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**On the rigged Hilbert space formalism of quantum mechanics**

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# **On the rigged Hilbert space formalism of quantum mechanics**

Memory carried out at the department of Mathematics  
Faculty of Sciences  
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aspiring to attain the title of Doctor in Mathematical Sciences.

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To my beloved Mother.

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# Abstract

Generalized eigenvectors are key tools in the theory of rigged Hilbert spaces. Let  $\mathcal{H}$  be a Hilbert space and let  $\Phi$  be a dense subspace of  $\mathcal{H}$ . Let  $A$  be a densely defined linear operator in  $\mathcal{H}$  such that  $\Phi \subset D(A)$  and  $A\Phi \subset \Phi$ . The generalized eigenvectors of  $A$  are the eigenvectors of the algebraic dual of  $\cdot : \Phi \rightarrow \Phi$ . In the case where  $\Phi$  is endowed with a topology  $\tau$  finer than the norm topology inherited from  $\mathcal{H}$ , generalized eigenvectors that are  $\tau$ -continuous may be of great interest. We discuss conditions which ensure the existence of representations associated to generalized eigenvectors of  $A$ . As an application, we review and refine Böhm's study of the algebra of the quantum harmonic oscillator. We also discuss canonical rigged Hilbert space constructions. We focus on cyclic self adjoint operators and use the one-dimensional free Hamiltonian on the half line as a model. We propose a nonstandard construction that can be generalized to many quantum systems. Our construction is motivated by the Stone-von Neumann uniqueness theorem.

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<sup>0</sup>**Key Words.** ; Rigged Hilbert space; nuclearity; representation; cyclic self-adjoint operators; Stone von Neumann theorem.

# Résumé

Les vecteurs propres généralisés sont des outils clés dans la théorie des triplets de Gelfand. Soit  $\mathcal{H}$  un espace de Hilbert et soit  $\Phi$  un sous-espace dense de  $\mathcal{H}$ . Soit  $A : D(A) \rightarrow \mathcal{H}$  un opérateur linéaire non borné à domaine dense défini dans  $\mathcal{H}$  tel que  $\Phi \subset D(A)$  et  $A\Phi \subset \Phi$ . Les vecteurs propres généralisés de  $A$  sont les vecteurs propres du dual algébrique de  $A : \Phi \rightarrow \Phi$ . Dans le cas où  $\Phi$  est muni d'une topologie  $\tau$  plus fine que la topologie induite par celle de  $\mathcal{H}$ , les vecteurs propres généralisés qui sont  $\tau$ -continus peuvent être d'un grand intérêt. Nous discutons des conditions qui garantissent l'existence de représentations associées aux vecteurs propres généralisés de  $A$ . À titre d'application, nous passons en revue et affinons l'étude de Böhm sur l'algèbre de l'oscillateur harmonique quantique. Nous discutons également des constructions canoniques de triplets de Gelfand. Nous nous concentrons sur les opérateurs cycliques auto-adjoints et utilisons l'Hamiltonien libre unidimensionnel sur la demi-droite comme modèle. Nous proposons une construction non standard qui peut être généralisée à de nombreux systèmes quantiques. Notre construction est motivée par le théorème d'unicité de Stone-von Neumann.

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<sup>0</sup>Mots clés ; Triplet de Gelfand; nuclearité; representation; opérateurs autoadjoint cycliques; Théorème de Stone-von Neumann

# Résumé étendu

Dans cette thèse, nous abordons des problèmes liés aux triplets de Gelfand en mécanique quantique non relativiste, en nous concentrant sur le cas simple du mouvement unidimensionnel d'une particule sans spin sous l'influence de quelques potentiels d'énergie basiques. Ces modèles servent de modèles simplifiés et fondamentaux pour comprendre le comportement des systèmes quantiques généraux. Nous mettons l'accent sur l'utilisation des vecteurs propres généralisés algébriques et tentons d'explorer les conditions garantissant l'existence de représentations associées à ces vecteurs propres généralisés pour un observable. Nous établissons rigoureusement la signification des bases orthonormales utilisées par les physiciens ainsi que les formules de changement de base de Dirac, qui, avec une légère modification, acquièrent une signification rigoureuse sans recourir aux fonctions généralisées. Nous traitons les opérateurs fondamentaux sur un pied d'égalité en utilisant les vecteurs propres généralisés, et nous explorons leurs propriétés de type cohérent. Trois exemples physiques clés - la particule libre, l'oscillateur harmonique quantique et le potentiel de barrière carrée - sont étudiés de manière rigoureuse. Ces exemples sont considérés comme des pierres angulaires de la mécanique quantique et de la théorie quantique des champs. Nous utilisons un langage aussi élémentaire que possible. En particulier, nous identifions clairement les questions mathématiques ouvertes. Nous nous concentrons sur les opérateurs auto-adjoints cycliques et utilisons l'hamiltonien libre comme modèle, pour lequel nous passons en revue une diagonalisation en utilisant des vecteurs propres généralisés algébriques d'une restriction spécifique. Pour plus de commodité, nous rappelons également la construction théorique d'une famille complète de vecteurs propres généralisés d'opérateurs auto-adjoints cycliques qui sont continus sur le triplet de Gelfand considéré. Enfin, nous discutons des constructions canoniques des espaces de triplet de Gelfand et proposons une construction non-standard qui peut être généralisée à de nombreux systèmes quantiques.

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<sup>0</sup>**Mots clés** ; Triplet de Gelfand; nuclearité; representation; opérateurs autoadjoint cycliques; Théorème de Stone-von Neumann

# Contents

Abstract	IV
Resumé	V
Resumé	VI
Introduction	1
<b>1 Three basic physical examples and the mathematical formalism of quantum mechanics</b>	<b>4</b>
1.1 A brief survey of basic one-dimensional Newtonian mechanics	4
1.2 The free particle	5
1.3 The harmonic oscillator	6
1.4 The square barrier potential	7
1.5 On Dirac braket formalism	8
1.6 The Hilbert space formalism of quantum mechanics	11
1.7 Introduction to the rigged Hilbert space formalism	13
<b>2 Mathematical tools of the formalism</b>	<b>15</b>
2.1 Preliminaries on some basic function spaces	15
2.2 The completion of a metric space	16
2.3 Unbounded operators in Hilbert space	18
2.3.1 Closed operators	18
2.3.2 Symmetry and self-adjointness	19
2.3.3 The spectrum	20
2.3.4 The projection-valued measure spectral theorem	21
2.3.5 Orthogonal decompositons	22
2.3.6 Cyclic vectors and spectral bases	23
2.3.7 The direct integral spectral theorem	26
2.3.8 The Stone-von Neumann uniqueness theorem	27
2.4 Basics on Sturm-Liouville differential equations	28
2.4.1 Basic existence and uniqueness results	28
2.4.2 The resolvent as an integral operator	30
2.5 The rigged Hilbert space structure	31
2.5.1 On locally convex topological vector spaces	31
2.5.2 The rigged Hilbert space structure	32
2.6 Generalized eigenvectors and the nuclear spectral theorem	33
2.7 On the one-dimensional moment problem	34
2.7.1 Statement of the problem and the basic criteria	34
2.7.2 Orthogonal polynomials and three-terms recurrence relations	35
2.7.3 Self-adjoint operators and the Hamburger moments problem	36
2.8 On Hermite and Laguerre polynomials	36
2.8.1 Hermite polynomials	36
2.8.2 Laguerre polynomials	38

<b>3</b>	<b>Generalized eigenvectors and the associated representations</b>	<b>39</b>
3.1	Some algebraic preliminaries . . . . .	39
3.2	Generalized eigenvectors and associated representations . . . . .	40
3.2.1	Completeness . . . . .	40
3.2.2	Coherence-like conditions . . . . .	40
3.2.3	Construction of the representation . . . . .	41
3.2.4	Change of bases formulas . . . . .	42
3.2.5	The spectral theorem and generalized eigenvectors . . . . .	43
3.3	True vectors for a self-adjoint operator . . . . .	44
<b>4</b>	<b>Case studies</b>	<b>46</b>
4.1	The algebra of the Harmonic oscillator . . . . .	46
4.2	Eigenstates of the Hamiltonian in function spaces . . . . .	49
4.3	Diagonalizing The free Hamiltonian by using algebraic generalized eigenvectors . . . . .	53
4.3.1	The Hilbert spaces $\mathcal{H}_a, \mathcal{H}_s, \mathcal{H}_b$ and $\iota : \mathcal{H}_b \rightarrow \mathcal{H}_s$ . . . . .	53
4.3.2	A basis of generalized eigenvectors of $P_a^2  _{\Psi_a}$ . . . . .	54
4.3.3	Generalized Laguerre polynomials and the measures $\sigma_1, \sigma_2$ . . . . .	55
4.3.4	Diagonalizing $P_s^2$ and $P_b^2$ . . . . .	56
4.4	A RHS construction based on the extension $\iota : \mathcal{H}_b \rightarrow \mathcal{H}_s$ . . . . .	56
4.4.1	The construction . . . . .	56
4.4.2	Continuity and strong continuity of generalized eigenvectors . . . . .	57
4.4.3	Diagonalizing via the regular solution: . . . . .	58
4.4.4	Calculations from $\Phi_b$ to $\Phi_s$ . . . . .	59
4.5	A similar RHS construction for the square barrier potential . . . . .	59
4.6	Algebraic manipulations . . . . .	60
4.6.1	The free Hamiltonian and the position observable in $\mathcal{H}_b$ . . . . .	60
4.6.2	The SBP and the free Hamiltonian in $\mathcal{H}_b$ . . . . .	61

# Introduction

Quantum Mechanics (QM) as we know it now was born in a period of a few years, roughly between 1924 and 1927, invented by Heisenberg and Schrödinger, with important contributions by Born, Pauli, Dirac and many others. Immediately after this, the mathematical foundations were laid by von Neumann. It has been roughly one hundred years since physicists began to realize that classical mechanics is fundamentally wrong at the atomic scale and hence cannot form a correct description of nature. A breakthrough was the paper of Heisenberg on the so-called matrix mechanics (1925). In 1926, Schrödinger proposed a wave equation for a quantum particle in a potential energy field, which also led to a successful description of atoms and other microscopic systems. In the two years following Heisenberg's *matrix mechanics* paper, the combined efforts of Born, Jordan, Schrödinger and Dirac led to a refinement of classical mechanics called QM. Next, in the late 1920's, Dirac proposed a new mathematical model of QM based on a remarkably elegant abstract algebra of linear operators defined on an infinite dimensional complex vector space equipped with an inner product which is proven to be of a significant heuristic value in the subsequent years, especially in dealing with Hamiltonians having a continuous spectrum. However, there were serious difficulties in finding a mathematical image making a precise sense of these linear algebra-type manipulations such as treating operators with continuous spectra as if they had actual eigenvectors, integral expansion formulas over those eigenvectors and so on.

Greatly inspired by Dirac transformation theory, in his book [1], von-Neumann proposed the first rigorous mathematical formulation of QM. It consisted in the use of the language of Hilbert Space (HS) with states being represented by unit vectors and observables (for instance the Hamiltonian of the system) by unbounded self-adjoint operators. More precisely, the basic properties of quantum mechanics can be expressed by a set of mathematical statements, *axioms*, together with their consequences. This is the so-called Hilbert Space (or, the standard) Formalism (HSF) of QM. Although some attempts to implement Dirac model within the HSF, serious mathematical difficulties were faced, especially in giving a sense to some singular objects such as Dirac delta function or to justify some expansions over *continuous* bases in Dirac model. Indeed, when the spectrum of an operator has a continuous component, the expansion formulas used in Dirac formalism are no longer valid since there are no vectors in the Hilbert space that are eigenvectors corresponding to points in the continuous component of the spectrum.

In 1939, Dirac published a paper [2] in which he introduced notations called *bras* and *kets*. These are special notations for linear algebra-type manipulations, vectors and operators in his mathematical model of QM. This is the so-called bra-ket formalism. For most physicists, the latter is considered to be simpler and more intuitive. It is consequently the one that is still used in standard textbooks. It is recalled that this formalism has been used with great success for quite some time by physicists and shown to be highly accurate in many practical applications. It is also worth to mention that Dirac was fully aware that his delta function for example is not a well-defined mathematical object. However, he was convinced that, as long as one follows the rules used in its definition, i.e. using it only under the integral sign and not asking for single point evaluations, no inconsistencies will arise. Moreover, the delta function can be replaced with well-defined mathematical expressions. However, according to Dirac, the drawback is that the latter substitution will lead to a more cumbersome expressions that will obscure the argument and thus a decrease of the understanding [3].

The HSF, with the spectral theorem for self-adjoint operators as a cornerstone, was fully appreciated by mathematicians. However, physicists considered it as difficult and not practical [4, 5, 6] and found the non-rigorous Dirac bra-ket formalism much more formally powerful for practical manipulations. This led to think that the Hilbert space framework for the spectral analysis might lack the flexibility making it possible to give a precise meaning to some singular objects (but of practical importance) such as Dirac bras and kets, delta function or Dirac basis vector expansions. These are essential key tools for physicists, especially when dealing with a continuous spec-

trum. There were several attempts to provide a rigorous mathematical justification of using state vectors that do not belong to the Hilbert space [7]. The most widely known among these approaches (and also the one that has led to the largest number of applications in QM) is the so-called rigged Hilbert space (RHS) structure. The general idea was to go beyond Hilbert space and provide an extension space  $\Phi^\times$  of the Hilbert space  $\mathcal{H}$  which should contain generalized eigenvectors associated to the points of the continuous spectrum of a self-adjoint operator  $A$  and thus replace the Hilbert space structure by a triplet  $\Phi \subset \mathcal{H} \subset \Phi^\times$  where  $\Phi$  is a dense subspace equipped with a topology  $\tau$  finer than the one induced by the Hilbert space structure and where  $\Phi^\times$  denotes its topological antidual linear space (i.e., the space of continuous anti-linear functionals on  $\Phi$ ). The RHS theory was developed in the 1950's, mainly by Gelfand, Kostutchenko, Vilenkin, Shilov and Maurin [8, 9, 10]. Starting with the RHS structure, together with von-Neumann's direct integral decomposition, they were able to prove the so-called nuclear spectral theorem, which provides more informations on the spectral properties of an observable forming an attempt to treat the discrete and the continuous spectrum on the same footing. Somewhat later, the use of the RHS for a rigorous mathematical formulation of Dirac's formalism was suggested and investigated by several authors in many papers. Among them we mention the work of Foias [11], Roberts [12, 13], Böhm [14] and Antoine [15]. In particular, the nuclear spectral theorem allows to justify some formulas that physicists use on expansions over bras and kets. For more details on the rigged Hilbert space formalism see for instance [7, 16, 17, 14, 18, 19, 20] and references therein. The basic tools of the theory are generalized eigenvectors of  $A$  that leave  $\Phi$  invariant : eigenvectors of the dual operator  $A^\times : \Phi^\times \rightarrow \Phi^\times$ . We refer the reader to [21, 22] for conditions that ensure tight rigging of the operator  $A$ , where the spectrum of the operator  $A$  coincides with an adequate set built from generalized eigenvalues of  $A$ . For the study of other constructions that generalize the RHS, see, e.g., [7, 23, 24]. Finally, let us mention the work of Bergeron [25], where another explanation of Dirac's formalism is proposed.

The RHS approach requires more mathematical hypotheses. It has the reputation of being much more delicate to rigorously handle, than the von-Neumann Hilbert space formulation. At this point, one might contend that physicists are not interested in that rigorous reformulation of something already evident for them. However, let us mention that Dirac's classic monograph, being advocated in the majority of modern treatises of QM, contains a fair amount of statements which are bare ambiguous or incorrect from the mathematical point of view. Or, in the formulation of a physical theory, a present lack of mathematical rigor can often and readily lead to apparent contradictions and forms a potential source of many surprises that is harder, if not impossible, to clarify all the inconsistencies within it [26]. These contradictions can only be discarded by making appeal to a more careful mathematical formulation of the problems under investigation, which will eventually allow to handle them in a more efficient manner. We believe that this should convey the idea that the use of the RHSF rather than just the HSF for the description of a quantum system will not only justify the mathematical undefined operations physicists have been accustomed to in their calculations, but also provide powerful means to solve certain mathematical problems of QM and thus lead to new results and deeper understanding of the behavior of the quantum system under study.

In this thesis, we discuss some problems related to the RHSF of non-relativistic QM, where we restrict our attention to the simple case of a one-dimensional motion of a non-relativistic spinless particle under the influence of some basic energy potentials. These serve as simplified and fundamental models for understanding the behavior of general quantum systems and grasping the fundamental principles before moving to higher dimensions. We focus on the role of using the language of algebraic generalized eigenvectors and try to investigate conditions which ensure the existence of representations associated to generalized eigenvectors of an observable (or, more generally, a fundamental operator in the case of the Quantum Harmonic Oscillator (QHO)) and provide the exact connection between generalized eigenvectors and the Hamiltonian eigenstates in different representations with a discussion of the important concept of change of representation. We define rigorously the meaning of orthonormal bases used by physicists and Dirac change of bases formulas, which, modulo a slight change, have a rigorous meaning without the use of generalized functions. We get that Dirac notations correspond to change of bases formulas. We treat fundamental operators on the same footing using generalized eigenvectors (for which we also discuss some coherent-like properties in the sense of Klauder-Skagerstam [27]) of suitable duals and use that to rigorously study three basic and generic physical examples : the free particle, the QHO and the square barrier potential. These are considered by physicists as cornerstones of QM and quantum field theory [4, 5, 6]. We also use an elementary language as much as possible. In particular, the open mathematical questions are clearly stated. We focus on

cyclic self-adjoint operators and use the free Hamiltonian as a model for which we review a diagonalization by using algebraic generalized eigenvectors of a specific restriction. For convenience, we also recall the theoretical construction of a complete family of generalized eigenvectors of cyclic self-adjoint operators that are continuous on the RHS. Finally, we discuss canonical rigged Hilbert space constructions and propose a non-standard construction that can be generalized to many quantum systems.

Next, we outline the content of the thesis :

- Chapter 1 : we briefly review some points in the most basic formulation of one-dimensional Newtonian mechanics and we present a brief study (as presented in standard textbooks, i.e., by solving the time-independent Schrödinger equation) of the three basic systems we worked on along this thesis, which form simple and illustrative examples that are used in many theoretical studies. Next, for convenience, we provide a short recap of some essential aspects of Dirac bra-ket formalism and state some of the most important axioms in von-Neumann HS formalism. We finish by some remarks and motivations towards the RHSF.
- Chapter 2 : we start with some mathematical preliminaries used in the HSF and the RHSF of QM such as spectral theory of unbounded self-adjoint operators in HS, locally convex topological vector spaces, the RHS structure and the nuclear spectral theorem. Next we review some of the material we will need on second-order Sturm-Liouville differential equations. We then finish by a section on some basics on orthogonal polynomials and the one-dimensional moment theory.
- Chapter 3 : we review the nuclear spectral theorem and we examine more closely the role of generalized eigenvectors (for which we also discuss some coherent-like conditions) of a fundamental operator and the exact link with the associated representations together with a discussion of the problems of change of representation and the change of basis formulas.
- Chapter 4 : a first part of this chapter is devoted to apply the material developed in chapter 3 to the three case studies we considered : the free particle, the QHO and the square barrier potential. We examine in it more closely the use of generalized eigenvectors and the construction of suitable representations. Moreover, we review the algebraic diagonalization of some suitable operators using the key tool of generalized eigenvectors of some suitable restrictions. Next we discuss some canonical RHS constructions for a self-adjoint restriction of the Hamiltonian by taking into consideration the fact that the initially considered Hilbert space may not be the best representation for the physical system and by adopting the point of view that the construction must be built and centered around a family of basic states of the system. We focus on cyclic self-adjoint operators and use the one-dimensional free Hamiltonian on the half-line as a model. Next, based on some suitable extension maps, we propose a non-standard construction that can be generalized to many quantum systems. To conduct our study, we first examine the one-dimensional free Hamiltonian and next treat in detail an analogue construction for the square barrier potential.

## THREE BASIC PHYSICAL EXAMPLES AND THE MATHEMATICAL FORMALISM OF QUANTUM MECHANICS

### 1.1 A brief survey of basic one-dimensional Newtonian mechanics

In Newtonian mechanics, a system refers to a finite collection of particles that are of interest for analysis (we say that Newtonian mechanics is a particle mechanics). Studying a given system means to identify and analyze the forces acting on each object within it and then apply Newton's second law to write equations of motion for each object within the system. These equations describe how the motion of the objects changes in response to the applied forces. The solutions determine the positions, velocities, and accelerations of the objects as functions of time. This allows to compute the value of any given observable at any given subsequent time and to make predictions about the future behavior of the system.

Suppose that a particle of mass  $m$  is moving in a straight line under the action of a conservative force  $F$ . The position of the particle is a function of time  $x(t) \in \mathbb{R}$ . The velocity is  $v(t) = \dot{x}(t)$ , and the speed  $v(t)$  of the particle is equal to the magnitude of its velocity. The acceleration is  $a = \ddot{x}(t)$ . We often write  $x, a, \dots$  instead of  $x(t), a(t), \dots$ . Newton's second law states that  $F = m\ddot{x}$ . Frequently the force  $F$  depends only on the position and can be expressed in the form  $F(x) = -V'(x)$ , where  $V$  is the potential energy and  $V'$  is its derivative with respect to the position  $x$ . So that the equation of motion takes the form  $m\ddot{x} = -V'(x)$ . i.e.  $\dot{p} = -V'(x)$  where  $p = mv$  is the momentum of the particle.

In its most basic form, Newtonian mechanics is formulated as follows :

The set  $\Gamma \subset \mathbb{R}$  of all possible pairs  $(x, p)$  is called the phase space and observables such as position, momentum or total energy are represented by smooth real-valued functions  $f : \Gamma \rightarrow \mathbb{R}$ .

The total energy observable, also called the Hamiltonian of the system, is often of the form

$$H = \frac{p^2}{2m} + V(x)$$

Where the first term refers to the kinetic energy and the second to the potential energy.

The (often implicate) time-dependence of a given observable  $f$  is expressed by

$$\frac{df}{dt} = \{f, H\}$$

where  $\{.,.\}$  is the so-called Poisson bracket, defined for any given smooth functions  $f_1(x, p), f_2(x, p)$  on  $\mathbb{R}^2$ , by

$$\{f_1, f_2\} = \frac{\partial f_1}{\partial x} \frac{\partial f_2}{\partial p} - \frac{\partial f_1}{\partial p} \frac{\partial f_2}{\partial x}$$

In particular, taking  $f = H$ , we see that  $\frac{dH}{dt} = 0$ , so that the total energy is conserved.

