sqrt{\frac{\pi}{\sigma}}\ .$$

Since for every $x \in \mathbb{R}$,

$$\sigma_1 x^2 = \sigma_1 |x|^2 \geqslant \begin{cases} \sigma_1|x| & \text{if } |x| \geqslant 1 \\ 0 & \text{if } |x| < 1 \end{cases} ,$$

we conclude for every $x \in \mathbb{R}$ that

$$|\,e^{-\sigma x^2}| = e^{-\sigma_1 x^2} \leqslant \begin{cases} e^{-\sigma_1 |x|} & \text{if } |x| \geqslant 1 \\ 1 & \text{if } |x| < 1 \end{cases} \leqslant \chi_{_{[-1,1]}}(x) + e^{-\sigma_1|\ |}(x)\ .$$

Hence

$$\left(\chi_{_{[-N,N]}} \cdot e^{-\sigma.\mathrm{id}_{\mathbb{R}}{}^2}\right)_{N\in\mathbb{N}^*}$$

is a sequence of Lebesgue-integrable functions that converges everywhere on $\mathbb{R}$ pointwise to $e^{-\sigma.\mathrm{id}_{\mathbb{R}}{}^2}$. In addition, each member of the corresponding sequence

$$\left(|\chi_{_{[-N,N]}} \cdot e^{-\sigma.\mathrm{id}_{\mathbb{R}}{}^2}|\right)_{N\in\mathbb{N}^*}$$

is dominated by the Lebesgue-integrable function

$$\chi_{_{[-1,1]}} + e^{-\sigma_1|\ |}\ .$$

Hence it follows from Lebesgue's dominated convergence theorem that

$$\int_{-\infty}^{\infty} e^{-\sigma x^2}\,dx = \lim_{N\to\infty}\int_{-N}^{N} e^{-\sigma x^2}\,dx = \sqrt{\frac{\pi}{\sigma}}\ .$$

□

Lemma 12.9.22. (**A Fourier Transform of a Gaussian I**) Let $\sigma = (\sigma_1, \sigma_2) \in (0,\infty)\times\mathbb{R}$. Then

$$F_1 e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2} = \sqrt{\frac{\pi}{\sigma}}\, e^{-\mathrm{id}_{\mathbb{R}}^2/(4\sigma)}\ .$$

Proof. For the proof, we define $g : \mathbb{R} \to \mathbb{C}$ by

$$g(x) := e^{-\sigma x^2}$$

for every $x \in \mathbb{R}$. As a consequence of the proof of Theorem 12.9.21,

$$g \in \mathcal{L}^1_{\mathbb{C}}(\mathbb{R})$$

and

$$|g| \leqslant \chi_{_{[-1,1]}} + e^{-\sigma_1 |\ |} \ .$$

Further, $g \in C^1(\mathbb{R}, \mathbb{C})$ and

$$g' = -2\sigma.\mathrm{id}_{\mathbb{R}} \cdot g \ .$$

Since for every $x \in \mathbb{R}$

$$\begin{aligned}
|\, xe^{-\sigma x^2}| = |x| e^{-\sigma_1 x^2} &\leqslant \begin{cases} |x| e^{-\sigma_1 |x|} & \text{if } |x| \geqslant 1 \\ |x| & \text{if } |x| < 1 \end{cases} \\
&\leqslant \begin{cases} |x| e^{-(\sigma_1/2)|x|}\, e^{-(\sigma_1/2)|x|} & \text{if } |x| \geqslant 1 \\ 1 & \text{if } |x| < 1 \end{cases} \\
&\leqslant \begin{cases} C\, e^{-(\sigma_1/2)|x|} & \text{if } |x| \geqslant 1 \\ 1 & \text{if } |x| < 1 \end{cases} \\
&\leqslant \max\{1, C\}.(\chi_{_{[-1,1]}} + e^{-\sigma_1 |\ |})(x) \ ,
\end{aligned}$$

we conclude that

$$\mathrm{id}_{\mathbb{R}} \cdot g \ , \ g' \in \mathcal{L}^1_{\mathbb{C}}(\mathbb{R}) \ .$$

Hence it follows from the properties of the Fourier Transformation F_1 that

$$\begin{aligned}
(F_1 g)' &= F_1(-i.\mathrm{id}_{\mathbb{R}} \cdot g) \\
F_1(-i.\mathrm{id}_{\mathbb{R}} \cdot g) &= \frac{i}{2\sigma}.F_1(-2\sigma.\mathrm{id}_{\mathbb{R}} \cdot g) = \frac{i}{2\sigma}.F_1 g' = \frac{i}{2\sigma}.i.\mathrm{id}_{\mathbb{R}} \cdot F_1 g \\
&= -\frac{1}{2\sigma}.\mathrm{id}_{\mathbb{R}} \cdot F_1 g
\end{aligned}$$

and hence that

$$(F_1 g)' = -\frac{1}{2\sigma}.\mathrm{id}_{\mathbb{R}} \cdot F_1 g \ .$$

Hence it follows, according to the Theory of Ordinary Differential Equations for complex-valued functions and as a consequence of Theorem 12.9.21, that

$$F_1 g = (F_1 g)(0)\, e^{-\mathrm{id}^2_{\mathbb{R}}/(4\sigma)} = \sqrt{\frac{\pi}{\sigma}}\, e^{-\mathrm{id}^2_{\mathbb{R}}/(4\sigma)} \ .$$

□

Corollary 12.9.23. (**A Fourier Transform of a Gaussian II**) Let $\sigma = (\sigma_1, \sigma_2) \in (0, \infty) \times \mathbb{R}$. Then

$$F_2 e^{-\sigma.\mathrm{id}^2_{\mathbb{R}}} = \frac{1}{\sqrt{2\sigma}}.e^{-\mathrm{id}^2_{\mathbb{R}}/(4\sigma)} \ .$$

Proof. For the proof, we note that

$$|e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2}|^2 \leqslant |e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2}|$$

and hence that

$$e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2} \in L^1_{\mathbb{C}}(\mathbb{R}) \cap L^2_{\mathbb{C}}(\mathbb{R}) \ .$$

As a consequence,

$$F_2 e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2} = \frac{1}{\sqrt{2\pi}}.F_1 e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2} = \frac{1}{\sqrt{2\pi}}.\sqrt{\frac{\pi}{\sigma}}.e^{-\mathrm{id}_{\mathbb{R}}^2/(4\sigma)} = \frac{1}{\sqrt{2\sigma}}.e^{-\mathrm{id}_{\mathbb{R}}^2/(4\sigma)} \ .$$

□

Corollary 12.9.24. (**A Fourier Transform of a Gaussian III**) Let $\sigma = (\sigma_1, \sigma_2) \in (0, \infty) \times \mathbb{R}$. Then

$$F_2 e^{-\sigma.|\ |^2} = (2\sigma)^{-n/2}.e^{-|\ |^2/(4\sigma)} \ .$$

Proof. First, since,

$$e^{-\sigma.\mathrm{id}_{\mathbb{R}}^2} \in L^1_{\mathbb{C}}(\mathbb{R}) \cap L^2_{\mathbb{C}}(\mathbb{R}) \ ,$$

we conclude from Tonelli's Theorem that

$$e^{-\sigma.|\ |^2} \in L^1_{\mathbb{C}}(\mathbb{R}^2)$$

and continuing in this manner that

$$e^{-\sigma.|\ |^2} \in L^1_{\mathbb{C}}(\mathbb{R}^n) \ .$$

Further, since

$$|\,e^{-\sigma.|\ |^2}|^2 \leqslant |\,e^{-\sigma.|\ |}| \ ,$$

we arrive at

$$e^{-\sigma.|\ |^2} \in L^1_{\mathbb{C}}(\mathbb{R}^n) \cap L^2_{\mathbb{C}}(\mathbb{R}^n) \ .$$

Hence it follows from Fubini's Theorem and Theorem 12.9.21 that

$$\begin{aligned} F_2 e^{-\sigma.|\ |^2} &= \left(\frac{1}{\sqrt{2\pi}}\right)^n \cdot F_1 e^{-\sigma.|\ |^2} = \left(\frac{1}{\sqrt{2\pi}}\right)^n \cdot \left(\sqrt{\frac{\pi}{\sigma}}\right)^n e^{-|\ |^2/(4\sigma)} \\ &= (2\sigma)^{-n/2}.e^{-|\ |^2/(4\sigma)} \ . \end{aligned}$$

□

Lemma 12.9.25 (An Application of Cauchy's Integral Theorem). Let $\sigma = (\sigma_1, \sigma_2) \in (0, \infty) \times \mathbb{R}$, $(z_1, \dots, z_n) \in \mathbb{C}^n$. Then,

$$[F_1 e^{-\sigma \sum_{j=1}^n (pr_j + z_j)^2}](v) = \left(\frac{\pi}{\sigma}\right)^{n/2} e^{i\sum_{j=1}^n z_j v_j} e^{-|v|^2/(4\sigma)} \ ,$$

$$[F_2 e^{-\sigma \sum_{j=1}^n (pr_j + z_j)^2}](v) = (2\sigma)^{-n/2}\, e^{i\sum_{j=1}^n z_j v_j} e^{-|v|^2/(4\sigma)} \ ,$$

for all $v \in \mathbb{R}^n$, where $pr_1, \dots, pr_n$ are the coordinate projections of $\mathbb{R}^n$.

Proof. For the proof, let $\sigma = (\sigma_1, \sigma_2) \in (0, \infty) \times \mathbb{R}$ and $z = (z_1, z_2) \in \mathbb{C}$. Then, it follows for $v \in \mathbb{R}$ that

$$\begin{aligned}\int_{\mathbb{R}} e^{-ivu} e^{-\sigma(u+z)^2}\, du &= \int_{\mathbb{R}} e^{-ivu} e^{-\sigma(u+z_1+iz_2)^2}\, du \\ &= e^{ivz_1} \int_{\mathbb{R}} e^{-ivu} e^{-\sigma(u+iz_2)^2}\, du \\ &= e^{ivz} \int_{\mathbb{R}} e^{-iv(u+iz_2)} e^{-\sigma(u+iz_2)^2}\, du \ ,\end{aligned}$$

and from Cauchy's integral theorem for rectangular paths, along the boundary of the rectangle $[-\nu, \nu] \times [0, z_2]$ and $[-\nu, \nu] \times [z_2, 0]$, if $z_2 \geqslant 0$ and $z_2 < 0$, respectively, where $\nu \in \mathbb{N}^*$, that

$$\begin{aligned}0 = &\int_{-\nu}^{\nu} e^{-ivu} e^{-\sigma u^2}\, du - \int_{-\nu}^{\nu} e^{-iv(u+iz_2)} e^{-\sigma(u+iz_2)^2}\, du \\ &+ i \left[\int_0^{z_2} e^{-iv(\nu+iu)} e^{-\sigma(\nu+iu)^2}\, du - \int_0^{z_2} e^{-iv(-\nu+iu)} e^{-\sigma(-\nu+iu)^2}\, du \right] \ .\end{aligned}$$

Since for every $v \in \mathbb{R}$ and $u = (u_1, u_2) \in \mathbb{C}$

$$\begin{aligned}&|\, e^{-ivu} e^{-\sigma u^2} | = |\, e^{-iv(u_1+iu_2)} e^{-\sigma(u_1+iu_2)^2} | \\ &= |\, e^{-iv(u_1+iu_2)} e^{-\sigma(u_1^2-u_2^2+2iu_1u_2)} | = e^{vu_2} |\, e^{-(\sigma_1+i\sigma_2)(u_1^2-u_2^2+2iu_1u_2)} | \\ &= e^{vu_2} e^{-\sigma_1(u_1^2-u_2^2)+2\sigma_2 u_1 u_2} \ ,\end{aligned}$$

we deduce that

$$|\, e^{-iv(\pm\nu+iu)} e^{-\sigma(\pm\nu+iu)^2} | = e^{vu} e^{-\sigma_1(\nu^2-u^2)\pm 2\sigma_2 \nu u} = e^{(v \pm 2\sigma_2 \nu) u} e^{-\sigma_1(\nu^2-u^2)} \ ,$$

for every $u \in [0, z_2]$ and $u \in [z_2, 0]$, respectively, from Lebesgue's dominated convergence theorem that

$$\int_{\mathbb{R}} e^{-iv(u+iz_2)} e^{-\sigma(u+iz_2)^2}\, du = \int_{\mathbb{R}} e^{-ivu} e^{-\sigma u^2}\, du = \sqrt{\frac{\pi}{\sigma}}\, e^{-v^2/(4\sigma)}$$

and hence that

$$\int_{\mathbb{R}} e^{-ivu} e^{-\sigma(u+z)^2}\, du = e^{ivz} \int_{\mathbb{R}} e^{-ivu} e^{-\sigma u^2}\, du = \sqrt{\frac{\pi}{\sigma}}\, e^{ivz} e^{-v^2/(4\sigma)} \ .$$