## 1.2 The free particle

The one-dimensional free particle is the simplest quantum mechanical system which allows to introduce and study the basic principles of quantum mechanics with neither the complexities of external forces or potential energy barriers nor internal degrees of freedom. It provides a foundational starting point for learning quantum mechanics and forms the simplest quantum system for which one can solve analytically the associated time-dependent Schrödinger equation. Also, understanding the behavior of a free particle is crucial for analyzing further the formalism of quantum mechanics.

The newtonian analysis of a free particle moving along a straight line parametrized by  $x \in \mathbb{R}$  is straightforward. Let  $x_0$  and  $v_0$  be respectively the initial position and velocity. Applying Newton's second law, we see that for a subsequent time  $t$  we have  $x(t) = v_0 t + x_0$ .

In most physics textbooks, the quantum mechanical analysis starts with the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = i\hbar \frac{\partial \psi}{\partial t}.$$

A separation of variables  $\psi(x, t) = \varphi(x)f(t)$  yields that  $\psi$  is a solution if and only if there is a constant  $E$  such that  $f(t) = e^{-i\frac{Et}{\hbar}}$  and  $\varphi$  is a solution of the so-called time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \varphi}{dx^2} = E\varphi.$$

Using a system of units for which  $\hbar = 1$  and  $m = 1/2$ , we have  $f(t) = e^{-iEt}$  and the above equation takes the form

$$\varphi'' + E\varphi = 0. \quad (\star)$$

We see that for each  $E \in [0, \infty)$  the space of solutions of  $(\star)$  is two-dimensional and for which a basis is given by the two linearly independent eigenfunctions

$$\varphi_E^\pm(x) = e^{\pm i\sqrt{E}x}, \quad \text{if } E \neq 0,$$

and

$$\varphi_0^- : x \mapsto 1, \quad \varphi_0^+ : x \mapsto x, \quad \text{if } E = 0.$$

So that each energy level  $E > 0$  is doubly degenerate, with the two solutions  $\varphi_E^\pm$  representing respectively particles travelling to the right and to the left. It is easy to see that the two eigenfunctions are also eigenfunctions of the momentum operators and therefore correspond to states with momentum  $\pm\sqrt{E}$ .

For  $E < 0$ , the solutions of  $(\star)$  are not bounded on the whole real axis and hence do not represent physical states (a wave function is, in particular, supposed to be a bounded function [4, 28]). Remark that this is also the case for  $\varphi_0^+$ .

For the values  $E \in [0, \infty)$ , we can rewrite the associated bounded eigenfunctions above in the following form  $(\varphi_k(x) = e^{ikx})_{k \in \mathbb{R}}$ . So that, for each  $k \in \mathbb{R}$ , the function  $\varphi_k$  is an eigenfunction with energy  $E = k^2$ .

For all  $k \in \mathbb{R}$ , by using the eigenfunction  $\varphi_k$ , define the stationary state  $\psi_k(x, t) := e^{-ik^2 t} \varphi_k(x)$ . These are non-normalizable (i.e., not belonging to the space  $L^2(\mathbb{R}, dx)$ ) energy eigenstates with energy  $E = k^2 \in [0, \infty)$ . Non-normalizable eigenfunctions do not have a direct physical interpretation in the sense that they do not represent physically realizable states.

The following result constructs square integrable solutions from the stationary states  $\psi_k$  for sufficiently nice initial conditions.

**Theorem 1.2.1.** *Let  $\psi_0 \in \mathcal{S}(\mathbb{R})$  and put  $\psi(x, t) = \int_{\mathbb{R}} \hat{\psi}_0(k) \psi_k(x, t) dk$ . Then  $\psi(x, t)$  is an  $L^2(\mathbb{R}, dx)$ -solution of the Schrödinger equation with initial condition  $\psi_0$ . Moreover,  $\|\psi(\cdot, t)\|_{L^2(\mathbb{R})} = \|\psi_0\|_{L^2(\mathbb{R})}$ .*

*Proof.* See [29, p. 93]. □

### 1.3 The harmonic oscillator

In classical mechanics, it is well known and easy to see (by using Taylor formula) that many potentials look basically like a simple harmonic oscillator if we are close to a local minimum. In quantum mechanics, the quantum harmonic oscillator (QHO) may approximate many physical phenomena. Dirac pointed out that the harmonic oscillator is an important example because it forms a cornerstone in the theory of radiation. The QHO is considered as a basic example in many studies concerning the formalism of quantum theory. It is a simple system for which one can solve analytically the associated Schrödinger equation. For instance, in his long paper about the rigged Hilbert space formalism, A. Bohm dealt only with the simple QHO as a basic example.

Consider a one dimensional particle, that is a particle constrained to move in one dimension, under the influence of a quadratic potential  $V(x) = \frac{1}{2}kx^2$ , where the spring constant  $k$  is positive and  $x$  represents the position of the particle. The force acting on the particle is  $F = -\nabla V = -kx$ , and serves to restore the particle to its equilibrium position  $x = 0$ .

The newtonian analysis of the harmonic oscillator is straightforward : From Newton's second law, the equation of motion of the harmonic oscillator is given by

$$m \frac{dx^2}{dt^2} + kx = 0,$$

where  $m$  is the mass of the particle and  $x = x(t)$  is position at time  $t$ . The solution to the equation of motion is given by

$$x(t) = a \cos(\omega t) + b \sin(\omega t)$$

where the characteristic frequency is  $\omega = \sqrt{\frac{k}{m}}$  and the initial conditions are  $x(0) = a$  and  $x'(0) = \omega b$ .

The total energy is a constant of the motion with well-defined contributions at each instant in time, the kinetic energy from the particle's speed and the potential energy from the particle's position in the potential well.

Often, the quantum mechanical analysis starts with the Schrödinger equation for the quantum harmonic oscillator

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi = i \hbar \frac{\partial \psi}{\partial t},$$

which operates on a suitable complex-valued function  $\psi(x, t)$  to give the quantum mechanical equation of motion. The primary problem is to find the eigenvectors and eigenvalues of the differential operator  $H$  defined by

$$H \varphi := -\frac{\hbar^2}{2m} \frac{\partial^2 \varphi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \varphi,$$

that is to solve the so-called time-independent Schrödinger equation

$$H \varphi = E \varphi.$$

The solutions are known to have the form

$$\varphi_n(x) = H_n(\sqrt{\omega} x) e^{-\frac{\omega x^2}{2}}, \quad n \in \mathbb{N},$$

where  $H_n(x)$  is the  $n$ th Hermite polynomial and with each eigenfunction  $\varphi_n$  corresponding to the eigenvalue  $(n + \frac{1}{2})\omega$ . It is well-known that the system of functions  $h_n(x) := \frac{1}{\sqrt{2^n n!}} H_n(x) e^{-\frac{x^2}{2}}$  form an orthonormal basis of  $L^2(\mathbb{R}, dx)$ . In particular, every square-integrable wavefunction  $\psi(x, t)$  is a superposition of the eigenfunctions  $(\varphi_n)_{n \in \mathbb{N}}$

$$\psi(x, t) = \sum_{n=0}^{\infty} \langle \varphi_n, \psi \rangle_{L^2(\mathbb{R}, dx)} \varphi_n(x),$$

where the convergence of the sum is that in  $L^2(\mathbb{R}, dx)$ .

## 1.4 The square barrier potential

The square barrier potential illustrates the behavior of a quantum particle encountering a potential energy barrier. It allows us to study the reflection and transmission of the particle's wave function at the barrier, which is a crucial concept in QM. It is also one of the very few problems in QM that can be solved analytically (i.e. without approximations) using elementary methods and which form an invaluable tool in the understanding of some fundamental concepts in QM. Moreover, it gives insights into how quantum particles can be bound or scattered by potential energy fields that can be obtained by considering models based on square wells and square barriers [30].

Consider a particle of mass  $m$  that is constrained to move on a half-line parametrized by  $\mathbb{R}^+$ . Let  $a, b \in (0, \infty)$  such that  $a < b$  and consider on  $\mathbb{R}^+$  a the potential barrier  $V$  of height  $V_0 > 0$  given by  $V(x) := V_0 \chi(a, b)$ . In classical mechanics, if for example the particle were to approach this barrier from the left, it would be reflected if its energy is below  $V_0$  and it would be transmitted if its energy is above  $V_0$ . However, in quantum mechanics, the outcome is uncertain ; it may be reflected or it may be transmitted. Most remarkably, the particle may be transmitted even when its energy is below the potential height  $V_0$  and continuing its travel as a wave on the other side and probability for this can be computed.

Often, the quantum mechanical behavior of a particle encountering such a potential energy barrier is described by a complex-valued function  $\psi$  (the wave function) which is a solution of the time-dependent Schroedinger equation

$$H\psi(x) := \left[-\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = i\hbar \frac{\partial \psi}{\partial t}$$

and which satisfies the Dirichlet boundary condition at  $x = 0$ , i.e.  $\psi(0, t) = 0$ .

When the particle has a definite energy  $E$ , the associated wave function has the form

$$\psi(x, t) = e^{-iEt/\hbar} \psi_E(x)$$

where  $\psi_E(x)$  is an eigenfunction of  $H$  with respect to  $E$  satisfying the Dirichlet boundary condition  $\psi_E(0) = 0$ .

By solving this eigenvalue equation in the three distinct regions  $(0, a)$ ,  $(a, b)$  and  $(b, \infty)$ , we find that for every  $E \in [0, \infty) \setminus \{0, V_0\}$ , a solution  $\psi_E(x)$  of  $H\psi = E\psi$  has the form

$$\begin{cases} \alpha_1 e^{ikx} + \alpha_2 e^{-ikx} & 0 < x < a \\ \beta_1 e^{iQx} + \beta_2 e^{-iQx} & a < x < b \\ \gamma_1 e^{ikx} + \gamma_2 e^{-ikx} & x > b \end{cases}$$

If  $E = 0$ , then  $\psi_E(x)$  has the form

$$\begin{cases} \alpha_1 + \alpha_2 x & 0 < x < a \\ \beta_1 e^{iQx} + \beta_2 e^{-iQx} & a < x < b \\ \gamma_1 + \gamma_2 x & x > b \end{cases}$$

and if  $E = V_0$ , then  $\psi_E(x)$  has the form

$$\begin{cases} \alpha_1 e^{ikx} + \alpha_2 e^{-ikx} & 0 < x < a \\ \beta_1 + \beta_2 x & a < x < b \\ \gamma_1 e^{ikx} + \gamma_2 e^{-ikx} & x > b \end{cases}$$

for appropriate coefficients  $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1, \gamma_2$  and where

$$k = \sqrt{\frac{2m}{\hbar^2} E} \quad \text{and} \quad Q = \sqrt{\frac{2m}{\hbar^2} (E - V_0)}$$

One can see that, for all  $E \in [0, \infty)$ , the equation  $H\psi = E\psi$  has no square integrable solutions. See [31].

The continuity of  $\psi_E$  and  $\psi'_E$  at  $x = a$  and  $x = b$  implies that, for every  $E \in [0, \infty)$ , the space of solutions of  $H\psi = E\psi$  has dimension two. In particular, every solution  $\psi_E$  is completely determined by  $\alpha_1$  and  $\gamma_1$ . Moreover, the boundary condition implies

$$\alpha_1 + \alpha_2 = 0 \quad \text{if } E > 0$$

and

$$\alpha_1 = 0 \quad \text{for } E = 0.$$

For  $E \in (0, \infty)$ , denote by  $\psi'_E$  and  $\psi''_E$  the two linearly-independent solutions induced respectively by  $(\alpha_1, \gamma_1) = (1, 0)$  and  $(\alpha_1, \gamma_1) = (0, 1)$  and denote by  $\psi_0$  the solution of  $H\psi = 0$  for which  $\alpha_2 = 1$ . Consider the functions  $(\varphi_k)_{k \in \mathbb{R}}$  given by

$$\varphi_k = \begin{cases} \psi_0 & \text{if } k = 0 \\ \psi'_k & \text{if } k \in (0, \infty) \\ \psi''_{-k} & \text{if } k \in (-\infty, 0). \end{cases}$$

Using the functions  $\varphi_k$ , define the stationary states  $\psi_k(x, t) = e^{-ik|x} \varphi_k(x)$ . These are non-normalizable energy eigenstates with energy  $E = |k| \in [0, \infty)$ . Again, as in the example of the free particle, we can ask if, using those eigenstates, we can construct normalizable eigenfunctions that can represent the state of the particle by considering solutions  $\psi(x, t)$  of the form

$$\psi(x, t) = \int_{\mathbb{R}} \varphi(k) \psi_k(x, t) dk$$

for some suitable functions  $\varphi(k)$ .

## 1.5 On Dirac bracket formalism

By the time Dirac started his investigations on the formal framework of quantum mechanics, this theory already existed in two distinct mathematical formulations: the Heisenberg-Born-Jordan "matrix mechanics" and Schrödinger's "wave mechanics" and for which a mathematical equivalence has been claimed by Schrödinger. These two approaches had been embedded as special cases in a more general formalism, often called "transformation theory", developed by Dirac and Jordan. In what follows, we present a description of some main ideas from Dirac's formalism, which are related to our work, as presented in his book [32].

Among the major principles in Quantum Mechanics and which are derived from experimental observations [32], there are the superposition principle and the intrinsic statistical nature of Quantum mechanics. The superposition principle suggests the mathematical formalisation of states as elements of a complex vector space  $\Psi$  [32]. A state vector  $\psi \in \Psi$  is then called a ket and denoted by  $|\psi\rangle$ . More precisely, a state is formalized as a ket  $|\psi\rangle \in \Psi \setminus \{0\}$  up to a numerical factor. It is also assumed that some more general processes are allowed such as the addition of an infinite sequence of kets or the integration of ket vectors  $|x\rangle$  parametrized by a variable  $x$  taking values in a 'range'  $X$  (a real interval for example). The result of the latter process is assumed to be a ket  $|s\rangle = \int_X |x\rangle dx$ . A set of kets is called independent if no one of them can be linearly expressed as a finite sum, a series or an integral of the others. It is called dependent otherwise.

An element  $\varphi$  of the dual space  $\Psi^*$  is called a bra and it is denoted by  $\langle\varphi|$ . Dirac assumed a one-to-one antilinear correspondance  $|\varphi\rangle \leftrightarrow \langle\varphi|$  between bras and kets (in particular, a bra do also correspond to a state of the system) and the existence of a 'scalar product' (the bracket)  $(\langle\varphi|, |\psi\rangle) \mapsto \langle\varphi|\psi\rangle$ .

Let  $A : \Psi \rightarrow \Psi$  be a linear operator. The concept of the adjoint operator  $A^*$  is defined in the usual way. By the identity  $\langle\varphi|A|\psi\rangle$ , the operator  $A$  can also be seen as acting to the left on the bra  $\langle\varphi|$  according to the relation  $\langle\varphi|A = \langle A^*\varphi|$ .

Linear operators correspond to dynamical variables of the quantum system (i.e. quantities such as the position, the momentum, the total energy etc. and complex-valued functions of these quantities) whereas self-adjoint operators correspond to real dynamical variables. Since we only measure real numbers, we restrict our attention to this class

## 1.5. ON DIRAC BRAKET FORMALISM

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of operators. However, not every real dynamical variable can be measured. The physical interpretation of the theory will in fact lead to further restrictions.

Let  $\lambda \in \mathbb{C}$  and consider the eigenvalue equation

$$A|\lambda\rangle = \lambda|\lambda\rangle.$$

If  $|\lambda\rangle \in \Psi$  is an eigenket with eigenvalue  $\lambda$  of  $A$ , observe that its conjugate  $\langle\lambda|$  satisfies  $\langle\lambda|A = \lambda\langle\lambda|$ . In this case,  $\langle\lambda|$  is said to be an eigenbra of  $A$  with eigenvalue  $\lambda$ . Similarly, if the latter equation holds true for a bra  $\langle\lambda| \neq 0$ , the associated ket  $|\lambda\rangle$  is an eigenket of  $A$  with eigenvalue  $\lambda$ . The corresponding state is then called an eigenstate of the system. The set of all eigenvalues is called the spectrum of  $A$  and it is denoted by  $\sigma(A)$  and which is real in the case of a self-adjoint operator.

Next, we list three essential postulates of the braket formalism :

1) If the quantum system is in a state  $|\lambda\rangle$  which is an eigenket of a real dynamical variable  $A$  with respect to an eigenvalue  $\lambda \in \mathbb{R}$ , a measurement of  $A$  will yield, with certainty, the value  $\lambda$  as a result. Conversely, if the system is in a state  $|\psi\rangle$  such that the measurement of a real dynamical variable  $A$  is certain to give the particular result  $\lambda \in \mathbb{R}$ , then the state  $|\psi\rangle \equiv |\lambda\rangle$  is an eigenket of  $A$  with the corresponding eigenvalue  $\lambda$ .

2) If a real dynamical variable  $A$  is measurable, the possible outcomes of a mesurement are the numbers in its spectrum  $\sigma(A)$ .

3) If the system is in a particular state and a real dynamical variable is measured, then, immediately after the measurement, the possible states in which the system can be, are such that the original state is linearly dependent of them.

In particular, any state in which the system can be is linearly dependent of the eigenkets of  $A$  and hence the eigenstates of a measurable real dynamical variable should form a complete set of states. An observable is therefore defined to be a self-adjoint operator whose eigenkets form a complete set.

Let  $A$  be an observable. The spectrum  $\sigma(A)$  may consist of a (finite or infinite) discrete set of numbers, or, alternatiely, of all numbers in a certain 'range' (an interval for example), or both together. That is to say, the spectrum of  $A$  may have the continuum cardinality. The condition for the eigenkets of  $A$  to form a complete set can be formulated as follows : Denote by  $|\lambda_d\rangle$  the eigenkets corresponding to the discrete part of the spectrum and  $|\lambda_c\rangle$  the ones corresponding to the continuum part. Then, any ket  $|\psi\rangle$  can be expressed in the following form

$$|\psi\rangle = \sum |\lambda_d\rangle + \int |\lambda_c\rangle d\lambda_c.$$

where  $\lambda_d$  in the (possibly infinite) sum runs over the discrete part of the spectrum and  $\lambda_c$  in the integral runs over the whole continuum range of the spectrum. Next, Dirac concluded that the eigenkets whose corresponding eigenvalues belong to the continuum range of the spectrum cannot have a finite length by arguing as follows : since, for two such kets  $|\psi\rangle$  and  $|\varphi\rangle$  such that

$$|\psi\rangle = \int |\lambda_c\rangle d\lambda \quad \text{and} \quad |\varphi\rangle = \int |\lambda'_c\rangle d\lambda'$$

one has

$$\langle\psi|\varphi\rangle = \int \int \langle\lambda_c|\lambda'_c\rangle d\lambda d\lambda',$$

considering the single integral

$$\int \langle\lambda_c|\lambda'_c\rangle d\lambda',$$

by orthogonality, the integrand must be zero for the whole range of integration except for the point  $\lambda'_c = \lambda_c$ . This entails that if the braket takes only finite values, we get  $\langle\psi|\varphi\rangle = 0$ , which is not the case in general. So the quantity  $\langle\lambda_c|\lambda_c\rangle$  ( i.e. the 'length' of  $|\lambda_c\rangle$  ) "*must be infinitely great in such a way as to make the integral non-vanishing and finite*". To reconciliate to this, the form of infinity was expressed by what he called the  $\delta$  function. This is "a quantity  $\delta(x)$  depending on a parameter  $x$  satisfying the conditions  $\int_{-\infty}^{\infty} \delta(x)dx = 1$  and  $\delta(x) = 0$  for every  $x \neq 0$ ". The most important property of  $\delta$  being

$$\int_{-\infty}^{\infty} f(x)\delta(x)dx = f(0),$$

where  $f(x)$  is any continuous function of  $x$ . Moreover, for a real number  $a$  and with a change of variable, the following formula is deduced

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a).$$

Next, let  $(\langle\lambda|)_{\lambda\in\Lambda}$  be a complete set of bra vectors. By completeness, each ket  $|\psi\rangle$  is characterized (i.e. completely determined) by the scalar products  $\langle\lambda|\psi\rangle$  ( $\lambda\in\Lambda$ ). That is, by the complex-valued function  $\psi$  on  $\Lambda$  defined by  $\psi(\lambda) := \langle\lambda|\psi\rangle$ . We say that the complete set  $(\langle\lambda|)_{\lambda\in\Lambda}$  induces a representation of the ket vectors (as complex-valued functions on  $\Lambda$ , which we would call wavefunctions). Elements of  $(\langle\lambda|)_{\lambda\in\Lambda}$  are called the basic bras of this representation. Although the basic bras of a representation do not have to be all independent, in most representation used in practice, they will satisfy the even more strong condition of being mutually orthogonal. In this case, the corresponding representation is called an orthogonal representation. The kets  $|\lambda\rangle$  ( $\lambda\in\Lambda$ ) corresponding to the basic bras of a representation are said to be the basic kets of that representation. Given an observable  $A$  for which each eigenvalue is of multiplicity one and using a complete set of corresponding eigenkets  $(|\lambda\rangle)_{\lambda\in\sigma(A)}$ , one can construct an orthogonal representation with those eigenkets as basic kets. Such an orthogonal representation is said to be induced by the observable  $A$ .

Given a complete set of orthogonal kets  $(|\lambda\rangle)_{\lambda\in\Lambda}$ , one can construct a one-to-one linear map  $|\psi\rangle\in\Psi\mapsto\psi(\lambda) := \langle\lambda|\psi\rangle$ . In particular, for a free particle moving along a straight line parametrized by  $x\in\mathbb{R}$ , and considering the position observable  $X$ , since the particle can occupy any position, the spectrum should be given by the range formed by all real numbers. Suppose moreover that for each eigenvalue  $x\in\sigma(X)$ , there is a unique associated normalized eigenket  $|x\rangle$ . Given a complete orthogonal set  $(|x\rangle)_{x\in\mathbb{R}}$  of eigenkets of  $X$ , the induced orthogonal representation  $|\psi\rangle\mapsto\psi(x) := \langle x|\psi\rangle$  is called the position representation. The latter representation has a special privilege since physical phenomena essentially concern the configuration space parametrized by  $x\in\mathbb{R}$  and boundary conditions directly concern the "wave function"  $\psi(x)$ . Similarly one can get the so-called momentum representation using a complete set  $(|p\rangle)_{p\in\mathbb{R}}$  of eigenkets of the momentum operator  $P$ . The induced complex-valued functions  $\psi(p)$  are called the momentum wavefunctions.

Dealing with an orthonormal representation, it is natural to have some normalization convention for the associated basic kets (bras). In the following, we assume this convention in the special case of an observable  $A$  for which each eigenvalue is of multiplicity one. In this case, with two eigenvalues  $\lambda_d$  and  $\lambda'_d$  belonging to the discrete part of the spectrum of  $A$ , we assume the following normalization condition

$$\langle\lambda_d|\lambda'_d\rangle = \delta_{\lambda_d,\lambda'_d},$$

where  $\delta_{\lambda_d,\lambda'_d}$  is the Kronecker delta symbol. Additionally, if  $\lambda_c$  and  $\lambda'_c$  are two eigenvalues of  $A$  belonging to a range, the corresponding eigenkets  $|\lambda_c\rangle$  and  $|\lambda'_c\rangle$  are supposed to be of an infinite length. The orthonormality condition is now assumed to be as follows

$$\langle\lambda_d|\lambda'_d\rangle = \delta(\lambda_c - \lambda'_d),$$

where  $\delta(\cdot)$  denotes the  $\delta$  function.

Labeling by a real parameter  $\lambda_d$  (resp.  $\lambda_c$ ) the eigenvalues of  $A$  in the discrete (resp. the range) part  $\sigma(A)$ , to each  $\lambda_d$  (resp.  $\lambda_c$ ) is associated a unique normalized eigenket  $|\lambda_d\rangle$  (resp.  $|\lambda_c\rangle$ ). Next, let  $|\lambda'_d\rangle$  and  $|\lambda'_c\rangle$  be fixed. It then follows that

$$|\lambda'_d\rangle = \sum_{\lambda_d} \langle\lambda_d|\lambda'_d\rangle |\lambda_d\rangle \quad , \quad |\lambda'_c\rangle = \int d\lambda_c \langle\lambda_c|\lambda'_c\rangle |\lambda_c\rangle.$$

Using the fact that the eigenkets  $|\lambda_d\rangle$  and  $|\lambda_c\rangle$  form a complete set of states, the following form of the identity operator (called the closure relation) is derived

$$I = \sum_{\lambda_d} |\lambda_d\rangle\langle\lambda_d| + \int d\lambda_c |\lambda_c\rangle\langle\lambda_c|,$$

and which, by means of it, any ket vector  $|\psi\rangle$  can be linearly expanded in terms of the basic kets of the orthonormal representation induced by  $A$  as

$$|\psi\rangle = \sum_{\lambda_d} \langle\lambda_d|\psi\rangle |\lambda_d\rangle + \int d\lambda_c \langle\lambda_c|\psi\rangle |\lambda_c\rangle.$$

Similarly for any bra vector  $\langle \psi |$  as

$$\langle \psi | = \sum_{\lambda_d} \langle \psi | \lambda_d \rangle \langle \lambda_d | + \int d\lambda_c \langle \psi | \lambda_c \rangle \langle \lambda_c |.$$

Also, with a ket  $|\psi\rangle$  and a bra  $\langle \varphi |$  one gets

$$\langle \varphi | \psi \rangle = \sum_{\lambda_d} \langle \varphi | \lambda_d \rangle \langle \lambda_d | \psi \rangle + \int d\lambda_c \langle \varphi | \lambda_c \rangle \langle \lambda_c | \psi \rangle.$$

## 1.6 The Hilbert space formalism of quantum mechanics

Greatly inspired by Dirac transformation theory formulation of QM, von Neumann proposed in 1932 a mathematically precise formulation of QM based on Hilbert space and linear operators. In his book, in which in fact the term 'Hilbert space' was first introduced and some of the important theorems in this area were first proved, von Neumann acknowledged that Dirac formalism provides a very elegant and powerful formal framework for quantum mechanics. He stated however that Dirac formulation in no way satisfies the necessary mathematical rigor due to the present and the central role of some *improper objects with self-contradictory properties* such as Dirac delta function and which von Neumann qualified as *mathematical fictions*.

In this section we shall present a brief introduction to some of the main postulates (or axioms) of Quantum Mechanics and its main ingredients : states, observables, measurement and quantum dynamics following von Neumann Hilbert space formalism. Mathematically, this was essentially handled by the general theory of operators, spectral theory and functional calculus for self-adjoint operators. The postulates were built through many efforts over several years, by many physicists. Mainly, Bohr, Born, De Broglie, Dirac, Heisenberg, Jordan, Schrödinger, von Neumann, to name but a few. About these postulates, we quote from [29] *These axioms are not to be understood in the mathematical sense as rules from which all other results are derived in a strictly deductive fashion. Rather, the axioms are the main principles of how quantum mechanics works.* They are the only ingredients necessary for being able to compute in QM.

We refer the reader to Section 2.3 for the needed material on unbounded operators.

### Postulate 1. (States )

The set of all possible physical states of a quantum system is represented by a Hilbert space  $\mathcal{H}$ . More precisely the states of a quantum system are represented by unit rays in a Hilbert space. These are equivalence classes of vectors that differ by a non-zero scalar multiplication. The states of the system are usually identified as normalized representatives of these classes. A state  $\psi$  contains all the physical information one can have about the system.

The above notion of states is called a pure state and it corresponds to the case where our knowledge of the system is complete. In the case where our knowledge is incomplete, but we know the statistical ensemble associated to the system, we have a more general notion of states called a mixed state and which is represented by a positive trace-class operator  $\rho : \mathcal{H} \rightarrow \mathcal{H}$  for which  $\text{tr}(\rho) = 1$ .

### Postulate 2. (Observables)

Physical quantities that could be observed by taking a measurement of the system such as position, velocity, total energy, spin etc are represented by selfadjoint operators in  $\mathcal{H}$ . These are called observables of the system.

The set of possible outcomes for the measurement of an observable  $A$  coincides with its spectrum  $\sigma(A)$  (which is real). In particular, for some quantum systems, the energy of the system may take values only in a given discrete set. This was in fact the origin of the name "Quantum Mechanics".

### Postulate 3. (Measurements)

The result of the measurement belongs to the set  $\sigma(A)$  but in general it cannot be predicted a priori. The only possible information one can be sure of is the probability distribution of the measurement outcome. This is described by the following :

Denote by  $P^A$  be the spectral measure associated to  $A$ .

If the system is in a pure state  $\psi$ , then the probability  $\mu_\psi^A(\Omega)$  of measuring, for the observable  $A$ , a value which lies in the Borel set  $\Omega \subset \mathbb{R}$  may be computed using the formula

$$\mu_\psi^A(\Omega) = \langle \psi, P^A(\Omega)\psi \rangle = \|P^A(\Omega)\psi\|^2$$

Furthermore, immediately after the measurement, the state of the system is changed and becomes

$$\psi' = \frac{P^A(\Omega)\psi}{\|P^A(\Omega)\psi\|}$$

This is the so-called reduction of the wave packet.

More generally, if the system is in a mixed state  $\rho$ , and we measure the observable  $A$ , then the probability  $\mu_\rho^A(\Omega)$  of measuring, for the observable  $A$ , a value which lies in the Borel set  $\Omega \subset \mathbb{R}$  may be computed using the formula

$$\mu_\rho^A(\Omega) = \text{tr}(P^A(\Omega)\rho).$$

Furthermore, immediately after the measurement, the state of the system is changed and becomes

$$\rho' = \frac{P^A(\Omega)\rho P^A(\Omega)}{\text{tr}(P^A(\Omega)\rho P^A(\Omega))}$$

In particular, if the observable satisfies  $\sigma(A) = \sigma_p(A)$ , and if the result of the measurement yields  $\lambda$ , then immediately after the measurement, the system will be in the state  $\rho'$ , such that

$$\rho' = \frac{P_\lambda^A \rho P_\lambda^A}{\text{tr}(P_\lambda^A \rho P_\lambda^A)},$$

where  $P_\lambda^A$  is the projection onto the  $\lambda$ -eigenspace of  $A$ .

Note also the important fact that, when measuring successively with respect to two different observables of a quantum system  $\mathcal{H}$ , the order in which the measurements are made is of importance in general.

**Postulate 4.** (Dynamics)

One observable of the system  $H$  has a particular status: the total energy  $H$  of the system. It is called the Hamiltonian of the system and it controls the way the system would evolve with time when no exterior intervention is present.

Suppose that the quantum system is isolated between times  $t_1$  and  $t_2$  and let  $H$  be the Hamiltonian of the system. Then, if the system is in a pure state  $\psi(t_1)$ , we have

$$\psi(t_2) = U(t_2 - t_1)\psi(t_1).$$

where  $U(t) = e^{-\frac{i}{\hbar}tH}$  can be computed using functional calculus. Note that the probability of measuring an observable  $A$  to be in a set  $\Omega$  at time  $t$  is thus equal to

$$\langle \psi(t), P^A(\Omega)\psi(t) \rangle = \langle U(t)\psi(0), P^A(\Omega)U(t)\psi(0) \rangle = \langle \psi(0), U(t)^* P^A(\Omega) U(t)\psi(0) \rangle$$

More generally, if the system is in a mixed state  $\rho(t_1)$ , we have

$$\rho(t_2) = U(t_2 - t_1)\rho(t_1)U(t_2 - t_1)^*$$

In the dynamics postulate above, the time dependence is carried by the states of the system whereas observables are supposed to be time-independent. This is the so-called Shroedinger picture. An alternative point of view is to suppose that the time dependence is instead carried by observables and that states stay time-independent. In this case the dynamics of an observable  $A(t)$  is supposed to be given by

$$A(t_2) = U(t_2 - t_1)^* A(t_1) U(t_2 - t_1)$$

where  $H(t) \equiv H$  is the Hamiltonian observable and which is in this case a constant of motion. This is the so-called Heisenberg picture.

## 1.7 Introduction to the rigged Hilbert space formalism

Till nowadays, most physicists and standard textbooks adopte the simpler and more intuitive braket formalism of Dirac within the framwork of the von Neumann Hilbert space formalism by, for example, using state vectors that do not belong to the considered Hilbert space (but which are of practical importance) such as plane waves or Dirac delta functions, although it is not mentionned that the Hilbert space methods cannot encorporate such concepts and manipulations. The original motivation for introducing the RHS structure in quantum mechanics was with the aim of reconciling the two approaches by providing a structure built around that of Hilbert space. It was obtained in the 60's, independently by Roberts [13], Antoine [15] and Bohm [14]. The use of the RHS for a rigorous mathematical formulation of Dirac's formalism was suggested and investigated by several authors, in many papers. Among them we mention the works of Foias [11], Roberts [12, 13], Bohm [14] and Antoine [15].

The rigged Hilbert space construction appeared in [8] and was motivated by the observation that many unitary or self-adjoint operators defined in  $L^2(\mathbb{R}, dx)$  have some "natural eigenvectors", which does not belong to  $L^2(\mathbb{R}, dx)$ . For instance the map  $\varphi$  defined by  $x \mapsto e^{i\lambda x}$  satisfies  $\varphi(x+a) = e^{i\lambda a} \varphi(x)$ . However, it cannot be a usual eigenvector of the translation operator

$$T_a : L^2(\mathbb{R}, dx) \rightarrow L^2(\mathbb{R}, dx), \quad \psi(x) \mapsto \psi(x+a),$$

since  $\varphi$  does not lie in  $L^2(\mathbb{R}, dx)$ . Other examples are given by the position and the momentum operators in the Schrödinger representation  $L^2(\mathbb{R}, dx)$

$$Q : D(Q) \rightarrow L^2(\mathbb{R}, dx), \quad \psi(x) \mapsto x\psi(x).$$

$$P : D(P) \rightarrow L^2(\mathbb{R}, dx), \quad \psi(x) \mapsto -i\hbar \frac{d\psi}{dx}(x).$$

For each  $\lambda \in \mathbb{R}$ , the differential equation

$$-i\hbar\psi'(x) = \lambda\psi(x)$$

is solved by scalar multiples of  $\psi_\lambda(x) := e^{-i\frac{\lambda}{\hbar}x} \notin L^2(\mathbb{R}, dx)$ . Hence  $P$  does not admit any eigenvalue. On the other hand, formally written, we have  $Q\delta(\lambda - x) = x\delta(\lambda - x) = \lambda\delta(\lambda - x)$  where  $\delta$  denotes the Dirac delta "function". Moreover, the authors in [8] observed that these natural eigenvectors satisfy a kind of completeness property. For example, using the Fourier transform, we have that

$$\forall \psi \in \mathcal{S}(\mathbb{R}), \quad \left( \int_{\mathbb{R}} \psi(x) e^{i\lambda x} dx = 0, \quad \forall \lambda \in \mathbb{R} \right) \Rightarrow \psi \equiv 0$$

In order to handle these natural eigenvectors in a rigorous way, the idea was to extend the Hilbert space  $L^2(\mathbb{R}, dx)$  to a larger space of functions or distributions where the eigenvectors will lie and then somehow extend the action of the considered operator to that bigger space. This can be formalized within the framework of Gelfand triples. These are structures of the form  $\Phi \subset \mathcal{H} \subset \Phi^\times$  where  $\Phi$  is a dense subspace of  $\mathcal{H}$  endowed with a locally convex topology  $\tau_\Phi$  finer than the one induced by the Hilbert space structure and where  $\Phi^\times$  denotes its topological antidual. By duality, each space in the latter structure is dense in the next one and all embeddings are lineaire and continuous. A standard example of a Gelfand triplet is given by  $\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dx) \subset \mathcal{S}^\times(\mathbb{R})$  where  $\mathcal{S}^\times(\mathbb{R})$  is the space of tempered distributions.

It turns out that there are subdomains  $\Phi$  of the Hilbert space that can be endowed with topologies that make observables of interest continuous [33]. Moreover, using the basic tools of the theory, namely the generalized eigenvectors of self-adjoint operators leaving the space  $\Phi$  invariant, the nuclear spectral theorem yields a rigourous formulation of many aspects of Dirac braket formalism which is routinely used by physicists but which cannot be justified solely within the Hilbert space structure, especially when a continuous spectrum is present. In this case, the RHS structure provide a natural mathematical framwork that give a precise sense to some main features of Dirac braket formalism such as the existence of eigenvectors corresponding to points in the continuous spectrum, the existence of sufficient eigenvectors ensuring some expansion formulas or the continuity of the algebra of observables. To some extent, this seems to be ensured by the nuclear spectral theorem for a continuous observable  $A : \Phi \rightarrow \Phi$  with a self-adjoint extension of  $\mathcal{H}$  [13]. Moreover, once the space  $\Phi$  is constructed, all physical quantities of

interest (such as expectation values, uncertainties, and commutators etc.) can be computed without having to worry about domain subtleties as in the von-Neumann Hilbert space formulation. In this regard,  $\Phi$  maybe interpreted as the space of states that are physically preparable [15] and it is sometimes called the space of wavefunctions [33]. In practice, most of the operators that one wants to use have a common dense and invariant domain  $\Phi$ . Elements of  $\Phi$  are most of the time represented by a set of well-behaved functions, in contrast to the elements of the Hilbert space, which are usually represented by sets of equivalent classes of functions. In this case, as a first impression, the space  $\Phi$  might seem too small to be of much use, but this will be somehow compensated by the fact that it will have a very large dual space and which will make precise sense of some singular objects of practical importance as elements of some special classes of distributions to which the operators of interest will be extended.

Consider the example of a non-relativistic one-dimensional spinless particle moving on a straight line parametrized by  $x \in \mathbb{R}$ . The spectrum of the position observable coincides with the set of all real numbers. For each  $x \in \mathbb{R}$ , the eigenkets  $|x\rangle$  of the position operator  $Q$  are not elements of the Hilbert space and thus somehow a larger linear space is needed to accommodate them. The RHS structure  $\Phi \subset \mathcal{H} \subset \Phi^\times$ , with a good choice of  $\Phi \subset D(Q)$ , can rigorously handle these eigenkets as generalized eigenvectors of the restriction  $Q|_\Phi$ . In general, the space  $\Phi$  will be such that, in particular, its antidual space  $\Phi^\times$  contains the eigenkets associated to the continuous spectrum of the observables of interest.

A main shortcoming of the RHS formalism is that it does not provide a prescription to construct the space  $\Phi$  nor the eigenkets associated to the continuous spectrum. The general statement of the nuclear spectral theorem [8] just assures the existence of a complete family of such eigenkets and assumes the spaces  $\Phi$  to be given a priori. Therefore, a systematic procedure to construct the RHS for a given quantum system is needed. As for standard constructions for nonrelativistic quantum systems, a prominent role is played by Robert's canonical construction for the algebra  $\mathcal{A}$  of observables in Schrödinger's representation associated to  $n$  interacting particles such that the position and momentum observables of the particles belong to  $\mathcal{A}$ , and the potential energy  $V(x)$  is almost everywhere infinitely differentiable [12, 13]. We sketch his construction as follows : Suppose given a Hilbert space  $\mathcal{H}$  with a collection of operators  $\mathcal{O} = \{A_i\}_{i \in I}$  of relevance ( called "labeled" observables ) which should be sufficient to describe the system (in particular, all the system's observables) and which are to be made continuous. We suppose that  $\mathcal{O}$  admits a common dense invariant domain. Denote by  $\Phi$  the maximal invariant domain for  $\mathcal{O}$  and consider the algebra with unite  $\mathcal{A}$  generated by  $\mathcal{O}^\circ \equiv \{A_i|_\Phi\}_{i \in I}$ . This domain  $\Phi$  is given by  $\Phi = \bigcap_{A \in \mathcal{A}} D(A)$ . Now to enable analytical methods, we equip  $\Phi$  with a topology  $\tau_\Phi$  making into a topological vector space and making  $\mathcal{O}^\circ$  into an algebra of continuous operators on  $\Phi$ . This topology is taken to be the initial topology on  $\Phi$  relatively to  $\mathcal{O}^\circ$  and it is uniquely determined by the following facts : it is the coarsest topology on  $\Phi$  making  $\mathcal{O}^\circ$  continuous and which is finer than the induced Hilbert space topology. It is in fact a locally convex topology that can also be seen as induced by the following family  $\{\|A^\circ \phi\|\}_{A^\circ \in \mathcal{O}^\circ}$  of seminorms. This topology makes  $\Phi$  into a complete topological vector space ( and a reflexive Frechet space once  $\mathcal{O}$  is countable ). Thus, from the so-called *labelled Hilbert space*  $(\mathcal{H}, \mathcal{O})$ , we derive (up to some identifications) a canonical triplet of spaces  $\Phi \subset \mathcal{H} \subset \Phi^\times$ . It is also worth pointing out that in [reference], the authors provided basis dependent RHS constructions on the half line by using generalized Laguerre polynomials.

## MATHEMATICAL TOOLS OF THE FORMALISM

### 2.1 Preliminaries on some basic function spaces

We recall in the following some basic function spaces that play an important role in the mathematical formulation of quantum mechanics.

Let  $X$  be a subset of  $\mathbb{C}$ . We denote by  $\mathcal{B}(X)$  the Borel  $\sigma$ -algebra on  $X$ . Let  $\mu$  be a positive regular Borel measure on  $X$ . Our Borel measures are supposed to be finite on compact sets. As usual,  $\chi_X$  denotes the characteristic function of  $X$  and  $\mathcal{L}^2(X, \sigma)$  denotes the function space

$$\mathcal{L}^2(X, d\mu) := \{\psi : X \rightarrow \mathbb{C}, \psi \text{ measurable and } \int_X |\psi(x)|^2 d\sigma < \infty\},$$

while  $L^2(X, d\mu)$  denotes the corresponding Hilbert space. It consists of equivalence classes of measurable functions in  $\mathcal{L}^2(X, \sigma)$  which are equal almost everywhere. Since there is no risk of ambiguity, we shall use the same notation for  $\psi \in \mathcal{L}^2(X, \sigma)$  and its corresponding equivalence class. For an everywhere defined function  $\psi$ ,  $\text{supp}(\psi)$  denotes its support. Its essential image is defined by

$$\text{ess.im}(\psi) = \{z \in \mathbb{C} : \forall \varepsilon > 0, \mu\{x \in X : |\psi(x) - z| < \varepsilon\} > 0\}.$$

Let  $I \subseteq \mathbb{R}$  be an interval. A function  $\psi : I \rightarrow \mathbb{C}$  is said to be absolutely continuous on  $I$  if there exists a Lebesgue integrable function  $\varphi : I \rightarrow \mathbb{C}$  such that

$$\psi(x) = \psi(a) + \int_a^x \varphi(y) dy$$

for all compact intervals  $[a, x] \subset I$ . In this case  $\psi$  is a.e. differentiable with  $\psi' = \varphi$ . We denote by  $AC(I)$  the set of such functions. The subset of functions  $\psi \in AC(I)$  whose derivative is absolutely continuous on  $I$  is denoted by  $AC^2(I)$ .

Let  $a < b$  be in  $\overline{\mathbb{R}}$ . The usual Sobolev spaces are defined by

$$H^m(a, b) := \{\psi \in L^2(a, b) : \psi^{(j)} \in AC(a, b), \psi^{(m)} \in L^2(a, b), 0 \leq j \leq m-1\}$$

where  $\psi^{(j)}$  is the  $j$ -th derivative of  $\psi$ .

The space of test functions is

$$\mathcal{D}(\mathbb{R}) = \{\psi \in \mathcal{C}^\infty(\mathbb{R}) : \text{supp}(\psi) \text{ is compact}\},$$

The Schwartz space  $\mathcal{S}(\mathbb{R})$  is defined as the set of infinitely differentiable functions on  $\mathbb{R}$  for which

$$\|\psi\|_{m,n} := \sup_{x \in \mathbb{R}} |x^m \psi^{(n)}(x)| < \infty, \quad \forall m, n \in \mathbb{N}$$

The  $(\|\cdot\|_{m,n})_{m,n}$  above is a family of seminorms on  $\mathcal{S}(\mathbb{R})$ . The induced locally convex topology is called the Schwartz topology on  $\mathcal{S}(\mathbb{R})$  and will be denoted by  $\tau_{\mathcal{S}}$ .

An equivalent countable family of seminorms (in fact norms) on  $\mathcal{S}(\mathbb{R})$  is given by

$$\|\psi\|_{m,n} := \sup_{x \in \mathbb{R}} |(1+|x|)^m \psi^{(n)}(x)| < \infty, \quad \forall m, n \in \mathbb{N}$$

The Schwartz topology is hence a metric topology on  $\mathcal{S}(\mathbb{R})$  and such a metric could be taken as

$$d(\psi, \varphi) = \sum_{m,n \in \mathbb{N}} 2^{-m-n} \frac{\|\psi - \varphi\|_{m,n}}{1 + \|\psi - \varphi\|_{m,n}} \quad \psi, \varphi \in \mathcal{S}(\mathbb{R})$$

Moreover, one can show that  $(\mathcal{S}(\mathbb{R}), d)$  is a complete metric space.