Finally, from Fubini's theorem, we infer further that

$$\int_{\mathbb{R}^n} e^{-iv \cdot \mathrm{id}_{\mathbb{R}^n}}\, e^{-\sigma \sum_{j=1}^n (pr_j + z_j)^2}\, dv^n = \left(\frac{\pi}{\sigma} \right)^{n/2} e^{\, i \sum_{j=1}^n z_j v_j} e^{-|v|^2/(4\sigma)} \ ,$$

where $pr_1, \dots, pr_n$ are the coordinate projections of $\mathbb{R}^n$. $\square$

Lemma 12.9.26. (An Inequality for Convolutions) For $f, g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$, $f * g \in C_\infty(\mathbb{R}^n, \mathbb{C})$ and

$$\|f * g\|_\infty \leqslant \frac{1}{(2\pi)^{n/2}} \cdot \|f\|_2 \cdot \|g\|_2 \ .$$

Proof. Let $f, g \in L^2_{\mathbb{C}}(\mathbb{R}^n)$. From the theory of the Fourier transformation, it follows that

$$f * g = F_1[(F_2^{-1} f) \cdot (F_2^{-1} g)] \ .$$

Hence, it follows for every $k \in \mathbb{R}^n$ that

$$\begin{aligned}
&|(f * g)(k)| = \left| \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ik.\mathrm{id}_{\mathbb{R}^n}} (F_2^{-1} f) \cdot (F_2^{-1} g) \, dv^n \right| \\
&\leqslant \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} |F_2^{-1} f| \cdot |F_2^{-1} g| \, dv^n \leqslant \frac{1}{(2\pi)^{n/2}} \cdot \|F_2^{-1} f\|_2 \cdot \|F_2^{-1} g\|_2 \\
&= \frac{1}{(2\pi)^{n/2}} \cdot \|f\|_2 \cdot \|g\|_2 \ ,
\end{aligned}$$

where the Cauchy-Schwarz inequality for $L^2_{\mathbb{C}}(\mathbb{R}^n)$ has been used. □

12.9.3 Special Functions

Lemma 12.9.27 (A Connection Between Confluent Hypergeometric Functions and Laguerre Polynomials). Let $l \in \mathbb{N}$, $n \in \{l+1, l+2, \dots\}$. Then,

$$M(l + 1 - n \, , \, 2(l+1) \, , x) = \binom{n+l}{2l+1}^{-1} \cdot L^{(2l+1)}_{n-(l+1)}(x) \ \ ,$$

for every $x \in \mathbb{R}$, where the confluent hypergeometric functions M and the generalized Laguerre polynomials L are defined according to [1]. See [1], Identities 22.3.9 and 22.5.54.

Proof. in the following, we are going to use Pochhammers symbol, defined according to [1], see Identity 6.1.22. First, we note that for all $k, n \in \mathbb{N}$:

$$(-n)_k = (-1)^k \cdot (n - (k-1))_k \ .$$

Indeed,

$$\begin{aligned}
1 &= (-n)_0 = (-1)^0 \cdot (n - (0-1))_0 \ , \\
-n &= (-n)_1 = (-1)^1 \cdot (n - (1-1))_1 \ ,
\end{aligned}$$

and for $k \geqslant 2$:

$$\begin{aligned}
(-n)_k &= (-n) \cdot (-n+1) \cdot \ldots \cdot (-n+k-1) \\
&= (-1)^k \cdot n \cdot (n-1) \cdot \ldots \cdot [n - (k-1)]
\end{aligned}$$

$$\begin{aligned} &= (-1)^k \cdot [n-(k-1)] \cdot \ldots \cdot (n-1) \cdot n \\ &= (-1)^k \cdot (n-(k-1))_k \ . \end{aligned}$$

Further, for $l \in \mathbb{N}$ and $n \in \{l+1, l+2, \ldots\}$, it follows that

$$\begin{aligned} &M(l+1-n\,,\, 2(l+1)\,, x) \\ &= M(-[n-(l+1)]\,,\, 2(l+1)\,, x) \\ &= \sum_{k=0}^{n-(l+1)} \frac{(-[n-(l+1)])_k}{(2(l+1))_k} \cdot \frac{x^k}{k!} \\ &= \sum_{k=0}^{n-(l+1)} \frac{(n-(l+1)-(k-1))_k}{(2(l+1))_k} \cdot \frac{(-x)^k}{k!} \\ &= \sum_{k=0}^{n-(l+1)} \frac{(n-(l+k))_k}{(2(l+1))_k} \cdot \frac{(-x)^k}{k!} \\ &= \sum_{k=0}^{n-(l+1)} \frac{\Gamma(n-l)/\Gamma(n-(l+k))}{\Gamma(2(l+1)+k)/\Gamma(2(l+1))} \cdot \frac{(-x)^k}{k!} \\ &= \Gamma(2(l+1)) \sum_{k=0}^{n-(l+1)} \frac{\Gamma(n-l)}{\Gamma(n-(l+k))\Gamma(2(l+1)+k)} \cdot \frac{(-x)^k}{k!} \end{aligned}$$

Further, since for $k \in \{0, \ldots, n-(l+1)\}$

$$\begin{aligned} \binom{n+l}{n-(l+k+1)} &= \frac{\Gamma(n+l+1)}{\Gamma(n-(l+k))\Gamma(2(l+1)+k)} \\ &= \frac{\Gamma(n+l+1)}{\Gamma(n-l)} \cdot \frac{\Gamma(n-l)}{\Gamma(n-(l+k))\Gamma(2(l+1)+k)} \ , \end{aligned}$$

it follows that

$$\begin{aligned} &M(l+1-n\,,\, 2(l+1)\,, x) \\ &= \frac{\Gamma(2(l+1))\Gamma(n-l)}{\Gamma(n+l+1)} \sum_{k=0}^{n-(l+1)} (-1)^k \binom{n+l}{n-(k+l+1)} \cdot \frac{x^k}{k!} \\ &= \frac{(2l+1)! \cdot (n-(l+1))!}{(n+l)!} \sum_{k=0}^{n-(l+1)} (-1)^k \binom{n+l}{n-(k+l+1)} \cdot \frac{x^k}{k!} \\ &= \binom{n+l}{2l+1}^{-1} \cdot L_{n-(l+1)}^{(2l+1)}(x) \ . \end{aligned}$$

$\square$

Lemma 12.9.28 (A Rodrigues' Type Formula for Laguerre Polynomials). Let $n \in \mathbb{N}$ and $\alpha > -1$. Then,

$$L_n^\alpha = \frac{1}{n!}\, x^{-\alpha} e^x \left(e^{-x} x^{n+\alpha}\right)^{(n)} ,$$

where x denotes the identical function on $\mathbb{N}$ and L the generalized Laguerre polynomials defined according to [1]. See [1], Identity 22.3.9.