Recall also that the Fourier transform  $\mathcal{F}$  is the unitary map defined on  $L^2(\mathbb{R}, dx)$  as a completion of the following map on the Schwartz space

$$\mathcal{F}\{f\}(\lambda) \equiv \hat{f}(\lambda) = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{-i\lambda x} f(x) dx, \quad f \in \mathcal{S}(\mathbb{R}).$$

The Bargmann-Fock space is defined by

$$\mathcal{F} = \left\{ \psi : \mathbb{C} \rightarrow \mathbb{C} : \psi \text{ is analytic and } \int_{\mathbb{C}} |\psi(z)|^2 e^{-|z|^2} dz < \infty \right\}$$

It is well known that  $\mathcal{F}$  is a Hilbert space for the usual  $L^2$  inner product with respect to the measure  $e^{-|z|^2} dz$  and that  $(\frac{z^n}{\sqrt{n!}})_n$  forms an orthonormal basis. In this basis, for  $\varphi = \sum_n \varphi_n z^n$ ,  $\psi = \sum_n \psi_n z^n \in \mathcal{F}$ , the inner product reads

$$\langle \varphi, \psi \rangle = \sum_{n=0}^{\infty} n! \overline{\varphi_n} \psi_n$$

For  $\omega, z \in \mathbb{C}$ , by putting  $e_{\omega}(z) = e^{\overline{\omega}z}$  we have for each  $\psi \in \mathcal{F}$  that

$$\psi(z) = \langle e_z, \psi \rangle$$

Additionally, by denoting  $K(\omega, z) = e^{\omega \overline{z}} = \langle e_{\omega}, e_z \rangle$ , we have

$$\psi(\omega) = \int_{\mathbb{C}} K(\omega, z) \psi(z) e^{-|z|^2} dz$$

## 2.2 The completion of a metric space

In this thesis, we will only be interested in the case of t.v.s. whose topologies are generated by a countable collection of norms. These spaces are in fact metric spaces. The so-called standard completion procedure, which generalizes the Cantor construction of the reals, enables to construct for any metric space a complete metric space in which the original space can be isometrically identified as a dense subset.

**Definition 2.2.1.** *Let  $(E, d)$  be a metric space. A complete metric space  $(F, \delta)$  is called a completion of  $(E, d)$  if there is an isometry  $i : E \rightarrow F$  such that the set  $i(E)$  is dense in  $F$ .*

**Theorem 2.2.1.** *Every metric space has a completion.*

## 2.2. THE COMPLETION OF A METRIC SPACE

*Proof.* Let  $E$  be a metric space. Denote by  $\mathcal{C}[E]$  the set of all Cauchy sequences in  $E$  and define on it the following equivalence relation :

$$(x_n) \sim (y_n) \Leftrightarrow \lim_n d(x_n, y_n) = 0$$

Let  $\bar{E}$  be the set of equivalence classes for  $\sim$  :

$$\bar{E} = \{[(x_n)] : (x_n)_n \in \mathcal{C}[E]\}$$

For  $\bar{x}, \bar{y} \in \bar{E}$  and  $(x_n)_n, (y_n)_n \in \mathcal{C}[E]$  such that  $\bar{x} = [(x_n)_n]$  and  $\bar{y} = [(y_n)_n]$ , we put

$$\bar{d}(\bar{x}, \bar{y}) := \lim_n d(x_n, y_n).$$

The reverse triangle inequality implies that  $(d(x_n, y_n))$  is a Cauchy sequence in  $\mathbb{R}$  and that the limit does not depend on the chosen representatives  $(x_n)_n$  and  $(y_n)_n$ . On the other hand, using the fact that  $d$  is a metric on  $E$ , we show that  $\bar{d}$  satisfies the triangle inequality. Moreover,  $\bar{d}(\bar{x}, \bar{y}) = 0$  clearly induces  $\bar{x} = \bar{y}$ . This shows that  $\bar{d}$  is well-defined metric on  $\bar{E}$ .

Let  $i : E \rightarrow \bar{E}$  be defined by  $x \mapsto [(x)_n]$ . It is easy to see that  $i$  is an isometry. Moreover, the set  $i(E)$  is dense in  $(\bar{E}, \bar{d})$ . Indeed : Let  $\varepsilon > 0$  and  $\bar{x} = [(x_n)_n] \in \bar{E}$ . There exists then  $m > 0$  such that for  $n \geq m$ ,  $d(x_n, x_m) < \varepsilon$ . We then have  $\lim_n d(x_n, x_m) < \varepsilon$ , i.e.  $\bar{d}(\bar{x}, [(x_m)_n]) < \varepsilon$ , where  $[(x_m)_n] = i(x_m) \in i(E)$ .

The metric space  $(\bar{E}, \bar{d})$  is complete : let  $(\bar{y}_n)_n$  be a Cauchy sequence in  $\bar{E}$ . By density of  $i(E)$ , there exists  $(x_n)_n \subset E$  such that  $\bar{d}(i(x_n), \bar{y}_n) < \frac{1}{n}$  for each  $n$ . We then see that the sequences  $(i(x_n))_n$  and  $(\bar{y}_n)_n$  either both converges or both diverges. On the other hand we have that  $(x_n)_n \subset E$  is a Cauchy sequence (see [34]). We thus have  $[(x_n)_n] \in \bar{E}$ . Now observing that  $\lim_n \bar{d}(i(x_n), [(x_n)_n]) = \lim_n \lim_m d(x_n, x_m) = 0$  gives that the sequence  $(i(x_n))_n$  converges to  $[(x_n)_n]$  in the metric space  $\bar{E}$ . The construction of the points  $x_n$  implies that the given Cauchy sequence too converges to  $[(x_n)_n]$ . This finishes the proof.  $\square$

**Remark 2.2.1.** *It follows easily from Definition 2.2.1 that if  $(\hat{E}, \hat{d})$  is another completion of  $(E, d)$ , then there is an isometry  $j : \bar{E} \rightarrow \hat{E}$  such that  $j(x) = x$  for all  $x \in E$ . ( $E$  being identified with  $i(E)$ )*

**Proposition 2.2.1.** *Let  $V$  be a normed linear space. Then  $V$  is complete if and only if every absolutely convergent series with terms in  $V$  is convergent.*

**Example 2.2.1.** 1. *Let  $X$  be a locally compact topological space,  $\mu$  a positive Borel measure on  $X$  and consider on the space  $\mathcal{C}_c(X)$  of continuous functions on  $X$  with compact support the following scalar product*

$$\langle f, g \rangle = \int_X f(x) \overline{g(x)} d\mu(x)$$

*Then  $L^2(X, d\mu)$  is a completion of  $(\mathcal{C}_c(X), \langle \cdot, \cdot \rangle)$ .*

*In the particular case where  $X$  is an open set of  $\mathbb{R}$ ,  $L^2(X, d\mu)$  is a completion of  $(\mathcal{C}_c^\infty(X), \langle \cdot, \cdot \rangle)$  where  $\mathcal{C}_c^\infty(X)$  is the space of infinitely differentiable functions with compact supports.*

2. *Consider on the space  $\mathcal{C}_c^\infty(\mathbb{R})$  of infinitely differentiable functions with compact supports the family  $(\|\cdot\|_{m,n})_{m,n \in \mathbb{N}}$  of semi-norms given by  $\|f\|_{m,n} := \sup_{x \in \mathbb{R}} |x^m f^{(n)}(x)|$ . Denote by  $d$  the distance on  $\mathcal{C}_c^\infty(\mathbb{R})$  defined by  $d(f, g) = \sum_{\alpha, \beta} 2^{-m-n} \frac{\|f-g\|_{m,n}}{1+\|f-g\|_{m,n}}$ . The Schwartz space  $\mathcal{S}(\mathbb{R})$  is then a completion of  $(\mathcal{C}_c^\infty(\mathbb{R}), d)$ . Put  $\Lambda = \text{span}\{h_n : n \in \mathbb{N}\}$  where  $(h_n)_n$  is the family of Hermite functions. Since  $(h_n)_n$  forms a Schauder basis of the Schwartz space  $\mathcal{S}(\mathbb{R})$ , the latter can also be seen as a completion of the metric space  $(\Lambda, d)$ .*

## On Initial topologies

Let  $E$  be a set and let  $\{S_\alpha\}_{\alpha \in A}$  be a family of subsets of  $E$ . Recall that the topology on  $E$  generated by the collection of subsets  $S_\alpha$  where  $\alpha$  runs through  $A$  is the intersection of all the topologies on  $E$  containing all the subsets  $S_\alpha$ . It is then the coarsest topology on  $E$  for which all the subsets  $S_\alpha$  are open. We denote it by  $\tau_i$ . Recall also that open sets for  $\tau_i$  are of the form  $\cup_I \cap_{J_{\text{finite}}} S_\alpha$ .

**Definition 2.2.2.** Let  $T_\alpha : E \rightarrow E_\alpha$  be mappings of  $E$  into topological spaces  $E_\alpha$ ; then the coarsest topology on  $E$  making the mappings  $T_\alpha$  ( $\alpha \in A$ ) continuous is called the initial topology with respect to the mappings  $T_\alpha$ .

**Example 2.2.2.** 1. The product topology on a product of topological spaces  $\prod_{i \in I} E_i$  is the initial topology with respect to the elementary projectors  $p_j : \prod_{i \in I} E_i \rightarrow E_j$

2. The induced topology on a subset  $F$  of a set  $E$  is the initial topology with respect to the canonical embedding  $i : F \rightarrow E$ .

3. The weak topology on a locally convex vector space is nothing else but the initial topology with respect to the topological dual.

The following are some basic properties of the initial topology

**Proposition 2.2.2.** Let  $E$  have the initial topology with respect to the mappings  $T_\alpha : E \rightarrow E_\alpha$  ( $\alpha \in A$ ) and let  $S : F \rightarrow E$  be a mapping from a topological space  $F$  into  $E$ . Then  $S$  is continuous if and only if  $T_\alpha S : F \rightarrow E_\alpha$  is continuous for all  $\alpha \in A$ .

*Proof.* Suppose that every  $T_\alpha S : F \rightarrow E_\alpha$  is continuous and let  $O_i \subset E_i$  be an open subset. Then  $S^{-1}(T_i^{-1}(O_i))$  is open in  $F$  and thus the same thing for any finite intersection  $\cap_{i \in I} S^{-1}(T_i^{-1}(O_i)) = S^{-1}(\cap_{i \in I} T_i^{-1}(O_i))$ . Hence, by taking unions, reverse image of an open subset of  $E$  (which is necessarily of the form  $\cup_J \cap_{i \in I} T_i^{-1}(O_i)$ ) is an open subset of  $F$   $\square$

One can also prove the following

**Proposition 2.2.3.** Let  $(x_n)_n$  be a sequence of elements of  $E$ . Then  $x_n \rightarrow x \in E$  in  $(E, \tau_i)$  if and only if  $T_\alpha(x_n) \rightarrow T_\alpha(x)$  in  $(E_\alpha, \tau_\alpha)$  for each  $\alpha \in A$ .

Another interesting property is the following

**Proposition 2.2.4.** Let  $\{T_\alpha\}_{\alpha \in A}$  be a semi-group of operators on a topological space  $E$ . If  $F$  denotes the space  $E$  with the initial topology with respect to the mappings  $T_\alpha : E \rightarrow E$  ( $\alpha \in A$ ), then each  $T_\alpha$  induces a continuous mapping  $T_\alpha : F \rightarrow F$ .

*Proof.* A mapping  $T_\beta : F \rightarrow F$  is continuous if and only if  $T_\alpha T_\beta : F \rightarrow E$  is continuous, for all  $\alpha \in A$ . As  $T_\alpha T_\beta \in \{T_\gamma\}_{\gamma \in A}$ , so the conclusion follows from Proposition 2.2.2.  $\square$

**Remark 2.2.2.** Let  $E$  be a vector space and let  $\{\|\cdot\|_i\}_{i \in I}$  be a family of norms on  $E$ . The topology on  $E$  generated by the family  $\{\|\cdot\|_i\}_{i \in I}$  is the initial topology on  $E$  with respect to the family of mappings  $\varphi \mapsto \|\varphi\|_i$ , ( $i \in I$ ).

## 2.3 Unbounded operators in Hilbert space

### 2.3.1 Closed operators

Let  $\mathcal{H}$  be a Hilbert space. An unbounded operator  $A$  in  $\mathcal{H}$  is any linear map  $A : D(A) \rightarrow \mathcal{H}$  where  $D(A)$  is a subspace of  $\mathcal{H}$  called the domain of  $A$  and which is usually assumed to be dense in  $\mathcal{H}$ . In this case we say that  $A$  is densely defined.

Let  $A, B$  be densely defined operators in  $\mathcal{H}$ . If  $D(A) \subset D(B)$  and if for all  $\psi \in D(A)$  it holds  $B\psi = A\psi$ , then  $B$  is called an extension of  $A$  and we write  $A \subset B$ .

The graph of  $A$  is the linear space

$$\Gamma(A) = \{(\psi, A\psi) : \psi \in D(A)\} \subset \mathcal{H} \times \mathcal{H}$$

## 2.3. UNBOUNDED OPERATORS IN HILBERT SPACE

If  $\Gamma(A)$  is closed in  $\mathcal{H} \times \mathcal{H}$ , then  $A$  is called a closed operator. The operator  $A$  is said to be closable if there exists a linear operator  $\bar{A}$  in  $\mathcal{H}$  such that  $\Gamma(\bar{A}) = \overline{\Gamma(A)}$ . In this case,  $\bar{A}$  is called the closure of  $A$ . It is easy to see that  $A$  is closable if and only if for any sequence  $(\psi_n)_n \subseteq D(A)$  such that  $\lim_{n \rightarrow \infty} \psi_n = 0$  and  $\lim_{n \rightarrow \infty} A\psi_n \rightarrow \varphi$ , where  $\varphi \in \mathcal{H}$ , it follows that  $\varphi = 0$ . Moreover, the operator  $A$  is closable if and only if it has a closed extension  $B$ . In this case, we have  $\bar{A} \subseteq B$ .

Let  $A$  be a closed operator and  $D$  a subspace of  $D(A)$ . We say that  $D$  is a core of  $A$  if  $\overline{A|_D} = A$ .

### 2.3.2 Symmetry and self-adjointness

Let  $A$  be a densely defined linear operator. The adjoint operator  $A^*$  is defined by:

$$D(A^*) = \{\psi \in \mathcal{H} : \exists \delta \in \mathcal{H}, \forall \varphi \in D(A), \langle \psi, A\varphi \rangle = \langle \delta, \varphi \rangle\}$$

and

$$A^*\psi = \delta$$

It is straightforward that  $A^*$  is well defined and that it is a closed operator.

The operator  $A$  is said to be self-adjoint if  $A = A^*$ . It is said to be symmetric if

$$\langle \varphi, A\psi \rangle = \langle A\varphi, \psi \rangle, \forall \varphi, \psi \in D(A).$$

That is,  $A \subseteq A^*$ .

By Hellinger-Toeplitz theorem, an everywhere defined symmetric operator is necessarily bounded. The proof follows immediately from the closed graph theorem.

A symmetric linear operator  $A$  is said to be essentially self-adjoint if  $\bar{A}$  is self-adjoint. That is,  $A$  can be rendered self-adjoint in a unique manner by extending its domain in a natural way. Clearly, a self-adjoint operator is essentially self-adjoint, but the converse is not true.

Let  $A$  be a symmetric operator. The deficiency indices  $d_+$ ,  $d_-$  are defined by  $d_{\pm}(A) := \dim \text{Ker}(A^* \pm i)$  where we used the shorthand notation  $i$  to denote the operator  $iId_{\mathcal{H}}$ . The following criterion by von Neumann provides a sufficient condition for symmetric operators to admit self-adjoint extensions [36].

**Proposition 2.3.1.** *A symmetric operator  $A$  has a self-adjoint extension if and only if its deficiency indices are equal.*

In practice, it is usually much easier to check that a given operator is symmetric than to show that it is self-adjoint or essentially self-adjoint, since the latter questions involve additional domain considerations. Next we give a criterion which determines whether a symmetric operator is essentially self-adjoint

**Proposition 2.3.2.** *Let  $A$  be a symmetric linear operator. Then the following properties are equivalent*

- (1)  $A$  is essentially self-adjoint.
- (2)  $d_{\pm}(A) = 0$ .
- (3)  $\overline{\text{Ran}(A+i)} = \overline{\text{Ran}(A-i)} = \mathcal{H}$ .

Let  $\mu$  be a Borel measure on  $\mathbb{R}$  and denote by  $Q$  the multiplication operator in  $L^2(\mathbb{R}, d\mu)$  defined by  $Qf(x) := xf(x)$  for  $f \in D(Q) = \{f \in L^2(\mathbb{R}, d\mu) : xf \in L^2(\mathbb{R}, d\mu)\}$ .

**Theorem 2.3.1.** *The operator  $Q$  in  $L^2(\mathbb{R}, d\mu)$  is self-adjoint.*

*Proof.* Let  $f \in L^2(\mathbb{R}, d\mu)$ ,  $n \in \mathbb{N}$ . It follows from dominated convergence theorem that the sequence  $(\chi_{[-n,n]}f)_n \subset D(Q)$  converges to  $f$  in  $L^2(\mathbb{R}, d\mu)$  and thus  $Q$  is densely defined. On the other hand, the operator  $Q$  is clearly symmetric and thus  $D(Q) \subset D(Q^*)$ . Let  $f \in D(Q^*)$ . Then

$$\int_{\mathbb{R}} \overline{(Q^*f - xf)}g d\mu = 0, \quad \forall g \in D(Q). \quad (\star)$$

Now observe that for or all  $n \in \mathbb{N}$  we have  $\chi_{[-n,n]}(Q^*f - xf) \in D(Q)$ . Thus, using  $(\star)$  and the fact that  $\chi_{[-n,n]}(Q^*f - xf) \in D(Q)$  for all  $n \in \mathbb{N}$  (by local integrability), we see that  $Q^*f = xf$   $\mu$ -almost everywhere in  $[-n, n]$  for all  $n \in \mathbb{N}$  and therefore  $\mu$ -almost everywhere in  $\mathbb{R}$ . This implies that  $f \in D(Q)$  and hence the self-adjointness of  $Q$ .  $\square$

More generally, given a real-valued Borel function  $f$ , similar arguments show that, on its usual domain, the multiplication operator  $M_f$  is self-adjoint. Such a multiplication operator will simply be denoted by  $f$ .

Let  $A : D(A) \rightarrow \mathcal{H}$  be a self-adjoint (respectively essentially self-adjoint) operator. It is clear that any unitary equivalent operator to  $A$  is self-adjoint (respectively essentially self-adjoint). In particular, using the Fourier transform, we see that the momentum operator  $P = -\mathcal{F}Q\mathcal{F}^{-1}$  is self-adjoint in  $L^2(\mathbb{R}, dx)$ . In particular, recall that  $P|_{\mathcal{S}(\mathbb{R})} = -i\frac{d}{dx}$ . Similarly, we see that, on its maximal domain  $H^2(\mathbb{R})$ , the Laplacian  $\frac{d^2}{dx^2}$  is self-adjoint. We have the following general result on the self-adjointness of some Schrödinger operators [37].

**Theorem 2.3.2.** *Let  $v(x)$  be a continuous and bounded function on  $\mathbb{R}$  satisfying  $v(x) \geq 0$  and  $v(x) \rightarrow 0$  as  $|x| \rightarrow 0$ . Then, considered on the domain  $H^2(\mathbb{R})$ , the Schrödinger operator  $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v$  is self-adjoint.*

### 2.3.3 The spectrum

Let  $A$  be a closed operator. The spectrum of  $A$  is defined by

$$\sigma(A) := \{\lambda \in \mathbb{C} : A - \lambda : D(A) \rightarrow \mathcal{H} \text{ is not bijective}\}$$

The resolvent set of  $A$  is defined by  $\rho(A) := \mathbb{C} \setminus \sigma(A)$ . Remark that via the closed graph theorem, if  $\lambda \in \rho(A)$ , the operator  $(A - \lambda)^{-1} : \mathcal{H} \rightarrow D(A)$  is bounded. The function  $R_A : \rho(A) \rightarrow \mathcal{B}(\mathcal{H})$  defined by  $R_A(z) = (A - z)^{-1}$  is called the resolvent of  $A$ .

In the case of a self-adjoint operator  $A$ , it is well known that

$$\sigma(A) = \{\lambda \in \mathbb{C} : (A - \lambda)D(A) \neq \mathcal{H}\}$$

and that  $\sigma(A) \subset \mathbb{R}$ .

Finally, a self-adjoint operator  $A$  is said to be positive if it satisfies

$$\langle \psi, A\psi \rangle \geq 0, \quad \forall \psi \in D(A)$$

In this case we have  $\sigma(A) \subset \mathbb{R}^+$ .

**Definition 2.3.1.** *Let  $A$  be a closed operator in  $\mathcal{H}$ .*

1. *The point spectrum of  $A$  is the set of eigenvalues of  $A$ . That is*

$$\sigma_p(A) = \{\lambda \in \mathbb{C} : A - \lambda \text{ is not one to one}\}$$

2. *The continuous spectrum of  $A$  is defined by*

$$\sigma_c(A) = \{\lambda \in \mathbb{C} : \lambda \notin \sigma_p(A), \overline{(A - \lambda)D(A)} = \mathcal{H}, (A - \lambda)^{-1} \text{ is not bounded}\}$$

3. *The residual spectrum of  $A$  is defined by*

$$\sigma_r(A) = \{\lambda \in \mathbb{C} : \lambda \notin \sigma_p(A), \overline{(A - \lambda)D(A)} \neq \mathcal{H}\}$$

## 2.3. UNBOUNDED OPERATORS IN HILBERT SPACE

It is clear that all these spectrum components are invariant under unitary transformations. Next let  $f$  be a complex-valued Borel function on  $\mathbb{R}$ . It can be shown that the spectrum of the usual multiplication operator  $M_f$  coincides with the essential image  $\text{ess.im}(f)$  of the function  $f$ . Moreover, in the case where  $f$  is continuous, we have  $\sigma(M_f) = \sigma_c(M_f) = \text{ess.im}(f)$ . In particular we have  $\sigma(Q) = \sigma_c(Q) = \sigma(P) = \sigma_c(P) = \mathbb{R}$ . and  $\sigma(-\Delta) = \sigma_c(-\Delta) = [0, \infty)$ .

In case of a self-adjoint operator  $A$ , it can be inferred that  $\sigma_r(A) = \emptyset$  and that, for  $\lambda \in \mathbb{R}$ , we have  $\lambda \in \sigma(A)$  if and only if there exists a sequence  $(\psi_n)_n \subseteq D(A)$  of normalized vectors such that  $\lim_{n \rightarrow \infty} (A - \lambda)\psi_n \rightarrow 0$ .

### 2.3.4 The projection-valued measure spectral theorem

Denote by  $\mathcal{P}(\mathcal{H})$  the set of projections on  $\mathcal{H}$ . A map  $P : \mathcal{B}(\mathbb{R}) \rightarrow \mathcal{P}(\mathcal{H})$  is called a projection-valued measure (PVM) if the following properties are satisfied.

- (1)  $P(\mathbb{R}) = id_{\mathcal{H}}$ .
- (2) If  $\{\Omega_j\}_j$  is a finite or a countable collection of pairwise disjoint measurable sets in  $\mathcal{B}(\mathbb{R})$ , then

$$P(\cup \Omega_j)\psi = \sum P(\Omega_j)\psi, \quad \forall \psi \in \mathcal{H}.$$

Let  $P : \mathcal{B}(\mathbb{R}) \rightarrow \mathcal{P}(\mathcal{H})$  be a PVM. We have the following basic properties :

**Proposition 2.3.3.** *Let  $\Omega_1, \Omega_2 \in \mathcal{B}(\mathbb{R})$ . Then :*

1.  $P(\emptyset) = 0$  and  $P(\mathbb{R} \setminus \Omega_1) = id_{\mathcal{H}} - P(\Omega_1)$ .
2.  $P(\Omega_1 \cup \Omega_2) = P(\Omega_1) + P(\Omega_2) - P(\Omega_1 \cap \Omega_2)$ .
3.  $P(\Omega_1 \cap \Omega_2) = P(\Omega_1)P(\Omega_2)$ .
4.  $P(\Omega_1) \leq P(\Omega_2)$  if  $\Omega_1 \subset \Omega_2$ .

Given two vectors  $\psi, \varphi \in \mathcal{H}$ , we define a finite complex Borel measure by  $P_{\varphi, \psi}(\Omega) := \langle \varphi, P(\Omega)\psi \rangle$ . In particular, for every  $\psi \in \mathcal{H}$  we have a finite positive Borel measure  $P_\psi := P_{\psi, \psi}$ . Moreover,  $P_\psi$  is the unique finite positive Borel measure on  $\mathbb{R}$  that satisfies

$$\langle \psi, (A - z)^{-1}\psi \rangle = \int_{\sigma(A)} (\lambda - z)^{-1} dP_\psi^A, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Let  $f$  be a complex-valued measurable function. The set

$$D(f) = \{\psi \in \mathcal{H} : f \in L^2(\mathbb{R}, P_\psi)\}$$

is a dense subspace of  $\mathcal{H}$  on which we define an operator  $\int_{\mathbb{R}} f dP$  via the identity

$$\langle \psi, (\int_{\mathbb{R}} f dP)\psi \rangle = \int_{\mathbb{R}} f(\lambda) P_\psi(d\lambda)$$

In the case of a real-valued function  $f$ , the operator  $\int_{\mathbb{R}} f dP$  is self-adjoint. Next we state the projection-valued version of the spectral theorem.

**Theorem 2.3.3.** *Let  $A : D(A) \rightarrow \mathcal{H}$  be a self-adjoint linear operator in  $\mathcal{H}$ . Then there exists a unique projection-valued measure  $P^A : \mathcal{B}(\mathbb{R}) \rightarrow \mathcal{P}(\mathcal{H})$  such that*

$$A = \int_{\mathbb{R}} \lambda dP^A$$

Moreover,

$$D(A) = \{\psi \in \mathcal{H} : \int_{\mathbb{R}} \lambda^2 dP_\psi^A(\lambda) < \infty\}.$$

Let  $\lambda$  be a real number. One can check the following

**Proposition 2.3.4.** 1.  $\lambda \in \sigma(A)$  if and only if, for every  $\varepsilon > 0$ ,  $P^A([\lambda - \varepsilon, \lambda + \varepsilon]) \neq 0$ . In particular we have  $P^A(\sigma(A)) = id_{\mathcal{H}}$ .

2.  $\lambda \in \sigma_p(A)$  if and only if  $P^A(\{\lambda\}) \neq 0$ .

**Example 2.3.1.** The projection valued measure associated with the self-adjoint operator  $Q$  in  $L^2(\mathbb{R}, dx)$  is given by  $P^Q(\Omega)f = \chi_{\Omega}f$  for all  $\Omega \in \mathcal{B}(\mathbb{R})$  and  $f \in L^2(\mathbb{R}, dx)$ .

For a self-adjoint operator  $A$  in  $\mathcal{H}$  and  $f : \mathbb{R} \rightarrow \mathbb{C}$  a measurable function we put

$$f(A) := \int_{\mathbb{R}} f(\lambda) dP^A$$

Recall that a strongly continuous one-parameter unitary group is a group homomorphism

$$U : \mathbb{R} \rightarrow \mathcal{U}(\mathcal{H}), \quad t \mapsto U(t)$$

where  $\mathcal{U}(\mathcal{H})$  is the group of unitary operators on  $\mathcal{H}$  and such that the family  $(U(t))_{t \in \mathbb{R}}$  is strongly continuous (i.e., for each  $\psi \in \mathcal{H}$ , the map  $t \mapsto U(t)\psi$  is continuous). Its infinitesimal generator is the linear operator  $A$  in  $\mathcal{H}$  defined by

$$iA\psi = \lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi)$$

with domain  $D(A) = \{\psi \in \mathcal{H} : \lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi) \text{ exists}\}$

Let  $A$  be a self-adjoint operator and put  $U(t) = e^{itA}$ . Then one can show that  $(U(t))_{t \in \mathbb{R}}$  is a strongly continuous one-parameter unitary group with infinitesimal generator  $A$ . Moreover,

$$U(t)D(A) = D(A) \quad \text{and} \quad AU(t) = U(t)A, \quad \forall t \in \mathbb{R}.$$

Conversely, all strongly continuous one-parameter unitary groups are of this form.

**Theorem 2.3.4 (Stone).** Let  $\{U(t)\}_t$  be a strongly continuous one-parameter unitary group and let  $A$  be its infinitesimal generator. Then  $A$  is self-adjoint and  $U(t) = e^{itA}$ .

### 2.3.5 Orthogonal decompositions

Let  $\mathcal{H}_1$  and  $\mathcal{H}_2$  be two Hilbert spaces,  $A_1 : D(A_1) \subset \mathcal{H}_1 \rightarrow \mathcal{H}_1$  and  $A_2 : D(A_2) \subset \mathcal{H}_2 \rightarrow \mathcal{H}_2$  two densely defined operators. We denote by  $A_1 \oplus A_2$  the operator with domain  $D(A_1 \oplus A_2) = D(A_1) \oplus D(A_2)$  and whose action is given by

$$A_1 \oplus A_2(\psi, \varphi) := (A_1\psi, A_2\varphi)$$

Let  $A$  be a linear operator on a Hilbert space  $\mathcal{H}$  and let  $\mathcal{H}_0$  be a closed subspace of  $\mathcal{H}$ . We say that  $\mathcal{H}_0$  is invariant for  $A$  if  $A$  maps  $D(A_0) := D(A) \cap \mathcal{H}_0$  into  $\mathcal{H}_0$ . In this case the operator  $A_0 := A|_{D(A_0)}$  is called the part of  $A$  on  $\mathcal{H}_0$ . The subspace  $\mathcal{H}_0$  is said to be reducing for  $A$  if it is invariant and if moreover the orthogonal projector  $P_0$  onto the subspace  $\mathcal{H}_0$  maps the domain  $D(A)$  into itself. Thus a closed subspace  $\mathcal{H}_0$  is reducing for  $A$  if and only if it satisfies  $P_0\psi \in D(A)$  and  $AP_0\psi \in \mathcal{H}_0$  for all  $\psi \in D(A)$ . Both conditions can be expressed through the condition that  $AP_0$  is an extension of the operator  $P_0A$ . Moreover, if  $\mathcal{H}_0$  reduces  $A$ , then one can check easily that  $\mathcal{H}_0^\perp := \mathcal{H}_0^\perp$  reduces  $A$  as well.

Suppose that  $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$  with each  $\mathcal{H}_j$  reduces  $A$ . Then  $A = A_0 \oplus A_1$  where, for each  $\psi \in D(A)$ ,  $A_j\psi = AP_j\psi$  and  $D(A_j) = P_jD(A)$  (for  $j = 0, 1$ ). Moreover, if  $A$  is self-adjoint we have that  $A_0$  and  $A_1$  are self-adjoint too and, for every  $\Omega \in \mathcal{B}(\mathbb{R})$ , their respective spectral measures satisfy  $P^{A_j}(\Omega) = P^A(\Omega)|_{\mathcal{H}_j}$  (for  $j = 0, 1$ ). We also have in this case that  $R_A(z) = R_{A_0}(z) \oplus R_{A_1}(z)$  and  $\sigma(A) = \sigma(A_0) \cup \sigma(A_1)$ .

The construction above generalizes straightforwardly to the case of a finitely many Hilbert spaces  $(\mathcal{H}_j)_{j=1}^n$  and densely defined operators  $(A_j)_{j=1}^n$ . [36].

### 2.3. UNBOUNDED OPERATORS IN HILBERT SPACE

Let  $A : D(A) \subset \mathcal{H} \rightarrow \mathcal{H}$  be a self-adjoint operator. We define the following subspaces

$$\mathcal{H}_{ac} := \{\psi \in \mathcal{H} : P_\psi^A \text{ is absolutely continuous}\},$$

$$\mathcal{H}_{sc} := \{\psi \in \mathcal{H} : P_\psi^A \text{ is singularly continuous}\},$$

and

$$\mathcal{H}_{pp} := \{\psi \in \mathcal{H} : P_\psi^A \text{ is pure point}\}$$

Each of those subspaces is reducing for  $A$  and one can show the following orthogonal decomposition

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

The absolutely continuous, singularly continuous, and pure point spectrum of  $A$  are defined by

$$\sigma_{ac}(A) := \sigma(A|_{D(A) \cap \mathcal{H}_{ac}}), \quad \sigma_{sc}(A) := \sigma(A|_{D(A) \cap \mathcal{H}_{sc}}) \quad \text{and} \quad \sigma_{pp}(A) := \sigma(A|_{D(A) \cap \mathcal{H}_{pp}})$$

In the case where  $\sigma(A) = \sigma_{ac}(A)$  (resp.  $\sigma(A) = \sigma_{sc}(A)$ ) we say that  $A$  has an absolutely continuous (resp. singular) spectrum. One can easily check that if, for every  $\psi \in \mathcal{H}$ , the spectral measure  $P_\psi^A$  is absolutely continuous with respect to Lebesgue measure, then  $A$  has an absolutely continuous spectrum.

### 2.3.6 Cyclic vectors and spectral bases

#### Cyclic vectors

Let  $\psi \in \mathcal{H}$ , The subspace  $\mathcal{H}_\psi := \{f(A)\psi : f \in L^2(\mathbb{R}, P_\psi^A)\}$  is a closed subspace of  $\mathcal{H}$  called the cyclic subspace generated by  $\psi$ . We collect in the following some key properties of these subspaces.

**Proposition 2.3.5.** 1.  $\mathcal{H}_\psi = \overline{\text{span}\{P^A(\Omega)\psi : \Omega \in \mathcal{B}(\mathbb{R})\}}$ .

2.  $\mathcal{H}_\psi$  is a reducing subspace for  $A$ .

3. Let  $\mathcal{D}^\infty(A) := \bigcap_{n \in \mathbb{N}} D(A^n)$ . Then  $\text{span}\{A^n \psi : n \in \mathbb{N}\} \subset \mathcal{H}_\psi$ .

4.  $\varphi \perp \psi \Leftrightarrow \mathcal{H}_\varphi \perp \mathcal{H}_\psi$ .

5.  $\{f(A)\psi : f \text{ bounded}\}$  is dense in  $\mathcal{H}_\psi$ .

*Proof.* Let us prove (4) for example :

$\Leftarrow$ : Trivial.

$\Rightarrow$ : Let  $f$  be a bounded function. We have  $f(A)\psi \perp \mathcal{H}_\varphi$ . Indeed, for  $g \in L^2(P_\varphi^A)$ , we have that  $\langle f(A)\psi, g(A)\varphi \rangle = \langle \psi, (\bar{f}g(A))\varphi \rangle = 0$ . We conclude using the density of  $\{f(A)\psi : f \text{ bounded}\}$  in  $\mathcal{H}_\psi$ .  $\square$

**Theorem 2.3.5.** Let  $A$  be a self-adjoint operator and  $\psi \in \mathcal{H}$ . Then the map  $U_\psi : \mathcal{H}_\psi \rightarrow L^2(\mathbb{R}, P_\psi^A)$  defined by  $f(A)\psi \mapsto f$  is a unitary operator which satisfies

$$U_\psi A|_{D(A) \cap \mathcal{H}_\psi} U_\psi^* = Q$$

where  $Q$  is the usual multiplication operator in  $L^2(\mathbb{R}, P_\psi^A)$ .

A vector  $\psi \in \mathcal{H}$  is said to be a cyclic vector for  $A$  if  $\mathcal{H}_\psi = \mathcal{H}$ . In this case  $A$  is said to be cyclic and we have a full diagonalization of our operator in the sense that the unitary operator  $U_\psi : \mathcal{H} \rightarrow L^2(\mathbb{R}, P_\psi^A)$  above satisfies

$$U_\psi A U_\psi = Q$$

In particular, we see that, for a self-adjoint operator  $A$ , the operator  $A|_{\mathcal{H}_\psi}$  is cyclic.

Let  $\varphi \in L^2(\mathbb{R}, d\mu)$  and put  $\Lambda_\varphi = \text{span}\{P^Q(\Omega)\varphi : \Omega \in \mathcal{B}(\mathbb{R})\}$ . We have the following

**Proposition 2.3.6.** *The function  $\varphi$  is a cyclic vector for  $Q$  if and only if  $\mu(\{\varphi = 0\}) = 0$ .*

*Proof.* Let  $\varphi \in L^2(\mathbb{R}, d\mu)$ .

$\Rightarrow$ : Suppose that  $\varphi$  is a cyclic vector for  $Q$  and that  $\mu(\{\varphi = 0\}) > 0$ . Let  $(\varphi_n)_n$  be a sequence of elements in  $\Lambda_\varphi$  such that  $\varphi_n \rightarrow \chi_{\{\varphi=0\}}$  in  $L^2(\mathbb{R}, d\mu)$  and consider a subsequence  $(\varphi_{\alpha(n)})_n$  that converges  $\mu$ -almost everywhere to  $\chi_{\{\varphi=0\}}$ . Since  $\varphi_{\alpha(n)}$  vanishes on  $\{\varphi = 0\}$  we see that  $\chi_{\{\varphi=0\}}$  vanishes  $\mu$ -almost everywhere on  $\{\varphi = 0\}$ , which is not the case.

$\Leftarrow$ : Suppose that  $\mu(\{\varphi = 0\}) = 0$  and let  $f \in \Lambda_\varphi^\perp$ . Put  $\Omega^+ = \{f \geq 0\}$ . Then  $f$  vanishes on  $\Omega^+ \cap \{\varphi > 0\}$  and  $\Omega^+ \cap \{\varphi < 0\}$  and hence on  $\Omega^+$ . A similar argument shows that  $f$  vanishes on  $\Omega^-$  too and thus everywhere. This implies that  $\varphi$  is a cyclic vector for  $Q$ .  $\square$

**Remark 2.3.1.** 1. *It is not difficult to see that a cyclic vector for  $Q$  in  $L^2(\mathbb{R}, d\mu)$  is given by  $\psi(x) = \sum_{-\infty}^{+\infty} 2^{-|k|} \mu([k, k+1])^{-\frac{1}{2}} \chi_{[k, k+1]}(x)$ .*

2. *If  $\mu$  is a finite Borel measure, the constant function  $x \mapsto 1$  is a cyclic vector for  $Q$ . Indeed, using the notations above, the subspace  $\Lambda_1$  coincides with the subspace of simple functions, which is dense in  $L^2(\mathbb{R}, d\mu)$ .*

3. *For  $Q$  in  $L^2(\mathbb{R}, d\mu)$ , a scalar  $\lambda \in \mathbb{R}$  is an eigenvalue for  $Q$  if and only if  $\mu(\{\lambda\}) \neq 0$ . In this case  $\lambda$  has multiplicity one. In particular, we see that for a cyclic self-adjoint operator, each eigenvalue has multiplicity one.*

For a detailed study of cyclic operators see [38, p. 83].

### Spectral bases

A family  $(\psi_j)_{j \in J}$  of vectors of  $\mathcal{H}$  is said to be a spectral basis of  $\mathcal{H}$  associated to  $A$  if it satisfies the following conditions

1.  $\|\psi_j\| = 1, \forall j \in J$
2.  $\forall i, j \in J, i \neq j \Rightarrow \mathcal{H}_{\psi_i} \perp \mathcal{H}_{\psi_j}$
3.  $\mathcal{H} = \bigoplus_{j \in J} \mathcal{H}_{\psi_j}$

**Theorem 2.3.6.** *Let  $A$  be a self-adjoint operator in a separable Hilbert space  $\mathcal{H}$ . Then  $A$  admits a spectral basis  $(\psi_j)_{j \in J}$  where the index set  $J$  is at most countable.*

*Proof.* See [36].  $\square$

In contradistinction to ordinary bases of the Hilbert space  $\mathcal{H}$ , two spectral bases of  $\mathcal{H}$  may have different cardinalities [36]. However, the cardinality of a spectral basis is at most equal to the cardinality of an ordinary Hilbert basis.

**Theorem 2.3.7.** *(The multiplication spectral theorem) Let  $A$  be a self-adjoint operator in a separable Hilbert space  $\mathcal{H}$ . Then there exists a spectral basis  $(\psi_j)_{j \in J}$  associated to  $A$  and a corresponding unitary operator*

$$U = \bigoplus_n U_{\psi_n} : \mathcal{H} \rightarrow \bigoplus_n L^2(\mathbb{R}, P_{\psi_n}^A)$$

such that

$$UAU^* = Q$$

where  $Q$  is the usual multiplication operator.

### 2.3. UNBOUNDED OPERATORS IN HILBERT SPACE

#### Analyticity and Nelson theorem

Let  $A$  be a cyclic self-adjoint operator. A vector  $\psi \in D^\infty(A)$  is said to be an analytic vector for  $A$  if

$$\sum_{n=0}^{\infty} \frac{\|A^n \psi\|}{n!} t^n < \infty \text{ for some } t > 0.$$

We denote by  $D^a(A)$  the set of analytic vectors of  $A$ .

The following theorem proves self-adjointness by means of growth estimates of  $\|A^n \psi\|$ .

**Theorem 2.3.8.** (Nelson's theorem) *Let  $A$  be a symmetric operator on  $\mathcal{H}$ . If the space  $D^a(A)$  of analytic vectors is dense, then  $A$  is essentially self-adjoint. If moreover  $A$  is closed, then  $A$  is self-adjoint if and only if  $\overline{D^a(A)} = \mathcal{H}$ .*

**Proposition 2.3.7.** *Let  $A$  be a cyclic self-adjoint operator,  $\psi \in \mathcal{H}$  and  $\alpha > 0$ . Then  $e^{-\alpha A^2} \psi$  is an analytic vector for  $A$ .*

*Proof.* see [39]. □

**Proposition 2.3.8.** *Let  $A$  be a closed symmetric operator on  $\mathcal{H}$ . Let  $D_0$  be a dense subspace of a closed subspace  $\mathcal{H}_0$  of  $\mathcal{H}$  such that  $D_0 \subset D(A)$ ,  $AD_0 \subset \mathcal{H}_0$  and let  $P_0$  denotes the orthogonal projection onto  $\mathcal{H}_0$ . Suppose moreover that  $A_0 := A|_{D_0}$  is essentially self-adjoint on  $\mathcal{H}_0$ . Then  $\mathcal{H}_0$  is a reducing subspace for  $A$  and  $A_0$  is the part of  $A$  on  $\mathcal{H}_0$ .*

We have the following result [39] :

**Theorem 2.3.9.** *Let  $A$  be a cyclic self-adjoint operator and  $\psi$  a cyclic vector. Then  $e^{-A^2} \psi$  is a cyclic vector of  $A$  which belongs to  $D^\infty(A)$ .*

*Proof.* Put  $\varphi = e^{-A^2} \psi$ . Observe that by the results above,  $\varphi$  is an analytic vector for  $A$ . Next put  $D_0 = \text{span}\{A^n \varphi : n \in \mathbb{N}\}$ ,  $\mathcal{H}_0 = \overline{D_0}$  and set  $P_n(t) = \sum_{k=0}^n \frac{t^{2k}}{k!}$  and  $f_n(t) = P_n(t)e^{-t^2}$ . Then  $f_n(t)$  converges monotonically to 1 on  $\mathbb{R}$ . Therefore, using functional calculus properties, we have that  $f_n(A)\psi = P_n(A)\varphi$  converges to  $\psi$  and hence  $\psi \in \mathcal{H}_0$ . On the other hand, as a restriction of a symmetric operator,  $A_0 := A|_{D_0}$  is a symmetric operator on  $\mathcal{H}_0$  and which satisfies  $A_0 D_0 \subset D_0$ . Remark that by construction we have  $D_0 \subset D^a(A)$  and hence  $D_0 = D^a(A_0)$ . Since  $\overline{A_0}$  has a dense subset of analytic vectors,  $\overline{A_0}$  is self-adjoint via Nelson's theorem and thus  $A$  decomposes as  $A = \overline{A_0} \oplus A_1$  with respect to the orthogonal direct sum  $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_0^\perp$ . In particular we have

$$P^{\overline{A_0}}(\Omega) = P^A(\Omega)|_{\mathcal{H}_0}, \quad \forall \Omega \in \mathcal{B}(\mathbb{R})$$

Now since  $\psi \in \mathcal{H}_0$ , we get  $P^A(\Omega)\psi = P^{\overline{A_0}}(\Omega)\psi \in \mathcal{H}_0$  and hence, using the fact that  $\psi$  is a cyclic vector for  $A$ , the span of vectors  $P^A(\Omega)\psi$  is dense in  $\mathcal{H}$ . Hence  $\mathcal{H} \subset \mathcal{H}_0$  and therefore  $\mathcal{H} = \mathcal{H}_0$ . In particular  $\varphi$  is a cyclic vector as desired. □

**Theorem 2.3.10.** *A self-adjoint operator  $A$  always admits a spectral basis  $(\varphi_n)_n$  formed by vectors of  $D^\infty(A)$ .*

*Proof.* Let  $(\psi_n)_n$  be a spectral basis associated to  $A$ . For every restriction  $A|_{\mathcal{H}_{\psi_n}}$ , one can pick a vector  $\varphi_n \in D^\infty(A) \cap \mathcal{H}_{\psi_n}$  such that  $\mathcal{H}_{\psi_n} = \overline{\text{span}\{A^k \varphi_n : k \in \mathbb{N}\}}$ . The family  $(\varphi_n)_n \subseteq D^\infty(A)$  is a spectral basis of  $A$ . Indeed : we have  $\varphi_n \in \mathcal{H}_{\psi_n}$  and the subspaces  $\mathcal{H}_{\psi_n}$  are pairwise orthogonal, so that the subspaces  $\mathcal{H}_{\varphi_n}$  are also pairwise orthogonal. On the other hand we have  $\mathcal{H}_{\psi_n} = \overline{\text{span}\{A^k \varphi_n\}} \subset \mathcal{H}_{\varphi_n}$  and which gives  $\mathcal{H} = \bigoplus_n \mathcal{H}_{\psi_n} \subset \bigoplus_n \mathcal{H}_{\varphi_n}$ . Remark that one can normalize the vectors  $\varphi_n$  if needed (since for every  $\psi \in \mathcal{H}$ , one has  $\mathcal{H}_\alpha \psi = \mathcal{H}_\psi$ ,  $\forall \alpha \neq 0$ ). □

### 2.3.7 The direct integral spectral theorem

The concept of direct integral of Hilbert spaces extends that of a direct sum of a countably many Hilbert spaces by relaxing the assumption of a countable number of terms. Consider a set  $X$  on which is defined a positive measure and suppose that to each point  $x \in X$  is associated a separable Hilbert space  $\mathcal{H}_x$  of dimension  $n(x) \in \mathbb{N}^* \cup \infty$ . Suppose moreover that the map  $x \mapsto n(x)$  is measurable with respect to the measure  $\mu$ .