Proof. According to Identity 22.3.9 in [1], for every $n \in \mathbb{N}$ and $\alpha > -1$:

$$L_n^\alpha = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{x^k}{k!} .$$

Further, we note for every $n \in \mathbb{N}$ and every C^∞-function f, defined on some open interval of $\mathbb{R}$, that

$$e^x \left(e^{-x} f\right)^{(n)} = \left(\frac{d}{dx} - 1\right)^n f . \tag{12.67}$$

The proof proceeds by induction on n. For $n = 0$, the previous is obviously satisfied. For the induction step, we assume that

$$e^x \left(e^{-x} f\right)^{(n)} = \left(\frac{d}{dx} - 1\right)^n f ,$$

for some $n \in \mathbb{N}$ and every C^∞-function f, defined on some open interval of $\mathbb{R}$. Then

$$\begin{aligned}
&e^x \left(e^{-x} f\right)^{(n+1)} = e^x \left(-e^{-x} f + e^{-x} f'\right)^{(n)} = -e^x \left(e^{-x} f\right)^{(n)} + e^x \left(e^{-x} f'\right)^{(n)} \\
&= -\left(\frac{d}{dx} - 1\right)^n f + \left(\frac{d}{dx} - 1\right)^n f' = -\left(\frac{d}{dx} - 1\right)^n f + \left(\frac{d}{dx} - 1\right)^n \frac{d}{dx} f \\
&= \left(\frac{d}{dx} - 1\right)^n \left(\frac{d}{dx} - 1\right) f = \left(\frac{d}{dx} - 1\right)^{n+1} f ,
\end{aligned}$$

for every C^∞-function, defined on some open interval of $\mathbb{R}$. Hence, (12.67) is true also for $n+1$, and the induction is complete. In the following, let $n \in \mathbb{N}$ and $\alpha > -1$. Using (12.67), it follows that

$$\begin{aligned}
&\frac{1}{n!}\, x^{-\alpha} e^x \left(e^{-x} x^{n+\alpha}\right)^{(n)} = \frac{1}{n!}\, x^{-\alpha} \left(\frac{d}{dx} - 1\right)^n x^{n+\alpha} \\
&= \frac{1}{n!}\, x^{-\alpha} \left[\sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{d^{n-k}}{dx^{n-k}}\right] x^{n+\alpha} \\
&= \frac{1}{n!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} x^{-\alpha} \frac{d^{n-k}}{dx^{n-k}} x^{n+\alpha} \\
&= \frac{1}{n!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} x^{-\alpha} \left[\prod_{m=0}^{n-k-1} (n+\alpha-m)\right] x^{n+\alpha-(n-k)}
\end{aligned}$$

$$= \frac{1}{n!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{(n+\alpha)!}{(k+\alpha)!} \, x^k = \sum_{k=0}^{n} (-1)^k \frac{(n+\alpha)!}{(n-k)! \cdot (k+\alpha)!} \, \frac{x^k}{k!}$$
$$= \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{x^k}{k!} = L_n^\alpha \; .$$

□

Lemma 12.9.29 (Integrals Involving Laguerre Polynomials). Let $\alpha > -1$. Then

$$\int_0^\infty x^m L_n^\alpha \, x^\alpha e^{-x} \, dx = (-1)^m \, \Gamma(m+\alpha+1) \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases} \; ,$$

for $n \in \mathbb{N}$ and $0 \leqslant m \leqslant n$. In addition,

$$\int_0^\infty x^m L_n^\alpha \, x^\alpha e^{-x} \, dx = (-1)^n \binom{m}{n} \Gamma(m+\alpha+1) \; ,$$

for $m, n \in \mathbb{N}$ satisfying $m > n$.

Proof. With the help of Lemma 12.9.28, it follows for $\alpha > -1$ and $m, n \in \mathbb{N}$ that

$$I_{mn} := \int_0^\infty x^m L_n^\alpha \, x^\alpha e^{-x} \, dx = \int_0^\infty x^m \, \frac{1}{n!} \, x^{-\alpha} e^x \, (e^{-x} x^{n+\alpha})^{(n)} \, x^\alpha e^{-x} \, dx$$
$$= \frac{1}{n!} \int_0^\infty x^m (e^{-x} x^{n+\alpha})^{(n)} \, dx \; .$$

In the case $n = 0$, the latter leads to

$$I_{m0} = \int_0^\infty x^{m+\alpha} e^{-x} \, dx = \Gamma(m+\alpha+1) \; .$$

In case that $n \in \mathbb{N}^*$, it follows for $m = 0$ that

$$I_{mn} = \frac{1}{n!} \int_0^\infty (e^{-x} x^{n+\alpha})^{(n)} \, dx = \frac{1}{n!} \int_0^\infty \left[(e^{-x} x^{n+\alpha})^{(n-1)} \right]' \, dx$$
$$= \frac{1}{n!} \int_0^\infty \left[e^{-x} \left(\frac{d}{dx} - 1 \right)^{n-1} x^{n+\alpha} \right]' \, dx = 0 \; ,$$

and for $m \neq 0$ that

$$I_{mn} = \frac{1}{n!} \int_0^\infty x^m (e^{-x} x^{n+\alpha})^{(n)} \, dx$$
$$= \frac{1}{n!} \int_0^\infty \left\{ \left[x^m (e^{-x} x^{n+\alpha})^{(n-1)} \right]' - m x^{m-1} (e^{-x} x^{n+\alpha})^{(n-1)} \right\} \, dx$$

$$
\begin{aligned}
&= \frac{1}{n!} \int_0^\infty \left[x^m e^{-x} \left(\frac{d}{dx} - 1 \right)^{n-1} x^{n+\alpha} \right]' dx \\
&\quad - \frac{m}{n!} \int_0^\infty x^{m-1} (e^{-x} x^{n+\alpha})^{(n-1)} \, dx \\
&= -\frac{m}{n!} \int_0^\infty x^{m-1} (e^{-x} x^{n+\alpha})^{(n-1)} \, dx \ ,
\end{aligned}
$$

where we used (12.67). In the following, we assume that $m, n \in \mathbb{N}^*$ and $m \leqslant n$. Repeating the above procedure, we obtain after m steps

$$
I_{mn} = (-1)^m \frac{m!}{n!} \int_0^\infty (e^{-x} x^{n+\alpha})^{(n-m)} \, dx \ .
$$

In particular, if $m < n$, we arrive at

$$
\begin{aligned}
I_{mn} &= (-1)^m \frac{m!}{n!} \int_0^\infty (e^{-x} x^{n+\alpha})^{(n-m)} \, dx \\
&= (-1)^m \frac{m!}{n!} \int_0^\infty \left[(e^{-x} x^{n+\alpha})^{(n-m-1)} \right]' dx \\
&= (-1)^m \frac{m!}{n!} \int_0^\infty \left[e^{-x} \left(\frac{d}{dx} - 1 \right)^{n-m-1} x^{n+\alpha} \right]' dx = 0 \ .
\end{aligned}
$$