Consider first the particular case where all the spaces  $\mathcal{H}_x$  have the same dimension and thus can be identified to a single Hilbert space  $\mathcal{H}$ . Denote by  $\mathbf{h}$  the space of equivalent classes (with respect to the equivalence relation of being equal  $\mu$ -almost everywhere on  $X$ ) of vector-valued functions  $h : x \in X \mapsto h(x) \in \mathcal{H}$  such that

1. for each  $h \in \mathcal{H}$ , the numerical function  $x \mapsto \langle h(x), h \rangle$  is measurable with respect to  $\mu$ .
2. The numerical function  $x \mapsto \|h(x)\|^2$  is square integrable with respect to  $\mu$ .

On the space  $\mathbf{h}$  we introduce a scalar product by setting [8, p. 115]

$$\langle h(x), g(x) \rangle_{\mathbf{h}} = \int_X \langle h(x), g(x) \rangle d\mu(x).$$

Equipped with the scalar product  $\langle \cdot, \cdot \rangle_{\mathbf{h}}$ , The space  $\mathbf{h}$  is a Hilbert space called the direct integral of the Hilbert spaces  $\mathcal{H}_x$  with respect to the measure  $\mu$  and it is denoted by  $\int_X^{\oplus} \mathcal{H}_x d\mu(x)$ .

Now for the general case, for each  $n \in \mathbb{N}^+ \cup \{\infty\}$ , put  $X_n := \{x \in X : \dim(\mathcal{H}_x) = n\}$ ,  $\mathbf{h}_n := \int_{X_n}^{\oplus} \mathcal{H}_x d\mu(x)$  and denote by  $\mathbf{h}$  the orthogonal direct sum of the Hilbert spaces  $\mathbf{h}_n$

$$\mathbf{h} := \bigoplus_{n=1}^{\infty} \mathbf{h}_n.$$

**Definition 2.3.2.** *The Hilbert space  $\mathbf{h}$  is called the direct integral of the Hilbert spaces  $\mathcal{H}_x$  with respect to the measure  $\mu$  and it is denoted by  $\int_X^{\oplus} \mathcal{H}_x d\mu(x)$ .*

**Remark 2.3.2.** *In the particular case where  $\mathcal{H}_x = \mathbb{C}$  for every  $x \in X$ , the obtained direct integral coincides with  $L^2(X, d\mu)$ . Remark also that if for every  $x, x' \in X$  we have  $\mathcal{H}_x = \mathcal{H}_{x'} \equiv \mathcal{H}$ , the obtained direct integral of the  $\mathcal{H}_x$ 's is nothing else but the space  $L^2(X, \mathcal{H}, d\mu)$  of square integrable  $\mathcal{H}$ -valued functions on  $X$ . The general direct integral is an extension of this that allows the Hilbert space to depend on the point  $x \in X$ . In this sense, a direct integral can be taught of as a more general version of a usual  $L^2$  space.*

Next we recall some details from the construction of such a direct integral representation [8, p. 130] and some notations :

Let  $\{\varphi^j\}_{j \in J}$  be a spectral basis of  $\mathcal{H}$  associated to  $A$ . By virtue of Theorem 2.3.10, we may suppose that  $\mathcal{H} = \bigoplus_j \mathcal{H}_j$ , where  $\mathcal{H}_j = \overline{\text{span}\{A^k \varphi^j\}}$ . Consider the representation  $\mathcal{H} \cong \bigoplus_{j \in J} L^2(\sigma(A), P_{\varphi^j}^A)$  associated to  $A$  and, for every Borel set  $\Omega$ , put  $\mu(\Omega) = \sum \frac{1}{2^j} P_{\varphi^j}^A(\Omega)$ . One can check that  $\mu$  is a well-defined positive measure on  $\sigma(A)$  and that for each  $j \in J$  we have  $P_{\varphi^j}^A \ll \mu$ . Moreover, we have  $\mathcal{H}_j \cong L^2(X_j, d\mu)$  where  $X_j \subset \sigma(A)$ . In particular  $\mathcal{H} \cong \bigoplus_{j \in J} L^2(X_j, d\mu)$ . For every  $x \in \sigma(A)$ , denote by  $n(x)$  the cardinality of  $J_x := \{j \in J : x \in X_j\}$ . Then  $n(x) \in \mathbb{N} \cup \{\infty\}$ . For every  $j \in J$ , denote by  $U^j : \mathcal{H}_j \rightarrow L^2(X_j, d\mu)$  the unitary map satisfying  $U^j(A^k \varphi^j) = x^k \varphi^j(x)$  and put  $\mathcal{H}_x = \{(U^{i_1} \psi_{i_1})(x), \dots, (U^{i_{n(x)}} \psi_{i_{n(x)}})(x)\}$ , where  $i_1 < i_2 < \dots < i_{n(x)}$  and  $\psi_j(\cdot) \in L^2(X_j, d\mu)$ . The map  $\hat{U} : \mathcal{H} \mapsto \int_{\sigma(A)} \mathcal{H}_x d\mu(x)$  defined by  $\psi \mapsto \xi_{\psi}$  where  $\xi_{\psi} : \sigma(A) \rightarrow \bigcup_{x \in \sigma(A)} \mathcal{H}_x$  is defined by  $x \mapsto (\psi_{i_1}(x), \dots, \psi_{i_{n(x)}}(x)) \in \mathcal{H}_x$ , is a unitary operator that sends  $A$  to the multiplication operator in  $\int_{\sigma(A)}^{\oplus} \mathcal{H}_x d\mu(x)$ . See [8, p. 133] for more details.

**Theorem 2.3.11.** *(The spectral theorem (Direct integral form)) Let  $A$  be a self-adjoint operator in  $\mathcal{H}$ . Then there exists a positive measure  $\mu$  on  $\sigma(A)$ , a direct integral*

$$\int_{\sigma(A)}^{\oplus} \mathcal{H}_x d\mu(x)$$

## 2.3. UNBOUNDED OPERATORS IN HILBERT SPACE

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and a unitary map

$$U : \mathcal{H} \rightarrow \int_{\sigma(A)}^{\oplus} \mathcal{H}_x d\mu(x)$$

, such that

$$(UAU^*(h))(x) = xh(x), \forall h \in U(D(A)).$$

### 2.3.8 The Stone-von Neumann uniqueness theorem

Let  $\mathcal{H}$  be a Hilbert space and  $A$  and  $B$  two self-adjoint operators in  $\mathcal{H}$ . If there is a common, dense and invariant subdomain  $\mathcal{D} \subset D(A) \cap D(B)$  on which it holds

$$[A, B] := AB - BA = -i1,$$

the operators  $A$  and  $B$  are said to satisfy the canonical commutation relation (CCR).

It is well-known that there is no realization of the canonical commutation relation by bounded operators. On the other hand, remark that for the usual position and momentum operators in the Schrödinger representation  $L^2(\mathbb{R}, dx)$ , on the Schwartz space  $\mathcal{S}(\mathbb{R})$  for example, one has

$$[P, Q] = -i\hbar 1.$$

We are asking about possible realizations of the canonical commutation relation. Using the spectral theorem, we associate to the position operators  $Q$  and the momentum operators  $P$  in the Schrödinger representation the following unitary operators

$$U(t) = e^{itQ} \quad V(t) = e^{itP}. \quad (\star)$$

That is

$$U(t)\psi(x) = e^{itx}\psi(x) \quad V(t)\psi(x) = \psi(x+t), \quad \forall \psi \in L^2(\mathbb{R}, dx).$$

Then  $(U(t))_{t \in \mathbb{R}}$  and  $(V(t))_{t \in \mathbb{R}}$  are strongly continuous one-parameter unitary groups on  $\mathcal{H}$ . These are known as the associated Weyl operators. One can also deduce the so-called Weyl form of the canonical commutation relations (or Weyl relations)

$$[U(s), U(t)] = [V(s), V(t)] = 0, \quad U(s)V(t) = e^{ist}V(t)U(s)$$

for all  $s, t \in \mathbb{R}$ .

Let us mention that the Weyl relations imply the CCR, but the opposite is not true [40, p. 275].

A pair  $(U(t), V(s))_{t, s \in \mathbb{R}}$  of strongly continuous one-parameter unitary groups on  $\mathcal{H}$  that satisfy the relation above is called a representation of the Weyl relations. The above cited representation  $(\star)$  of Weyl relations is called the Schrödinger representation.

We say that a family of unitary operators  $\mathcal{A}$  acts irreducibly on  $\mathcal{H}$  if every nonzero closed subspace of  $\mathcal{H}$  which is invariant under  $\mathcal{A}$  is equal to  $\mathcal{H}$ . We have the following

**Proposition 2.3.9.** *The Schrödinger representation of the Weyl relations on the Hilbert space  $L^2(\mathbb{R}, dx)$  is irreducible.*

The importance of the Schrödinger representation is highlighted by the well-known Stone-von Neumann theorem.

**Theorem 2.3.12.** *(Stone-von Neumann)*

*Any irreducible representation of the Weyl relation is unitarily equivalent to the Schrödinger representation.*

## 2.4 Basics on Sturm-Liouville differential equations

### 2.4.1 Basic existence and uniqueness results

Let  $I = (a, b)$  be an interval of  $\mathbb{R}$ ,  $v(x) \in L^1_{loc}(I, dx)$  and consider the following differential operator  $\tau y = -y'' + v(x)y$  on  $AC^2(I)$ . The left endpoint  $a$  is said to be regular if it is finite and if  $x \mapsto v(x)$  is summable on every interval of the form  $[a, \beta]$ . Otherwise it is said to be singular. We define the regularity and singularity for the right endpoint in a similar way. The differential operator  $\tau$  is said to be regular if both endpoints are regular.

For a given function  $f$ , a solution  $y$  of  $\tau y = f$  is supposed to be an element of  $AC^2(a, b)$ .

Consider on  $I$  a linear system of differential equations

$$Y' = A(x)Y + f(x), \quad (E)$$

where  $Y = (y_1(x), \dots, y_N(x))$ ,  $A(x) = (a_{i,j}(x))_{1 \leq i, j \leq N}$  and  $f(x) = (f_1(x), \dots, f_N(x))$ . We suppose that  $x \mapsto A(x)$  and  $x \mapsto f(x)$  are locally integrable on  $I$ .

A solution of (E) is by definition an absolutely continuous function  $Y : (a, b) \rightarrow \mathbb{C}^N$  satisfying (E).

We recall the fundamental theorem on existence and uniqueness. We provide a sketch of proof for completeness.

**Theorem 2.4.1.** *Let  $x_0 \in I$  and  $Y_0$  be an arbitrary vector in  $\mathbb{C}^n$ . The initial value problem*

$$(P) \quad \begin{cases} Y'(x) = A(x)Y(x) + f(x) \\ Y(x_0) = Y_0 \end{cases}$$

*has a unique solution on  $I$ .*

*Proof.* It is clear that an absolutely continuous function  $Y : I \rightarrow \mathbb{C}^n$  is a solution of (P) if and only if it is a solution of the following integral equation

$$Y = Y_0 + \int_{x_0}^x [A(t)Y(t) + f(t)] dt., \quad (F)$$

To construct a solution of (F), we use the well-known method of successive approximations:

Consider the sequence  $(Y_n(x))_n$  of (vector-valued) functions defined by

$$Y_0(x) = Y_0, \quad Y_n(x) = Y_0 + \int_{x_0}^x A(t)Y_{n-1}(t) dt.$$

One can check that the sequence of functions  $(Y_n(x))_n$  converges uniformly to a limit function  $Y(x)$  in every compact interval of  $I$ . Such a limit function is then clearly a solution of (F). Hence the existence part of the theorem.

The uniqueness of the solution is easy to see using the integral equation (F). □

We get the following existence and uniqueness result.

**Theorem 2.4.2.** *Let  $f$  be in  $L^1_{loc}(I)$  and  $x_0 \in I$ . Then for every  $\alpha, \beta \in \mathbb{C}$ , the equation  $\tau y = f$  has in the interval  $I$  a unique solution  $y(x)$  which satisfies the conditions  $y(x_0) = \alpha$ ,  $y'(x_0) = \beta$ .*

*Proof.* Denote the following

$$Y = (y, y'), \quad \bar{f} = (0, f), \quad Y_0 = (\alpha, \beta), \quad A(x) = \begin{bmatrix} 0 & 1 \\ v(x) & 0 \end{bmatrix}.$$

We then have that  $\tau y = f$  is equivalent to  $Y' = A(x)Y + \bar{f}$ . The functions  $x \mapsto A(x)$  and  $x \mapsto \bar{f}(x)$  do satisfy the conditions in the above theorem. Therefore the equation  $\tau y = f$  has in  $I$  one and only one solution  $y(x)$  satisfying the initial condition

$$y(x_0) = \alpha, \quad y'(x_0) = \beta. \quad \square$$

## 2.4. BASICS ON STURM-LIOUVILLE DIFFERENTIAL EQUATIONS

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Let  $c, d \in I$  and  $f, g \in AC^2(I)$ . A twice integration by parts gives the so-called Lagrange identity

$$\int_c^d [g(x)(\tau f)(x) - f(x)(\tau g)(x)] dx = W(f, g)(d) - W(f, g)(c), \quad (\star),$$

where

$$W(f, g)(x) = (fg' - f'g)(x)$$

is the Wronskian.

It is an absolutely continuous function with derivative

$$W(f, g)(x)' = g(x)(\tau f)(x) - f(x)(\tau g)(x), \quad x \in I.$$

In particular we see that two solutions  $y_1$  and  $y_2$  of the homogenous equation  $\tau y = 0$  are linearly independent if and only if their Wronkian vanishes in the interval  $I$ . Moreover, for two solutions  $y_1$  and  $y_2$  of  $\tau y = 0$ ,  $W(y_1, y_2)$  is constant. It is then denoted by  $W(y_1, y_2)$  from now on.

We thus at least have two linearly independent solutions  $y_1$  and  $y_2$  of  $\tau y = 0$ . Indeed, it suffices to take  $(\alpha, \beta) \neq (\alpha', \beta')$  in the existence theorem above. A linearly independent system of solutions  $\{y_1, y_2\}$  is called a fundamental system for the equation  $\tau y = 0$ .

**Theorem 2.4.3.** *The linear space of solutions of  $\tau y = 0$  is two-dimensional.*

*Proof.* Let  $\{y_1, y_2\}$  be a fundamental system for the equation  $\tau y = 0$  and let  $y$  be a solution. Let  $c_1, c_2 \in \mathbb{C}$  such that, at a point  $x_0 \in (a, b)$ , we have

$$(S) \begin{cases} y(x_0) = c_1 y_1(x_0) + c_2 y_2(x_0) \\ y'(x_0) = c_1 y_1'(x_0) + c_2 y_2'(x_0) \end{cases}$$

This is possible since the determinant of the above system is not zero.

The system (S) implies that the functions  $y$  and  $c_1 y_1 + c_2 y_2$  are solutions of  $\tau y = 0$  and that they satisfy the same initial conditions. Hence, since such a solution is unique, we necessarily have  $y \equiv c_1 y_1 + c_2 y_2$ .  $\square$

Now for the inhomogenous case, let  $\{y_1, y_2\}$  be a fundamental system of solution of the homogeneous equation  $\tau y = 0$ . Let

$$y(x) = c_1(x)y_1(x) + c_2(x)y_2(x)$$

with  $c_1(x), c_2(x)$  satisfying the equation

$$c_1'(x)y_1(x) + c_2'(x)y_2(x) = 0.$$

For each fixed  $x \in (a, b)$ , we hence get the system

$$\begin{cases} c_1'(x)y_1(x) + c_2'(x)y_2(x) = 0 \\ c_1'(x)y_1'(x) + c_2'(x)y_2'(x) = f(x) \end{cases}$$

Solving for  $c_1'(x)$  and  $c_2'(x)$  gives us the following result

**Theorem 2.4.4.** *The general solution of the equation  $\tau y = f$  has the form*

$$y(x) = [\alpha - \int_{x_0}^x \frac{y_2(t)}{W(y_1, y_2)} f(t) dt] y_1(x) + [\beta + \int_{x_0}^x \frac{y_1(t)}{W(y_1, y_2)} f(t) dt] y_2(x)$$

where  $\{y_1, y_2\}$  is a fundamental system of solutions of  $\tau y = f$  and  $\alpha, \beta \in \mathbb{C}$  are arbitrary constants.

We say that a function  $f : (a, b) \rightarrow \mathbb{C}$  is  $L^2$  near  $a$  if it is square integrable on  $(a, c)$  for some  $c \in (a, b)$ . Similarly we say that  $f$  is  $L^2$  near  $b$  if it is square integrable on  $(c, b)$  for some  $c \in (a, b)$ . If  $\tau$  is regular at  $a$  and  $f$  is  $L^2$  near  $a$ , then we can chose  $x_0 = a$ .

**Definition 2.4.1.** The differential operator  $\tau$  is said to be in the limit circle case (l.c.c.) at  $a$  if for all  $z \in \mathbb{C}$ , all the solutions of  $(\tau - z)y = 0$  are  $L^2$  near  $a$ . Otherwise it is said to be limit point (l.p.c.) at  $a$ . Similarly for the endpoint  $b$ .

**Proposition 2.4.1.** (Weyl alternative) At each of the endpoints,  $\tau$  is on the l.c. case if and only if for one  $z_0 \in \mathbb{C}$  all solutions of  $(\tau - z_0)y = 0$  are  $L^2$  near that endpoint.

Thus, if  $\tau$  is regular at some endpoint, it is limit circle at this endpoint. Indeed, in this case each solution of  $(\tau - z_0)y = 0$  has a continuous extension to this endpoint [41, p. 90] :

**Lemma 2.4.1.** Let  $\tau$  be regular at  $a$ ,  $z \in \mathbb{C}$  and  $g$  summable on  $(a, c)$  for every  $c \in (a, b)$ . Then for every solution  $f$  of  $(\tau - z)f = g$ , The limits  $\lim_{x \rightarrow a^+} f(x)$  and  $\lim_{x \rightarrow a^+} f'(x)$  exist and are finite.

## 2.4.2 The resolvent as an integral operator

Let  $I = (0, \infty)$  and denote by  $A_{max}$  the restriction of  $\tau$  to the following domain

$$\mathcal{D}_{max} = \{f \in L^2(I, dx) : f, f' \in AC(I), \tau f \in L^2(I, dx)\}$$

Denote by  $A_c$  the symmetric operator given by the restriction of  $A_{max}$  to compactly supported functions of  $\mathcal{D}_{max}$ . One can check that  $A_{min} := \overline{A_c}$  is a symmetric operator that satisfies  $A_{min}^* = A_{max}$  and that, if  $A$  is a self-adjoint extension of  $A_{min}$ , we have  $A_{min} \subset A \subset A_{max}$ . Suppose moreover that 0 is a regular endpoint and that  $\tau$  is in the limit point case at  $\infty$ . In this case  $A_{min}$  has deficiency indices  $(1, 1)$  or  $(2, 2)$  and its self-adjoint extensions are given by the one parameter family  $(A_\alpha)_{\alpha \in [0, \pi)}$  of the restrictions of  $A_{max}$  to the domains

$$D_\alpha := \{f \in \mathcal{D}_{max} : f(0)\cos(\alpha) - f'(0)\sin(\alpha) = 0\}$$

See [42, p.137].

Denote by  $A$  the self-adjoint extension of  $A_{min}$  given by the Dirichlet boundary condition, i.e.  $A = A_0$ . We have the following result expressing the resolvent of  $A$  as an integral operator [36].

**Theorem 2.4.5.** Let  $z \in \rho(A)$  and  $g \in L^2(0, \infty)$ . Then there exists a solution  $y_0$  of  $\tau y = zy$  which is  $L^2$  near 0 and satisfying the Dirichlet boundary condition  $y_0(0) = 0$  and there exists  $y_\infty$  a solution of  $\tau y = zy$  which is  $L^2$  near  $\infty$ . The resolvent of  $A$  is given by

$$(A - z)^{-1}g(x) = \int_0^\infty G(z, x, y)g(y)dy$$

where

$$G(z, x, y) = \frac{1}{W(y_0, y_\infty)} \begin{cases} y_\infty(z, x)y_0(z, y), & x \geq y \\ y_0(z, x)y_\infty(z, y), & x \leq y \end{cases}$$

*Proof.* Given  $g$  supported in some  $[c, d] \subset (0, \infty)$  and  $\{y_1, y_2\}$  a fundamental system of solutions of the equation  $(\tau - z)y = 0$ , we put  $f = (A - z)^{-1}g$ . We then have  $(\tau - z)f = g$  and thus  $f$  is of the form

$$f = y_1[\alpha + \int_0^x \frac{y_2}{W(y_1, y_2)}g] + y_2[\beta + \int_x^\infty \frac{y_1}{W(y_1, y_2)}g]$$

for some  $\alpha, \beta \in \mathbb{C}$ .

Thus, near 0, we have  $f = \alpha y_1 + \tilde{\beta} y_2$  and near  $\infty$  we have  $f = \tilde{\alpha} y_1 + \beta y_2$  where  $\tilde{\alpha} = \alpha + \int_0^\infty y_2 g$  and  $\tilde{\beta} = \beta + \int_0^\infty y_1 g$ . Now suppose that  $f$  vanishes identically both near 0 and near  $\infty$ . We then necessarily have  $\alpha = \beta = \tilde{\alpha} = \tilde{\beta} = 0$ . In particular we have  $\lambda_i := \int_0^\infty y_i(t)g(t)dt = 0$  for  $i = 1, 2$ . So if  $g$  is chosen so that  $(\lambda_1, \lambda_2) \neq (0, 0)$ , the function  $f$  is not vanishing identically at least near one endpoint and thus we get either  $y_\infty$  or  $y_0$  by putting it equal to  $f$  near to that endpoint and then extending it using the differential equation. Suppose we get  $y_\infty$ . (i.e. a non-trivial solution of  $(\tau - z)u = 0$  which is  $L^2$  near  $\infty$ ). Now choose  $y_1 = y_\infty$  and consider the behavior near  $\infty$  : if

## 2.5. THE RIGGED HILBERT SPACE STRUCTURE

$y_2$  is not  $L^2$  near  $\infty$ , since  $\beta y_2 = f - \tilde{\alpha} y_\infty$  is  $L^2$  near  $\infty$ , we must have  $\beta = 0$ . If  $y_2$  is  $L^2$  near  $\infty$ , we get that  $\tau$  is l.c. at  $\infty$  and  $0 = \lim_{\infty} W(y_\infty, f)(x) = \lim_{\infty} W(y_\infty, \tilde{\alpha} y_\infty + \beta y_2)(x) = \beta W(y_\infty, y_2)$ . Thus  $\beta = 0$  in both cases and we have

$$f(x) = y_\infty \left[ \alpha + \int_0^x y_2 g \right] + y_2 \int_x^\infty y_\infty g$$

Hence, near 0, we get  $f = \alpha y_\infty + \tilde{\beta} y_2$ . If  $f$  vanishes identically near  $a$  we get in particular that  $\tilde{\beta} = \int_0^\infty y_\infty g = 0$ . Thus, by choosing  $g$  such that  $\int_0^\infty y_\infty g \neq 0$ , we necessarily have that  $f$  is not identically zero near 0 and thus we can get  $y_0$ . Now, choosing  $y_2 = y_0$  and considering the behavior near 0, by a similar reasoning we infer that  $\alpha = 0$  and thus, for any compactly supported  $g$ , we have

$$(A - z)^{-1} g(x) = f(x) = y_\infty \int_0^x y_0 g + y_0 \int_x^\infty y_\infty g = \int_0^\infty G(x, y) g(y) dy$$

where  $G$  is of the form above. Since  $L^2_{loc}(0, \infty)$  is dense in  $L^2(0, \infty)$  and by the  $L^2$ -continuity of the resolvent operator we have the result  $\square$

Let  $\mathcal{H}$  be a Hilbert space and  $T$  a cyclic self-adjoint operator on  $\mathcal{H}$ . Recall that by the multiplicative spectral theorem, there exists a finite Borel measure  $\mu$  on  $\mathbb{R}$  and a unitary operator  $U : \mathcal{H} \rightarrow L^2(\mathbb{R}, d\mu)$  such that  $U$  transforms  $T$  to the usual multiplication operator  $Q$  in  $L^2(\mathbb{R}, d\mu)$ .

Suppose in the following that the potential function  $x \mapsto v(x)$  is so that  $A$  is a cyclic self-adjoint operator. We then have the following result :

**Theorem 2.4.6.** *Let  $U : L^2(0, \infty) \rightarrow L^2(\mathbb{R}, d\mu)$  be a unitary operator such that  $UAU^* = Q$  where  $Q$  is the usual multiplication operator in  $L^2(\mathbb{R}, d\mu)$ . Then  $U$  can be expressed in the following form*

$$U(f)(\lambda) = \int_0^\infty u_\lambda(x) f(x) dx$$

where, for  $\mu$ -a.e.  $\lambda$ ,  $u_\lambda(\cdot)$  is a solution of  $\tau u = \lambda u$  satisfying  $u(0) = 0$ . Furthermore, the inverse is given by

$$(U^{-1}F)(x) = \int_{\mathbb{R}} \overline{u_\lambda(x)} F(\lambda) \mu(d\lambda)$$

.

*Proof.* See [36, p.238].  $\square$

## 2.5 The rigged Hilbert space structure

### 2.5.1 On locally convex topological vector spaces

Let  $\Phi$  be a vector space endowed with a family  $(\|\cdot\|_i)_{i \in I}$  of seminorms. The sets of the form  $B_{x, i_1, \dots, i_n, r} := \{y \in \Phi : \|y - x\|_{i_k} < r; k = 1, 2, \dots, n\}$  where  $x \in \Phi, r > 0$  and  $\{i_1, i_2, \dots, i_n\} \subseteq I$ , form a basis of a topology  $\tau$ . It is easy to see that  $\tau$  is the weakest topology on  $\Phi$  making all the seminorms  $\|\cdot\|_i$  continuous. This topology is metrizable if and only if the set  $I$  is at most countable. A topological vector space  $(\Phi, \tau)$  is said to be locally convex if its topology can be generated by a family of seminorms  $(\|\cdot\|_i)_{i \in I}$ . In this case  $\tau$  is said to be a locally convex topology on  $\Phi$ . Let  $(\Phi, (\|\cdot\|_i)_{i \in I})$  be a locally convex topological vector space. The topological space  $\Phi$  is Hausdorff if and only if for every  $x \in \Phi \setminus \{0\}$  there exists  $i \in I$  such that  $\|x\|_i \neq 0$ .

In this thesis, we will only deal with locally convex topological vector spaces for which the topology is induced by a countable family of seminorms  $(\|\cdot\|_n)_n$ . These are in fact metrizable spaces and in this case the locally convex topology can be seen as induced by the following metric

$$d(\varphi, \psi) = \sum_{k=0}^{\infty} 2^k \frac{\|\varphi - \psi\|_k}{1 + \|\varphi - \psi\|_k}$$

Given a locally convex topological space  $(\Phi, (\|\cdot\|_n)_n)$ , we may define an alternative system  $(p_n(\cdot))_n$  of semi-norms on  $\Phi$ , by

$$p_n(\cdot) = \sum_{k=0}^{k=n} \|\cdot\|_k$$

One can easily check that the system  $(p_n(\cdot))_n$  induces the same locally convex topology on  $\Phi$ . Moreover, it has the advantage of satisfying the following increasing property

$$p_0(\varphi) \leq p_2(\varphi) \leq p_3(\varphi) \leq \dots$$

For all  $\varphi \in \Phi$ .

Thus, we may, and always will, suppose without loss of generality that our system  $(\|\cdot\|_n)_n$  of seminorms satisfies this increasing property.

Recall the following result on continuity

**Proposition 2.5.1.** *Let  $(\Phi, (\|\cdot\|_n)_n)$  and  $(\Psi, (p_n)_n)$  be locally convex topological vector spaces and  $A : \Phi \rightarrow \Psi$  be a linear operator. Then  $A$  is continuous if and only if for each  $n \in \mathbb{N}$  there exists  $m \in \mathbb{N}$  and  $C \geq 0$  such that for every  $\varphi \in \Phi$  we have*

$$p_n(A\varphi) \leq C\|\varphi\|_m$$

## 2.5.2 The rigged Hilbert space structure

Recall that a Frechet space is a vector space  $\Phi$  endowed with a countable family of semi-norms  $(\|\cdot\|_n)_n$  such that  $\Phi$  is complete with respect to the associated locally convex topology.

**Definition 2.5.1.** *A Frechet space  $(\Phi, (\|\cdot\|_n)_{n \in \mathbb{N}^*})$  for which each seminorm  $\|\cdot\|_n$  is actually a norm which is defined by a scalar product  $(\cdot, \cdot)_n$  is called a countably Hilbert space.*

Let  $\Phi$  be a countably Hilbert space. Denote by  $\Phi_n$  the  $\|\cdot\|_n$ -completion of  $\Phi$ . We then see that the spaces  $\{\Phi_n\}_n$  form a decreasing chain

$$\dots \Phi_{n+1} \subset \Phi_n \cdots \subset \Phi_2 \subset \Phi_1$$

and  $\Phi = \bigcap_{n \in \mathbb{N}^*} \Phi_n$  [8].

Denote by  $\Phi'$  and  $\Phi'_n$  the topological dual spaces of  $\Phi$  and  $\Phi_n$ , (i.e., the spaces of continuous linear functionals resp. on  $\Phi$  and  $\Phi_n$ ). Usually,  $\Phi'$  and  $\Phi'_n$  are equipped with the weak\*-topology. It is then easy to see that the spaces  $\{\Phi'_n\}_n$  form an increasing chain

$$\Phi'_1 \subset \Phi'_2 \subset \dots \subset \Phi'_n \subset \Phi'_{n+1} \dots$$

and  $\Phi' = \bigcup_{n \in \mathbb{N}^*} \Phi'_n$ .

Further, consider additionally a Hilbert space  $(\mathcal{H}, (\cdot, \cdot))$  together with a continuous linear embedding  $i : \Phi \rightarrow \mathcal{H}$  with dense range. The latter induces a continuous linear embedding  $i^* : \mathcal{H} \rightarrow \Phi'$  given by  $x \mapsto (x, i(\cdot))$ . The induced structure  $\Phi \xrightarrow{i} \mathcal{H} \xrightarrow{i^*} \Phi'$  is called a Gelfand triple. If moreover,  $\Phi$  is nuclear, that is for every  $n$ , there exists  $m > n$  such that the canonical injection

$$\iota_{mn} : \Phi_m \rightarrow \Phi_n, \quad u \mapsto u$$

is trace class, the triple  $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$  is called a rigged Hilbert space (RHS). Next we recall the concept of a trace-class operator by using canonical decompositions.

Let  $\mathcal{H}$  and  $\mathcal{K}$  be two complex separable Hilbert spaces and let  $A : \mathcal{H} \rightarrow \mathcal{K}$  be a linear operator. Then  $A$  is compact if and only if there exists a null sequence  $(\lambda_k)_k$  of positive numbers and orthonormal families  $(u_k)_k \subset \mathcal{H}$  and  $(v_k)_k \subset \mathcal{K}$  such that

$$A = \sum \lambda_k \langle u_k, \cdot \rangle v_k.$$

The numbers  $(\lambda_k)_k$  correspond to the singular values of  $A$  (i.e., the non-zero eigenvalues of  $|A|$ ). If  $\sum_1^\infty \lambda_k^2 < \infty$ ,  $A$  is called a trace-class (or nuclear) operator. Recall that every nuclear operator is the product of two Hilbert-Schmidt operators. In particular, every nuclear operator is Hilbert-Schmidt.

## 2.6. GENERALIZED EIGENVECTORS AND THE NUCLEAR SPECTRAL THEOREM

Perhaps the most important example of a rigged Hilbert space is the following

$$\mathcal{S}(\mathbb{R}) \xrightarrow{i} L^2(\mathbb{R}, dx) \xrightarrow{i^*} \mathcal{S}'(\mathbb{R})$$

where  $i$  is the natural inclusion and  $i^*(f)(\varphi) = \int_{\mathbb{R}} \overline{f(x)}\varphi(x)dx$ . The Schwartz topology  $\tau_{\mathcal{S}(\mathbb{R})}$  can be seen as induced by the following family of inner products

$$(f, g)_n = \int_{\mathbb{R}} (1+x^2)^{2n} \sum_{0 \leq k \leq n} \overline{f^{(k)}(x)} g^{(n)}(x) dx, \quad n \in \mathbb{N}^*, \quad (f, g \in \mathcal{S}(\mathbb{R}))$$

Observe that if  $U : \mathcal{H} \rightarrow \mathcal{H}$  is a unitary map between Hilbert spaces  $\mathcal{H}$  and  $\mathcal{H}$ , then any RHS structure on  $\mathcal{H}$  induces an equivalent RHS structure on  $\mathcal{H}$ . In this thesis we shall sometimes use the notation  $\Phi$  without further specification to refer to a RHS  $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$  and we shall use the symbol  $\tau$  to refer to its topology.

### 2.6 Generalized eigenvectors and the nuclear spectral theorem

**Definition 2.6.1.** Let  $A$  be a self-adjoint operator  $A$  in  $\mathcal{H}$ . We say that  $A$  is a self-adjoint operator in a RHS  $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$  (or that the latter is a RHS for  $A$ ) if  $\Phi \subset D(A)$ ,  $A\Phi \subset \Phi$ ,  $A|_{\Phi}$  is essentially self-adjoint and  $A : \Phi \rightarrow \Phi$  is  $\tau$ -continuous.

Let  $A$  be a linear operator in  $\mathcal{H}$  and  $\Lambda \subset A$  a dense linear subspace of  $\mathcal{H}$ . Suppose moreover that  $A\Lambda \subset \Lambda$ . A generalized eigenvector of  $A : \Lambda \rightarrow \Lambda$  with respect to a generalized eigenvalue  $\lambda \in \mathbb{C}$  is a linear functional  $F \in \Lambda' \setminus \{0\}$  such that  $F(A\varphi) = \lambda F(\varphi)$  for every  $\varphi \in \Lambda$ . That is,  $F$  is an eigenvector for the dual operator  $A' : \Lambda' \rightarrow \Lambda'$ , defined by  $A'F = FA$ , with associated  $\lambda$  as an eigenvalue. A family  $\mathcal{G}$  of generalized eigenvectors of  $A : \Lambda \rightarrow \Lambda$  is said to be complete if for every  $\varphi \in \Lambda$ ,

$$(F\varphi = 0, \quad \forall F \in \mathcal{G}) \Rightarrow \varphi = 0.$$

Now going back to the example of the momentum operator  $P$  in the Schrödinger representation  $L^2(\mathbb{R}, dx)$  and considering the RHS  $\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dx) \subset \mathcal{S}'(\mathbb{R})$ , it is well-known that  $P$  is a self-adjoint operator in the latter RHS. For each  $\lambda \in \mathbb{R}$ , denote by  $T_{\lambda}$  the regular distribution associated with the locally integrable function  $e^{-i\lambda x}$ . One can then easily check that  $(T_{\lambda})_{\lambda \in \mathbb{R}}$  forms a complete family of generalized eigenvectors of  $P$  in  $\mathcal{S}'(\mathbb{R})$ . Similarly, with the Dirac delta tempered distribution  $\delta$ , one can check that  $(\delta(x - \lambda))_{\lambda \in \mathbb{R}}$  forms a complete family of generalized eigenvectors of the position operator  $Q$  on  $\mathcal{S}'(\mathbb{R})$ .

Let  $A$  be a self-adjoint operator in a RHS  $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$ . The nuclear spectral theorem [8, 9] says that one can always find a complete system of generalized eigenvectors for  $A|_{\Phi}$ . For the convenience, we provide in this section a proof for cyclic self-adjoint operators, obtained via a closer look at the arguments in [8] and [43]. In particular, the proof describes how to construct generalized eigenvectors by using nuclearity. Remark that the spectral theorem implies that the study of many properties of cyclic self-adjoint operators on a RHS may be conducted in RHS structures of the form  $\Phi \hookrightarrow L^2(\mathbb{R}, d\mu) \hookrightarrow \Phi'$ , such that  $Q\Phi \subset \Phi$  and  $Q|_{\Phi}$  is essentially self-adjoint.

**Theorem 2.6.1.** Let  $\Phi \subset \mathcal{H} = L^2(\mathbb{R}, \sigma) \subset \Phi'$  be a RHS for  $Q$ . Then for every  $s \geq n$  in  $\mathbb{N}^*$  such that  $\iota_{s,n}$  is nuclear and  $Q : (\Phi, \|\cdot\|_s) \rightarrow (\Phi, \|\cdot\|_n)$  is continuous, there exists a family of linear functionals  $\{F_x\}_{x \in \mathbb{R}} \subset \Phi'_s$  and a negligible subset  $Y$  of  $\mathbb{R}$  such that for  $\tilde{\varphi} \in \Phi_s$ ,  $\tilde{\varphi}(x) = F_x(\tilde{\varphi})$  a.e., and for every  $x \in \mathbb{R} \setminus Y$  and  $\varphi \in \Phi$ ,  $F_x(Q\varphi) = xF_x(\varphi)$ .

*Proof.* Let  $\{\lambda_k\}_k \subset \mathbb{R}^+$ , such that

$$\iota_{s,n} = \sum_k \lambda_k \langle u_k, \cdot \rangle_s v_k, \quad \sum_k \lambda_k < \infty,$$

where  $\{u_k\}_k$  is an orthonormal basis of  $\Phi_s$ ,  $\{v_k\}_k$  is a family of everywhere defined functions such that  $\{v_k\}_k$  is an orthonormal basis of  $\Phi_n$ .

It follows from [8, Lemma 1, p. 111] that the set  $X$  of real values  $x$  for which the series  $\sum_k \lambda_k |v_k(x)|$  does not converge is  $\sigma$ -negligible. Put

$$F_x = \sum_k \lambda_k v_k(x) \langle u_k, \cdot \rangle_s, \quad \text{if } x \in \mathbb{R} \setminus X, \quad F_x = 0 \quad \text{if } x \in X.$$

Since the functional  $\langle u_k, \cdot \rangle_s$  has norm 1, we check easily that  $F_x \in \Phi'_s$  for every  $x \in \mathbb{R}$ . Let  $\psi \in \Phi_s$ . Then

$$\psi = \iota_{s,n}(\psi) = \sum_k \lambda_k \langle u_k, \psi \rangle_s v_k.$$

On the other hand,

$$F_x(\psi) = \sum_k \lambda_k v_k(x) \langle u_k, \psi \rangle_s, \quad x \in \mathbb{R} \setminus X.$$

Thus  $\psi(x) = F_x(\psi)$  a.e.

Next choose  $t \geq s$  such that  $Q : (\Phi, \|\cdot\|_t) \rightarrow (\Phi, \|\cdot\|_s)$  is continuous and let  $\{g_k\}_k \subset \Phi$  such that  $\Lambda = \text{span}\{g_k\}_k$  is dense in  $\Phi_t$ . Then  $Qg_k \in \Phi$  and

$$(Qg_k)(x) = F_x(Qg_k) \quad \text{a.e.}, \quad g_k(x) = F_x(g_k) \quad \text{a.e.}$$

Hence there exists a negligible subset  $Y_k$  of  $\mathbb{R}$  such that

$$F_x(Qg_k) = xF_x(g_k), \quad x \in \mathbb{R} \setminus Y_k.$$

Put  $Y = X \cup (\cup_k Y_k)$ . Let  $\psi \in \Phi$ . Choose  $\{h_k\}_k \subset \Lambda$  such that  $\psi = \lim_k h_k$  for  $\|\cdot\|_t$ . Then  $\psi = \lim_k h_k$  for  $\|\cdot\|_s$ . We have  $Q\psi \in \Phi$  and

$$Q\psi = Q(\lim_k h_k) = \lim_k Qh_k.$$

Fix  $x \in \mathbb{R} \setminus Y$ . Then

$$F_x(Q\psi) = F_x(\lim_k Qh_k) = \lim_k F_x(Qh_k) = \lim_k xF_x(h_k) = xF_x(\psi).$$

□

By using unitary equivalence and the spectral theorem for cyclic self-adjoint operators, we deduce the following version of the nuclear spectral theorem in the cyclic case.

**Corollary 2.6.1.** *Let  $A$  be a cyclic self-adjoint operator in a RHS  $\Phi \subset \mathcal{H} \subset \Phi'$ . Then  $A|_{\Phi}$  has a complete family of generalized eigenvectors.*

## 2.7 On the one-dimensional moment problem

### 2.7.1 Statement of the problem and the basic criteria

Consider the following problem ( $\mathcal{P}$ ): Given a closed subset  $K$  of  $\mathbb{R}$  and a sequence  $s = (s_n)_{n \in \mathbb{N}} \subset \mathbb{R}$ , provide criteria that ensure the existence of a positive Borel measure  $\mu$  on  $\mathbb{R}$  such that  $\text{supp}(\mu) \subset K$  and

$$\int_{\mathbb{R}} x^n d\mu = s_n$$

If such a Borel measure exists,  $(s_n)_{n \in \mathbb{N}}$  is said to be a  $K$ -moment sequence. We say that  $(s_n)_n$  is a Hamburger (resp. Stieltjes) moment sequence if moreover  $K = \mathbb{R}$  (resp.  $K = [0, \infty)$ ). The problem is said to be determinate if the measure is unique. Otherwise, the problem is said to be indeterminate. The two basic questions in the theory of moments are existence and determinacy.

## 2.7. ON THE ONE-DIMENSIONAL MOMENT PROBLEM

Given a linear functional  $F$  on  $\mathbb{R}[X]$ , we associate to  $F$  the sequence  $(s_n)_{n \in \mathbb{N}}$  of moments defined by  $s_n = F(x^n)$  for all  $n \in \mathbb{N}$  (we identify a polynomial with its associated polynomial function). We also associate to  $F$  a symmetric bilinear form defined on  $\mathbb{R}[X]$  by  $\langle P, Q \rangle_F := F(PQ)$ . It is clear that a linear functional  $F$  on  $\mathbb{R}[X]$  is uniquely determined by its sequence of moments.

Let  $K$  be a closed set of  $\mathbb{R}$ . We say that a polynomial  $P$  is positive on  $K$  if  $P(x) \geq 0$  for all  $x \in K$ . A linear functional  $F$  is said to be positive on  $K$  if  $F(P) \geq 0$  whenever  $P$  is positive on  $K$ . If moreover we have that  $F(P) > 0$  for every positive polynomial  $P \in \mathbb{R}[X] \setminus \{0\}$ , we say that  $F$  is positive definite on  $K$ . A real sequence  $(s_n)_{n \in \mathbb{N}}$  is said to be positive (resp. positive definite) on  $K$  if the linear functional  $F_s$  defined on  $\mathbb{R}[X]$  by  $F_s(x^n) := s_n$  is positive (resp. positive definite) on  $K$ . In the case of  $K = \mathbb{R}$ , we simply say that  $(s_n)_n$  and  $F_s$  are positive (positive definite). Remark that the sequence  $(s_n)_n$  is positive if and only if we have

$$\sum_{0 \leq i, j \leq m} s_{i+j} x_i x_j \geq 0, \quad x_i \in \mathbb{R}, \quad m \in \mathbb{N}.$$

We have the following basic criteria of existence.

**Theorem 2.7.1.** *A real sequence  $(s_n)_n$  is a  $K$ -moment sequence if and only if the linear functional  $F_s$  is positive on  $K$ .*

*Proof.* See [39]. □

In particular we get the following

**Corollary 2.7.1.** *1. A real sequence  $(s_n)_n$  is a Hamburger-moment sequence if and only if it is positive.*

*2. A real sequence  $(s_n)_n$  is a Stieltjes-moment sequence if and only if  $(s_n)_n$  and  $(s_{n+1})_n$  are positive.*

### 2.7.2 Orthogonal polynomials and three-terms recurrence relations

Let  $s = (s_n)_n$  be a positive definite sequence. In this case  $(s_n)_n$  generates a scalar product on  $\mathbb{R}[X]$  given by  $\langle x^m, x^n \rangle_s = s_{m+n}$ . Now, applying the Gram-Schmidt process on the canonical polynomial basis, we get the so-called orthonormal family of polynomials  $(P_n)_n$  associated to  $s$  and which then forms an orthonormal basis for the pre-Hilbert space  $(\mathbb{R}[X], \langle \cdot, \cdot \rangle_s)$ . Moreover, we have  $\deg(P_n) = n$ .