If $m = n$, then

$$
I_{nn} = (-1)^n \int_0^\infty e^{-x} x^{n+\alpha} \, dx = (-1)^n \, \Gamma(n + \alpha + 1) \ .
$$

Summarizing the above results, we showed that

$$
\int_0^\infty x^m L_n^\alpha \, x^\alpha e^{-x} \, dx = (-1)^m \, \Gamma(m + \alpha + 1) \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases} \ ,
$$

for $n \in \mathbb{N}$ and $0 \leqslant m \leqslant n$. In the following, we calculate I_{mn}, for $m, n \in \mathbb{N}^*$ and $m > n$. If $n = 0$, see above, it follows that

$$
I_{m0} = \Gamma(m + \alpha + 1) \ .
$$

If $n > 0$, again, repeating the above procedure, we obtain after n steps

$$
\begin{aligned}
I_{mn} &= (-1)^n \frac{m \cdot (m-1) \cdot \ldots \cdot [m - (n-1)]}{n!} \int_0^\infty x^{m-n} e^{-x} x^{n+\alpha} \, dx \\
&= (-1)^n \frac{m \cdot (m-1) \cdot \ldots \cdot [m - (n-1)]}{n!} \int_0^\infty x^{m+\alpha} e^{-x} \, dx \\
&= (-1)^n \frac{m \cdot (m-1) \cdot \ldots \cdot [m - (n-1)]}{n!} \, \Gamma(m + \alpha + 1)
\end{aligned}
$$

$$= (-1)^n \, \frac{m!}{n!(m-n)!} \, \Gamma(m+\alpha+1) = (-1)^n \binom{m}{n} \Gamma(m+\alpha+1) \; .$$

□

Lemma 12.9.30 (Orthogonality and Normalization of Laguerre Polynomials). Let $\alpha > -1$. Then

$$\int_0^\infty L_m^\alpha L_n^\alpha \, x^\alpha e^{-x} \, dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{\Gamma(n+\alpha+1)}{n!} & \text{if } m = n \end{cases} \; ,$$

for all $m, n \in \mathbb{N}$. In addition,

$$\int_0^\infty (L_n^\alpha)^2 \, x^{\alpha+1} e^{-x} \, dx = \frac{2n+\alpha+1}{n!} \, \Gamma(n+\alpha+1) \; ,$$

for all $n \in \mathbb{N}$.

Proof. For the proof, let $m, n \in \mathbb{N}$. Without loss of generality, we can assume that $m \leqslant n$. If $m < n$, then

$$\int_0^\infty L_m^\alpha L_n^\alpha \, x^\alpha e^{-x} \, dx = \sum_{k=0}^m \frac{(-1)^k}{k!} \binom{m+\alpha}{m-k} \int_0^\infty x^k L_n^\alpha \, x^\alpha e^{-x} \, dx = 0 \; .$$

If $m = n$, then

$$\begin{aligned}
&\int_0^\infty L_n^\alpha L_n^\alpha \, x^\alpha e^{-x} \, dx = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} \int_0^\infty x^k L_n^\alpha \, x^\alpha e^{-x} \, dx \\
&= \frac{(-1)^n}{n!} \int_0^\infty x^n L_n^\alpha \, x^\alpha e^{-x} \, dx = \frac{(-1)^n}{n!} \, (-1)^n \, \Gamma(n+\alpha+1) \\
&= \frac{\Gamma(n+\alpha+1)}{n!} \; .
\end{aligned}$$

In addition,

$$\begin{aligned}
&\int_0^\infty L_n^\alpha L_n^\alpha \, x^{\alpha+1} e^{-x} \, dx = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} \int_0^\infty x^k L_n^\alpha \, x^{\alpha+1} e^{-x} \, dx \\
&= \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} \int_0^\infty x^{k+1} L_n^\alpha \, x^\alpha e^{-x} \, dx \\
&= \sum_{k=0}^{n-2} \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} \int_0^\infty x^{k+1} L_n^\alpha \, x^\alpha e^{-x} \, dx \\
&\quad + \frac{(-1)^{n-1}}{(n-1)!} \, (n+\alpha) \int_0^\infty x^n L_n^\alpha \, x^\alpha e^{-x} \, dx \\
&\quad + \frac{(-1)^n}{n!} \int_0^\infty x^{n+1} L_n^\alpha \, x^\alpha e^{-x} \, dx
\end{aligned}$$

$$
\begin{aligned}
&= \frac{(-1)^{n-1}}{(n-1)!}\,(n+\alpha)\,(-1)^n\,\Gamma(n+\alpha+1) \\
&\quad + \frac{(-1)^n}{n!}\,(-1)^n\,\frac{(n+1)\cdot\ldots\cdot 2}{n!}\,\Gamma(n+\alpha+2) \\
&= -\frac{n+\alpha}{(n-1)!}\,\Gamma(n+\alpha+1) + \frac{n+1}{n!}\,\Gamma(n+\alpha+2) \\
&= -\frac{n(n+\alpha)}{n!}\,\Gamma(n+\alpha+1) + \frac{(n+1)(n+\alpha+1)}{n!}\,\Gamma(n+\alpha+1) \\
&= \frac{(n+1)(n+\alpha+1) - n(n+\alpha)}{n!}\,\Gamma(n+\alpha+1) \\
&= \frac{n+\alpha+n+1}{n!}\,\Gamma(n+\alpha+1) = \frac{2n+\alpha+1}{n!}\,\Gamma(n+\alpha+1)\ .
\end{aligned}
$$

□

Theorem 12.9.31 (The Hypergeometric Series as a Function of its Parameters). By

$$F(a,b,c,z) := \sum_{n=0}^{\infty} \frac{(a)_n\,(b)_n}{(c)_n}\,\frac{z^n}{n!} = 1 + \frac{ab}{c}\,z + \frac{a\,(a+1)\,b\,(b+1)}{c\,(c+1)}\,\frac{z^2}{2!} + \cdots\ ,$$

for every $(a,b,c,z) \in \mathbb{C}^2 \times (\mathbb{C}\setminus(-\mathbb{N})) \times U_1(0)$, there is defined a continuous function $F : \mathbb{C}^2 \times (\mathbb{C}\setminus(-\mathbb{N})) \times U_1(0) \to \mathbb{C}$. The convergence of the series is uniform on compact subsets of $\mathbb{C}^2 \times (\mathbb{C}\setminus(-\mathbb{N})) \times U_1(0)$.

Proof. For the proof, we define for every $n \in \mathbb{N}$ the continuous function

$$h_n := \left(\mathbb{C}^2 \times (\mathbb{C}\setminus(-\mathbb{N})) \times U_1(0) \to \mathbb{C}, (a,b,c,z) \mapsto \frac{(a+n)\cdot(b+n)}{(c+n)\cdot(n+1)}\cdot z\right)$$

as well as the continuous function

$$h_\infty := \left(\mathbb{C}^2 \times (\mathbb{C}\setminus(-\mathbb{N})) \times U_1(0) \to \mathbb{C}, (a,b,c,z) \mapsto z\right)\ .$$

We claim that for every non-empty compact subset K of $\mathbb{C}^2 \times (\mathbb{C}\setminus(-\mathbb{N})) \times U_1(0)$, it follows that

$$\lim_{n\to\infty} \left\|(h_n - h_\infty)\big|_K\right\|_\infty = 0\ . \tag{12.68}$$

For the proof, let K be such a subset. For every $j \in \{1,2,3,4\}$, we denote by K_j be the projection of K onto the j-th coordinate. Since K_j is the image of a compact set under a continuous map, K_j is a compact subset of $\mathbb{C}$. Hence there is $C_j \in (0,\infty)$ such that $|u| \leqslant C_j$, for every $u \in K_j$. Further, since K_4 is a compact subset of $U_1(0)$, we can assume without loss of generality that $C_4 < 1$. Also, since K_3 is a compact subset of $\mathbb{C}\setminus(-\mathbb{N})$, there is $\delta > 0$ such that $|u+n| \geqslant \delta$ for all

$u \in K_3$ and $n \in \mathbb{N}$. Hence, we conclude for $n \in \mathbb{N}$ satisfying $n \geqslant 2C_3$ and every $u \in K_3$

$$\begin{aligned}\left|1+\frac{u}{n}\right| &= \frac{1}{n}\cdot|u+n| = \frac{1}{n}\,|n-(-u)| \geqslant \frac{1}{n}\cdot(n-|u|\,) = 1-\frac{|u|}{n} \\ &\geqslant 1-\frac{C_3}{n} \geqslant 1-\frac{1}{2} = \frac{1}{2}\ .\end{aligned}$$

Since for every $n \in \mathbb{N}^*$ and every $u \in K_3$,

$$\left|1+\frac{u}{n}\right| = \frac{1}{n}\cdot|u+n| \geqslant \frac{\delta}{n}\ ,$$

we conclude that

$$\left|1+\frac{u}{n}\right| \geqslant \delta' := \min\left\{\frac{1}{2},\frac{\delta}{2C_3}\right\}\ ,$$

for all $u \in K_3$ and $n \in \mathbb{N}^*$. Hence for $n \in \mathbb{N}^*$ and every $(a,b,c,z) \in K$, it follows that

$$\begin{aligned}&|h_n(a,b,c,z)-h_\infty(a,b,c,z)| = \left|\frac{\left(1+\frac{a}{n}\right)\cdot\left(1+\frac{b}{n}\right)}{\left(1+\frac{c}{n}\right)\cdot\left(1+\frac{1}{n}\right)}-1\right|\cdot|z| \\ &= \frac{1}{\left|1+\frac{c}{n}\right|\cdot\left(1+\frac{1}{n}\right)}\cdot\left|a+b-c-1+\frac{ab-c}{n}\right|\cdot\frac{|z|}{n} \\ &\leqslant \frac{C_4}{\delta'}\cdot(C_1+C_2+2C_3+1+C_1C_2)\cdot\frac{1}{n}\end{aligned}$$

and hence (12.68). Furthermore, from (12.68), it follows that

$$\lim_{n\to\infty}\left|\left\|h_n|_K\right\|_\infty - \left\|h_\infty|_K\right\|_\infty\right| = 0$$

and hence that

$$\lim_{n\to\infty}\left\|h_n|_K\right\|_\infty = \left\|h_\infty|_K\right\|_\infty\ \ (\leqslant C_4)\ .$$

Hence, there is $n_0 \in \mathbb{N}$ such that

$$\begin{aligned}\|\,h_n|_K\|_\infty &= \left|\,\|h_n|_K\|_\infty\right| \leqslant \left|\,\|h_n|_K\|_\infty - \|h_\infty|_K\|_\infty\right| + \|\,h_\infty|_K\|_\infty \\ &< \frac{1-C_4}{2}+C_4 = \frac{1+C_4}{2}\ \ (<1)\ ,\end{aligned}$$

for every $n \in \mathbb{N}$ such that $n \geqslant n_0$. As a consequence, for $n \in \mathbb{N}$ such that $n \geqslant n_0+2$, it follows that

$$\begin{aligned}\left\|\prod_{l=0}^{n-1} h_l|_K\right\|_\infty &\leqslant \left[\prod_{l=0}^{n_0}\|\,h_l|_K\|_\infty\right]\cdot\left[\prod_{l=n_0+1}^{n-1}\|\,h_l|_K\|_\infty\right] \\ &\leqslant \left[\prod_{l=0}^{n_0}\|\,h_l|_K\|_\infty\right]\cdot\left(\frac{1+C_4}{2}\right)^{n-(n_0+1)}\ .\end{aligned}$$

Thus, it follows for any finite subset M of $\mathbb{N}$ that

$$
\begin{aligned}
&\sum_{n \in M} \left\| \prod_{l=0}^{n-1} h_l\big|_K \right\|_\infty \\
&\leqslant \sum_{n=0}^{n_0+1} \left\| \prod_{l=1}^{n-1} h_l\big|_K \right\|_\infty + \left[\prod_{l=0}^{n_0} \| \, h_l\big|_K \|_\infty \right] \cdot \sum_{n=0}^{\infty} \left(\frac{1+C_4}{2} \right)^{n-(n_0+1)} \\
&= \sum_{n=0}^{n_0+1} \left\| \prod_{l=1}^{n-1} h_l\big|_K \right\|_\infty + \left[\prod_{l=0}^{n_0} \| \, h_l\big|_K \|_\infty \right] \left(\frac{1+C_4}{2} \right)^{-(n_0+1)} \cdot \frac{1}{1 - \frac{1+C_4}{2}} \\
&= \sum_{n=0}^{n_0+1} \left\| \prod_{l=1}^{n-1} h_l\big|_K \right\|_\infty + \frac{2}{1-C_4} \left(\frac{1+C_4}{2} \right)^{-(n_0+1)} \cdot \left[\prod_{l=0}^{n_0} \| \, h_l\big|_K \|_\infty \right]
\end{aligned}
$$

and hence that

$$
\left(\prod_{l=0}^{n-1} h_l\big|_K \right)_{n \in \mathbb{N}}
$$

is absolutely summable in $(C(K, \mathbb{C}), \| \, \|_\infty)$. Since the latter is true for every non-empty compact subset K of $\mathbb{C}^2 \times (\mathbb{C} \setminus (-\mathbb{N})) \times U_1(0)$, we conclude that F is continuous. □

Theorem 12.9.32 (The Confluent Hypergeometric Series as a Function of its Parameters). By

$$
M(a,b,z) := \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{z^n}{n!} = 1 + \frac{a}{b}\, z + \frac{a\,(a+1)}{b\,(b+1)} \frac{z^2}{2!} + \cdots \ ,
$$

for every $(a,b,z) \in \mathbb{C} \times (\mathbb{C} \setminus (-\mathbb{N})) \times \mathbb{C}$, there is defined a continuous function $M : \mathbb{C} \times (\mathbb{C} \setminus (-\mathbb{N})) \times \mathbb{C} \to \mathbb{C}$. The convergence of the series is uniform on compact subsets of $\mathbb{C} \times (\mathbb{C} \setminus (-\mathbb{N})) \times \mathbb{C}$.

Proof. For the proof, we define for every $n \in \mathbb{N}$ the continuous function

$$
h_n := \left(\mathbb{C} \times (\mathbb{C} \setminus (-\mathbb{N})) \times \mathbb{C} \to \mathbb{C}, (a,b,z) \mapsto \frac{(a+n)}{(b+n) \cdot (n+1)} \cdot z \right) .
$$

We claim that for every non-empty compact subset K of $\mathbb{C} \times (\mathbb{C} \setminus (-\mathbb{N})) \times \mathbb{C}$, it follows that

$$
\lim_{n \to \infty} \| \, h_n\big|_K \|_\infty = 0 \ . \tag{12.69}
$$

For the proof, let K be such a subset. For every $j \in \{1,2,3\}$, we denote by K_j be the projection of K onto the j-th coordinate. Since K_j is the image of a compact set under a continuous map, K_j is a compact subset of $\mathbb{C}$. Hence there is $C_j \in (0, \infty)$ such that $|u| \leqslant C_j$, for every $u \in K_j$. Further, since K_2 is a compact subset of

$\mathbb{C}\backslash(-\mathbb{N})$, there is $\delta > 0$ such that $|u+n| \geqslant \delta$ for all $u \in K_2$ and $n \in \mathbb{N}$. Hence, we conclude for $n \in \mathbb{N}$ satisfying $n \geqslant 2C_2$ and every $u \in K_2$

$$\begin{aligned} \left|1 + \frac{u}{n}\right| &= \frac{1}{n} \cdot |u+n| = \frac{1}{n}\,|n-(-u)| \geqslant \frac{1}{n} \cdot (n - |u|\,) = 1 - \frac{|u|}{n} \\ &\geqslant 1 - \frac{C_2}{n} \geqslant 1 - \frac{1}{2} = \frac{1}{2} \ . \end{aligned}$$

Since for every $n \in \mathbb{N}^*$ and every $u \in K_2$,

$$\left|1 + \frac{u}{n}\right| = \frac{1}{n} \cdot |u+n| \geqslant \frac{\delta}{n} \ ,$$

we conclude that

$$\left|1 + \frac{u}{n}\right| \geqslant \delta' := \min\left\{\frac{1}{2}, \frac{\delta}{2C_2}\right\} \ ,$$

for all $u \in K_2$ and $n \in \mathbb{N}^*$. Hence for $n \in \mathbb{N}^*$ and every $(a,b,z) \in K$, it follows that

$$\begin{aligned} |\,h_n(a,b,z)| &= \left|\frac{1+\frac{a}{n}}{\left(1+\frac{b}{n}\right) \cdot \left(1+\frac{1}{n}\right)}\right| \cdot |z| = \frac{1}{\left|1+\frac{b}{n}\right| \cdot \left(1+\frac{1}{n}\right)} \cdot \left|1 + \frac{a}{n}\right| \cdot \frac{|z|}{n} \\ &\leqslant \frac{C_3}{\delta'} \cdot (1 + C_1) \cdot \frac{1}{n} \end{aligned}$$

and hence (12.69). As a consequence, for $\varepsilon \in (0,1)$, there is $n_0 \in \mathbb{N}$ such that

$$\|\,h_n|_K\|_\infty < 1 - \varepsilon \ ,$$

for every $n \in \mathbb{N}$ such that $n \geqslant n_0$, and for $n \in \mathbb{N}$ such that $n \geqslant n_0 + 2$, it follows that

$$\begin{aligned} \left\|\prod_{l=0}^{n-1} h_l|_K\right\|_\infty &\leqslant \left[\prod_{l=0}^{n_0} \|\,h_l|_K\|_\infty\right] \cdot \left[\prod_{l=n_0+1}^{n-1} \|\,h_l|_K\|_\infty\right] \\ &\leqslant \left[\prod_{l=0}^{n_0} \|\,h_l|_K\|_\infty\right] \cdot (1-\varepsilon)^{n-(n_0+1)} \ . \end{aligned}$$

Thus, it follows for any finite subset S of $\mathbb{N}$ that

$$\begin{aligned} &\sum_{n \in S} \left\|\prod_{l=0}^{n-1} h_l|_K\right\|_\infty \\ &\leqslant \sum_{n=0}^{n_0+1} \left\|\prod_{l=1}^{n-1} h_l|_K\right\|_\infty + \left[\prod_{l=0}^{n_0} \|\,h_l|_K\|_\infty\right] \cdot \sum_{n=0}^{\infty} (1-\varepsilon)^{n-(n_0+1)} \\ &= \sum_{n=0}^{n_0+1} \left\|\prod_{l=1}^{n-1} h_l|_K\right\|_\infty + \left[\prod_{l=0}^{n_0} \|\,h_l|_K\|_\infty\right] (1-\varepsilon)^{-(n_0+1)} \cdot \frac{1}{1-(1-\varepsilon)} \end{aligned}$$

$$= \sum_{n=0}^{n_0+1} \left\| \prod_{l=1}^{n-1} h_l\big|_K \right\|_\infty + \frac{1}{\varepsilon}\,(1-\varepsilon)^{-(n_0+1)} \cdot \left[\prod_{l=0}^{n_0} \| \, h_l\big|_K \|_\infty \right]$$

and hence that

$$\left(\prod_{l=0}^{n-1} h_l\big|_K \right)_{n \in \mathbb{N}}$$

is absolutely summable in $(C(K,\mathbb{C}), \| \, \|_\infty)$. Since the latter is true for every non-empty compact subset K of $\mathbb{C} \times (\mathbb{C} \backslash (-\mathbb{N})) \times \mathbb{C}$, we conclude that M is continuous. $\square$

Bibliography

[1] Abramowitz M and Stegun I A (ed), 1984, *Pocketbook of Mathematical Functions*, Thun: Harri Deutsch. 115, 117

[2] Adams R A, Fournier J J F 2003, *Sobolev spaces*, 2nd ed., Academic Press: New York.

[3] Baez J C, Segal I E, Zhou Z 1992, *Introduction to algebraic and constructive quantum field theory*, Princeton University Press: Princeton.

[4] Beals R, Wong R 2016, *Special functions and orthogonal polynomials*, Cambridge University Press: Cambridge.

[5] Belleni-Morante A, McBride A C 1998, *Applied nonlinear semigroups: An introduction*, Wiley: New York. 97

[6] R. Bellman 1949, *A survey of the theory of the boundedness, stability, and asymptotic behaviour of solutions of linear and nonlinear differential and difference equations*, NAVEXOS P-596, Office of Naval Research: Washington, DC. 73

[7] Beyer H R 2007, *Beyond partial differential equations: On linear and quasi-linear abstract hyperbolic evolution equations*, Lecture Notes in Mathematics 1898, Springer: Berlin. 97, 99, 102, 105

[8] Brezis H 1983, *Analyse fonctionnelle: Théorie et applications*, Collection Mathématiques Appliquées pour la Maîtrise, Masson: Paris.

[9] Chernoff P R 1968, *Note on product formulas for operator semigroups*, Journal of Functional Analysis, Vol. **2**, 238-242.

[10] Chihara T S 1978, *An introduction to orthogonal polynomials*, Gordon and Breach: New York.

[11] Dixmier J, 1977, $\mathbb{C}^*$-*Algebras*, North-Holland: Amsterdam.

[12] Dunford N, Schwartz J T 1957, *Linear operators, Part I: General theory*, Wiley: New York.

[13] Dunford N, Schwartz J T 1963, *Linear operators, Part II: Spectral theory: Self adjoint operators in Hilbert space theory*, Wiley: New York.

[14] Dunkel O 1912-1913, *Regular singular points of a system of homogeneous linear differential equations of the first order*, Am. Acad. Arts Sci. Proc. **38**, 341–370. 73

[15] Engel K-J, Nagel R 2000, *One-parameter semigroups for linear evolution equations*, Springer: New York. 97

[16] Erdelyi A (ed.) 1981, *Higher Transcendental Functions Volume II*, Robert Krieger: Florida.

[17] Goldberg S 1985, *Unbounded linear operators* Dover: New York.

[18] Goldstein J A 1985, *Semigroups of linear operators and applications*, Oxford University Press: New York. 97

[19] Goldstein J A 1972, *Lectures on semigroups of nonlinear operators*, Tulane University: New Orleans. 97

[20] Hille E 1969, *Lectures on ordinary differential equations*, Addison-Wesley: Reading. 73

[21] Hirzebruch F, Scharlau W 1971, *Einführung in die Funktionalanalysis*, BI: Mannheim.

[22] Hutson V, Pym J S, Cloud, M J 2005, *Applications of functional analysis and operator theory*, 2nd ed., Elsevier : Amsterdam.

[23] Joergens K, Rellich F 1976, *Eigenwerttheorie gewoehnlicher Differentialgleichungen*, Springer: Berlin Heidelberg.

[24] Kato T 1966, *Perturbation theory for linear operators*, Springer: New York.

[25] Lang S 1996, *Real and functional analysis*, 3rd ed., Springer: New York.

[26] Lebedev N N 1965, *Special functions and their applications*, Prentice-Hall: Englewood Cliffs.

[27] Levinson N 1948, *The asymptotic nature of the solutions of linear systems of differential equations*, Duke Math. J. **15**, 111–126. 73

[28] Miyadera I 1992, *Nonlinear semigroups*, AMS: Providence. 97

[29] Von Neumann J 1930, *Allgemeine Eigenwerttheorie Hemitescher Funktionaloperatoren*, Mathematische Annalen, Vol. **102**, 49–131.

[30] Von Neumann J 1932, *Mathematische Grundlagen der Quantenmechanik*, Springer: Berlin.

[31] Olver F W J, Lozier D W, Boisvert R F, and Clark C W (eds), 2010 *NIST Handbook of Mathematical Functions*, Cambridge University Press: New York.

[32] Olver F W J, Olde Daalhuis A B, Lozier D W, Schneider B I, Boisvert R F, Clark C W, Miller B R, Saunders B V, Cohl H S, and McClain M A, eds., 2022, *NIST Digital Library of Mathematical Functions*, http://dlmf.nist.gov/, Release 1.1.6 of 2022-06-30.

[33] Pazy A 1983, *Semigroups of linear operators and applications to partial differential equations*, Springer: New York. 97

[34] Reed M and Simon B, 1980, 1975, 1979, 1978, *Methods of modern mathematical physics*, Volume I, II, III, IV, Academic: New York. 1, 11

[35] Renardy M and Rogers R C 1993, *An introduction to partial differential equations*, Springer: New York.

[36] Riesz F and Sz-Nagy B 1955, *Functional analysis*, Unger: New York. 1

[37] Rudin W 1991, *Functional analysis*, 2nd ed., MacGraw-Hill: New York. 1

[38] Schäfke W 1963, *Einführung in die Theorie der speziellen Funktionen der mathematischen Physik*, Springer: Berlin.

[39] Schechter M 2003, *Operator methods in quantum mechanics*, Dover Publication: New York.

[40] Simon B 2015, *A Comprehensive Course in Analysis Part 4: Operator Theory*, AMS: Providence.

[41] Stein E M, Shakarchi R 2003, *Fourier analysis: An introduction*, Princeton University Press: Princeton and Oxford.

[42] Szegö G 1939, *Orthogonal polynomials*, AMS: Providence.

[43] Weidmann J 1980, *Linear Operators in Hilbert spaces*, Springer: New York. 1

[44] Weidmann J 2000, *Lineare Operatoren in Hilberträumen: Teil I: Grundlagen*, Teubner: Stuttgart.

[45] Weidmann J 2003, *Lineare Operatoren in Hilberträumen: Teil II: Anwendungen*, Teubner: Stuttgart.

[46] Yosida K 1968, *Functional analysis*, 2nd ed., Springer: Berlin. 1

[47] Ziemer W P 1989, *Weakly differentiable functions*, Springer: New York.

Index of Symbols

Index