We also associate to  $s$  the sequence of Hankel matrices  $(H_n)_n$  and Hankel determinants  $(D_n)_n$  defined by

$$H_n = \begin{bmatrix} s_0 & \dots & s_n \\ s_1 & \dots & s_{n+1} \\ \vdots & \vdots & \vdots \\ s_n & \dots & s_{2n} \end{bmatrix} \quad D_n = \det(H_n), \quad \forall n \in \mathbb{N}$$

The sequence  $s$  is said to be normalized if  $s_0 = 1$ . We suppose that  $s$  is normalized from now on.

**Proposition 2.7.1.** *We have that  $P_0(x) = 1$  and the leading coefficient of  $P_n(x)$  is*

$$a_n = \sqrt{\frac{D_{n-1}}{D_n}}$$

Moreover, the  $P_n$ 's are given by the explicit formula

$$P_n(x) = \frac{1}{\sqrt{D_{n-1}D_n}} \begin{vmatrix} s_0 & s_1 & \dots & s_n \\ \vdots & \vdots & \vdots & \vdots \\ s_{n-1} & s_n & \dots & s_{2n-1} \\ 1 & x & \dots & x^n \end{vmatrix}, \quad (n \in \mathbb{N}^*)$$

**Proposition 2.7.2.** *The orthonormal polynomials  $(P_n(x))_{n \in \mathbb{N}}$  associated to  $s$  satisfy the following three-terms relation*

$$xP_n(x) = d_n P_{n+1}(x) + c_n P_n(x) + d_{n-1} P_{n-1}(x), \quad d_{-1} = 0, \quad n \in \mathbb{N}$$

where

$$c_n = F_s(xP_n(x)^2), \quad d_n = \frac{\sqrt{D_{n-1}D_{n+1}}}{D_n}$$

Moreover, the leading coefficient of  $P_n$  is  $(d_0 d_1 \dots d_{n-1})^{-1}$ .

For each  $n \in \mathbb{N}$ , denote by  $p_n$  the monic polynomial associated to  $P_n$ .

**Corollary 2.7.2.** *The monic orthonormal polynomials  $(p_n(x))_{n \in \mathbb{N}}$  associated to  $s$  satisfy a three-terms relation of the form*

$$p_{n+1}(x) = (x - c_n)p_n(x) - d_{n-1}^2 p_{n-1}(x), \quad p_0(x) = 1, \quad p_{-1}(x) = 0, \quad n \in \mathbb{N}$$

where  $c_n$  and  $d_{n-1}$  are as in the above proposition.

Conversely, we have the following

**Proposition 2.7.3.** *(Favard's theorem) Let  $(d_n)_n$  be a strictly positive real sequence,  $(c_n)_n$  be a real sequence and  $(P_n)_n$  a family of polynomials defined by the induction relation in the proposition 2.7.2 with  $P_{-1} = 0, P_0 = 1$  and  $d_{-1} = 0$ . Then there exists a positive definite real sequence  $s = (s_n)_n$  such that  $(P_n)$  are the orthonormal polynomials associated to  $s$ .*

### 2.7.3 Self-adjoint operators and the Hamburger moments problem

Let  $(s_n)_n$  be a positive definite sequence and consider the complex scalar product  $\langle \cdot, \cdot \rangle$  which extends the real scalar product  $\langle \cdot, \cdot \rangle_s$  induced by  $(s_n)_n$  on  $\mathbb{R}[X]$ . Hence the family  $(P_n(x))_n$  is orthonormal for this scalar product. Denote by  $\mathcal{H}$  the Hilbert space completion of  $(\mathbb{C}[X], \langle \cdot, \cdot \rangle)$  and consider the linear operator defined on  $\mathbb{C}[X]$  by  $Af(x) = xf(x)$ . It is easy to see that  $A$  is symmetric. Moreover, using the conjugation criterion, we infer that  $A$  admits self-adjoint extensions.

**Theorem 2.7.2.** *Every self-adjoint extension  $B$  of  $A$  in  $\mathcal{H}$  provides a solution  $\mu = P_1^B$  of the moment problem  $(\mathcal{P})$ . Conversely, let  $\mu$  be a solution of the moment problem  $(\mathcal{P})$ , then  $A \subset Q$  and  $\mu = P_1^Q$ , where  $Q$  is the usual position operator in  $L^2(\mathbb{R}, d\mu)$ .*

We have the following result on determinacy

**Theorem 2.7.3.** *The moment problem associated to  $(s_n)_n$  is determinate if and only if  $Q: \mathbb{C}[X] \rightarrow \mathcal{H}$ ,  $P(x) \mapsto xP(x)$  is essentially self-adjoint. In this case, if  $\mu$  denotes such a unique positive measure on  $\mathbb{R}$ ,  $\mathbb{C}[X]$  is dense in  $L^2(\mathbb{R}, d\mu)$ .*

*Proof.* See [39]. □

## 2.8 On Hermite and Laguerre polynomials

### 2.8.1 Hermite polynomials

We shall use the following form of the real and complex Hermite polynomials (see [44] and [45] for the complex case)

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

We have the following recurrence relation

$$H_n(x) = 2xH_{n-1}(x) - H_n'(x) \quad (*)$$

## 2.8. ON HERMITE AND LAGUERRE POLYNOMIALS

which allows one to compute  $H_n$  by induction on  $n$ . In particular,  $H_n$  is a polynomial of degree  $n$  whose leading term is  $(2x)^n$ . Moreover,  $H_n$  is even or odd depending on whether  $n$  is even or odd.

Remark that

$$H_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n!(-1)^k}{k!(n-2k)!} (2x)^{n-2k} \quad (2.1)$$

We now investigate orthogonality properties of the Hermite polynomials. We shall be working with the spaces  $L^2(\mathbb{R}, dx)$  and  $L^2(\mathbb{R}, e^{-x^2} dx)$

**Theorem 2.8.1.** *The family  $(H_n)_n$  forms an orthonormal basis for  $L^2(\mathbb{R}, e^{-x^2} dx)$ .*

We have the following

**Theorem 2.8.2.** *For any  $x \in \mathbb{R}$  and  $z \in \mathbb{C}$  we have*

$$\sum_0^\infty H_n(x) \frac{z^n}{n!} = e^{2xz - z^2}$$

Differentiating the identity above with respect to  $x$  yields

$$\sum_0^\infty H'_n(x) \frac{z^n}{n!} = 2ze^{-2xz - z^2} = 2 \sum_0^\infty H_n(x) \frac{z^{n+1}}{n!} = 2 \sum_1^\infty H_{n-1}(x) \frac{z^n}{(n-1)!}$$

Now polynomial identification yields

$$H'_0 = 0, \quad H'_n = 2nH_{n-1} \quad \text{for } n > 0.$$

Combining this with  $(\star)$ , one gets the recurrence formula

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x)$$

as well as the differential equation

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$$

We will also use the following result called Mehler's formula

**Proposition 2.8.1.** *Let  $r \in (-1, 1)$  and  $x, y \in \mathbb{R}$ . We have*

$$\sum_{n=0}^\infty r^n \frac{H_n(x)H_n(y)}{2^n n!} = (1-r^2)^{-1/2} \exp\left(\frac{2xyr - r^2(x^2 + y^2)}{1-r^2}\right).$$

For many purposes it is preferable to replace the Hermite polynomials by the Hermite functions defined by

$$h_n(x) = e^{-x^2} H_n(x)$$

The Hermite functions  $(h_n)_n$  form an orthonormal basis for  $L^2(\mathbb{R}, dx)$  and they satisfy

$$\begin{aligned} xh_n(x) + h'_n(x) &= 2nh_{n-1}(x) \\ xh_n(x) - h'_n(x) &= h_{n+1}(x) \\ h''_n(x) - x^2h_n(x) + (2n+1)h_n(x) &= 0 \end{aligned}$$

**Definition 2.8.1.** (Schauder basis) *Let  $E$  be a topological vector space. A family  $(e_n)_n$  of elements of  $E$  is said to be a Schauder basis of  $E$  if for all  $x \in E$ , there exists a unique sequence  $(a_n)_n$  of scalars such that  $x = \sum_{n=0}^\infty a_n e_n$ , where the convergence of the infinite sum is in the sense of the topology of  $E$ .*

**Theorem 2.8.3.** *The Hermite functions  $(h_n)_n$  form a Schauder basis of the Schwartz space  $\mathcal{S}(\mathbb{R})$ .*

### 2.8.2 Laguerre polynomials

Let  $\alpha$  be a real number such that  $\alpha > -1$ . The  $n$ th Laguerre polynomial  $L_n^\alpha$  corresponding to the parameter  $\alpha$  is defined by

$$L_n^\alpha(x) = \frac{x^{-\alpha} e^x}{n!} \frac{d^n}{dx^n} (x^{\alpha+n} e^{-x})$$

We have

$$L_n^\alpha(x) = x^\alpha e^x \sum_{k=0}^n \frac{1}{k!(n-k)!} \frac{d^k}{dx^k} \frac{d^{n-k} x^{\alpha+n}}{dx^{n-k}} = \sum_{k=0}^n \frac{(n+\alpha)(n-1+\alpha)\dots(k+1-\alpha)}{k!(n-k)!} (-x)^k$$

Thus  $L_n^\alpha$  is a polynomial of degree  $n$  and its leading coefficient is given by  $\frac{(-1)^n}{n!}$ .

The family  $(L_n^\alpha)_n$  forms an orthogonal basis of the Hilbert space  $L^2(\mathbb{R}^+, x^\alpha e^{-x})$ . Moreover

$$\|L_n^\alpha\|_{L^2(\mathbb{R}^+, x^\alpha e^{-x})} = \frac{\Gamma(n+1+\alpha)}{n!}$$

We now derive the generating function for the Laguerre polynomials

**Theorem 2.8.4.** For  $x > 0$  and  $|z| < 1$ ,

$$\sum_{n=0}^{\infty} L_n^\alpha(x) z^n = \frac{e^{-xz/(1-z)}}{(1-z)^{\alpha+1}}$$

Recall the following formulas connecting Hermite and Laguerre polynomials (see for instance [46])

$$H_{2n}(x) = (-1)^n 2^{2n} n! L_n^{-1/2}(x^2), \quad H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{1/2}(x^2).$$

## GENERALIZED EIGENVECTORS AND THE ASSOCIATED REPRESENTATIONS

### 3.1 Some algebraic preliminaries

Let  $\Lambda$  be a complex vector space and let  $T : \Lambda \rightarrow \Lambda$  be a linear map. The spectrum of  $T$  is

$$\sigma(T, \Lambda) = \{\lambda \in \mathbb{C} : T - \lambda \text{ is not bijective}\}.$$

We denote by  $\Lambda^*$  the dual space of  $\Lambda$ , elements of  $\Lambda^*$  are the linear functionals  $F : \Lambda \rightarrow \mathbb{C}$ . Denote by  $T^\circ : \Lambda^* \rightarrow \Lambda^*$  the dual of  $T$ , which is defined by  $T^\circ F = FT$ . It is easy to see that if the range of  $T$  has finite codimension  $n$ , then the dimension of  $\text{Ker} T^\circ$  is equal to  $n$ . If  $F$  is an eigenvector of  $T^\circ$  with respect to the eigenvalue  $\lambda$ , we say that  $(F, \lambda)$  (or  $F$ ) is an algebraic generalized eigenvector of  $T$  and  $\lambda$  is an algebraic generalized eigenvalue of  $T$ . Suppose that  $\Lambda$  is endowed with a linear topology  $\tau$ . Suppose moreover that  $\Lambda$  is endowed with a scalar product which is  $\tau$ -continuous in each variable. Then  $\Lambda \subseteq \Lambda'$  via  $u \mapsto \langle u, \cdot \rangle$  (we assume that our scalar products are antilinear in the first argument). Denote by  $\mathcal{H}$  the Hilbert space completion of  $(\Lambda, \langle \cdot, \cdot \rangle)$ . Clearly we have  $\mathcal{H} \subseteq \Lambda'$ . Since we want to deal with linear embeddings, we shall also deal with antidual spaces. We denote by  $\overline{\Lambda^*}$  the algebraic antidual space of  $\Lambda$  (i.e., the space of antilinear functionals on  $\Lambda$ ), and by  $\Lambda^\times$  the topological antidual space (with respect to  $\tau$ ). Clearly, elements of  $\overline{\Lambda^*}$  (resp.  $\Lambda^\times$ ) are of the form  $\overline{F}$  where  $F \in \Lambda^*$  (resp.  $\Lambda'$ ) and  $\overline{Fu} = \overline{F}u$  for every  $u$ . Analogously, we define  $T^\times : \overline{\Lambda^*} \rightarrow \overline{\Lambda^*}$  by  $T^\times \overline{F} = \overline{FT}$  and  $T^\times : \Lambda^\times \rightarrow \Lambda^\times$  by  $T^\times \overline{F} = \overline{FT}$ . We have

$$\Lambda \subset \mathcal{H} \subset \Lambda^\times \subset \overline{\Lambda^*}.$$

Moreover, let  $T^*$  be the Hilbert adjoint of  $T$ , then it is easy to see that

$$D(T^*) = \{u \in \mathcal{H} : T^\times u \in \mathcal{H}\} = (T^\times)^{-1}(\mathcal{H}) \cap \mathcal{H}, \quad T^* = T^\times |_{D(T^*)}.$$

For  $F \in \overline{\Lambda^*}$  and  $\varphi \in \Lambda$ , we shall use the notations  $F(|\varphi\rangle) = (\varphi, F) = \overline{\langle F|\varphi\rangle}$ . We shall deal with topological, algebraic, linear or antilinear generalized eigenvectors. The words "linear, antilinear, topological and algebraic" can be omitted when there is no risk of ambiguity.

Let  $\Lambda, \Omega$  be complex linear spaces and let  $T : \Lambda \rightarrow \Omega$  be a bijective linear map. Then it is clear that  $\Omega^* = \{FT^{-1} : F \in \Lambda^*\}$ . In particular, if  $\Lambda$  and  $\Omega$  are linear topological spaces and if  $T$  is a topological isomorphism, then  $\Omega' = \{FT^{-1} : F \in \Lambda'\}$ .

For any linear map  $T$  defined on a linear space having a countable basis  $\{e_n\}_n$ , we denote by  $M(T, \{e_n\}_n)$  the matrix of  $T$  with respect to the basis  $\{e_n\}_n$

Finally, given a set of functions  $\Lambda$  defined on the real line, we denote by  $\mathcal{Z}(\Lambda)$  its zero set, that is

$$\mathcal{Z}(\Lambda) = \{x \in \mathbb{R} : g(x) = 0 \forall g \in \Lambda\}.$$

## 3.2 Generalized eigenvectors and associated representations

Throughout this section,  $X$  is a subset of  $\mathbb{C}$  and  $\mathcal{H}$  is a Hilbert space. To deal freely with evaluation maps, we first consider general spaces of functions. We shall say that a complex linear space  $\Omega$  is a space of functions on  $X$  if all elements of  $\Omega$  are functions  $f : X \rightarrow \mathbb{C}$ ; in particular,  $f = 0$  if and only if  $f(x) = 0$  for every  $x \in X$ . In the following, for all  $x \in X$ , we denote by  $\delta_x$  the evaluation map on  $\Omega$  defined by  $\delta_x : f \mapsto f(x)$ .

Our discussion is based on the following elementary lemma.

**Lemma 3.2.1.** *Let  $\Omega$  be a space of functions on  $X$ ,  $f : X \rightarrow \mathbb{C}$  a function, and  $A : \Omega \rightarrow \Omega$  be a linear map. Then  $A$  is defined by  $A\psi = f\psi$  for all  $\psi \in \Omega$  if and only if for every  $x \in X$ , either  $\delta_x$  is a generalized eigenvector for  $A$  with respect to  $f(x)$  or  $\delta_x = 0$ .*

*Proof.* This is straightforward. Just observe that for every  $\psi \in \Omega$  and  $x \in X$ ,

$$A\psi(x) = f(x)\psi(x) \Leftrightarrow \delta_x(A\psi) = f(x)\delta_x(\psi) \Leftrightarrow (A^\circ \delta_x)(\psi) = f(x)\delta_x(\psi).$$

□

### 3.2.1 Completeness

From now on, in this section we suppose that  $A$  is a linear operator in  $\mathcal{H}$ ,  $\Lambda$  is a dense linear subspace of  $\mathcal{H}$  such that  $\Lambda \subset D(A)$  and  $A\Lambda \subset \Lambda$ . Let  $\{(F_x, f(x))\}_{x \in X}$  be a family of generalized eigenvectors of  $A|_\Lambda$ . For every  $\varphi \in \Lambda$ , consider the function  $\tilde{\varphi}$  defined on  $X$  by  $\tilde{\varphi}(x) = F_x(\varphi)$  and put  $\Omega = \{\tilde{\varphi} : \varphi \in \Lambda\}$ . Then it is easy to see that  $\Omega$  is a space of functions on  $X$  and that for every  $x \in X$ ,  $\delta_x \neq 0$ . Moreover, the map  $T : \Lambda \rightarrow \Omega$  defined by  $T\varphi = \tilde{\varphi}$  is linear and surjective by construction.

Here and subsequently, we suppose that  $\delta_x \neq 0$  for all  $x \in X$  in every considered space of functions on  $X$ . Let us consider the following general definition of completeness (see [8, p.120]). A family  $\{F_\lambda\}_\lambda$  of elements of  $\Lambda^*$  (or  $\overline{\Lambda^*}$ ) is said to be complete if for every  $\varphi \in \Lambda$ ,  $F_\lambda(\varphi) = 0$  for every  $\lambda$  implies that  $\varphi = 0$ .

**Lemma 3.2.2.** *The following assertions are equivalent:*

(i) *The family  $\{F_x\}_{x \in X}$  is complete.*

(ii) *The map  $T : \Lambda \rightarrow \Omega$  defined by  $T\varphi = \tilde{\varphi}$  is injective.*

*In this case, for every  $\psi \in \Omega$ , we have  $TAT^{-1}(\psi(x)) = f(x)\psi(x)$ . Moreover, if  $\Lambda$  is a linear topological space, and  $\Omega$  is endowed with the final topology induced by  $T$ , then for every  $x$ , the evaluation map on  $\Omega$  is continuous if and only if  $F_x$  is continuous.*

*Proof.* The implication (ii)  $\Rightarrow$  (i) is obvious. Let us show that (i)  $\Rightarrow$  (ii): Suppose that for some  $\varphi \in \Lambda$ ,  $T\varphi = 0$ . Then  $\tilde{\varphi}(x) = 0$  for every  $x$ . That is,  $F_x(\varphi) = 0$  for every  $x$ . By completeness of the family  $\{F_x\}_x$ , we get  $\varphi = 0$ . Hence  $T$  is injective.

Next suppose that  $\Lambda$  is a topological space and that  $\Omega$  is equipped with the topology induced by  $T$ . Then the map  $T$  is continuous. Since  $\delta_x = F_x T^{-1}$ , we obtain the desired conclusion. □

### 3.2.2 Coherence-like conditions

In [27], Klauder and Skagerstam observed that coherent states share two basic properties : strong continuity and completeness. Next we generalise those two properties to the case of a family of generalized eigenvectors. We shall say that  $\{F_x\}_{x \in X}$  is strongly continuous if for every sequence  $\{x_n\} \subseteq X$  satisfying  $\lim_n x_n = x$  where  $x \in X$ , we have  $\lim_n F_{x_n}(\varphi) = F_x(\varphi)$  for every  $\varphi \in \Lambda$ . On the other hand we shall say that  $\{F_x\}_{x \in X}$  is measure-complete if there exists a positive measure  $\mu$  on  $X$ , a closed subspace  $\mathcal{H}$  of  $L^2(X, d\mu)$  and a unitary map  $U : \mathcal{H} \rightarrow \mathcal{H}$  such that  $(U\varphi)(x) = F_x(\varphi)$  for every  $\varphi \in \Lambda$ . Observe that this is equivalent to the fact that there exists a Hilbertian basis  $\{e_n\}_n$  of  $\mathcal{H}$  contained in  $\Lambda$  and a positive measure  $\mu$  such that the functions  $\{F_x(e_n)\}_n$  form an orthonormal family of  $L^2(X, d\mu)$ . In the case where  $F_x \in \mathcal{H}$  for every  $x \in X$ , we recover Klauder-Skagerstam's conditions.

The next proposition provides a criterion of completeness for a family of generalized eigenvectors of  $A$ . It may be used to construct new representations using generalized eigenvectors of certain operators.

### 3.2. GENERALIZED EIGENVECTORS AND ASSOCIATED REPRESENTATIONS

**Proposition 3.2.1.** *Suppose that  $\{F_x\}_{x \in X}$  is measure-complete. Then it is complete. Suppose moreover that  $\Lambda$  is endowed with a metrizable linear topology  $\tau$  finer than that of the norm of  $\mathcal{H}$  such that the maps  $F_x$  are  $\tau$ -continuous, and let  $\Lambda'$  be the completion of  $(\Lambda, \tau)$ . Then the family  $\{\tilde{F}_x\}_{x \in X}$  is complete, where  $\tilde{F}_x$  is the continuous extension of  $F_x$  to  $\Lambda'$ .*

*Proof.* Let  $\varphi$  be an element of  $\Lambda$  and suppose that for every  $x$ ,  $F_x(\varphi) = 0$ . Let  $\mu$  be a positive measure on  $X$  associated to the measure-complete family  $\{F_x\}_x$  and let  $\mathcal{H}$  be a closed subspace of  $L^2(X, \mu)$  such that there exists a unitary map  $U : \mathcal{H} \rightarrow \mathcal{H}$  satisfying  $(U\psi)(x) = F_x(\psi)$  for every  $\psi \in \Lambda$ . Then  $(U\varphi)(x) = 0$  for every  $x$ . That is,  $U\varphi = 0$ . Since  $U$  is unitary, we get  $\varphi = 0$ . Next let us prove the second assertion. Let  $\varphi \in \Lambda'$  and suppose that for every  $x$ ,  $\tilde{F}_x(\varphi) = 0$ . In the case that  $\varphi \in \Lambda$ , we have  $\tilde{F}_x(\varphi) = F_x(\varphi)$  and we are done. Next suppose that  $\varphi \in \Lambda' \setminus \Lambda$  and consider a sequence  $\{\varphi_n\}_n \subseteq \Lambda$  such that  $\lim_n \varphi_n = \varphi$  for the topology  $\tau$ . Since  $\tau$  is finer than the topology induced by the norm  $\|\cdot\|$  on  $\Lambda$ , the sequence  $\{\varphi_n\}_n$  converges to  $\varphi$  in  $\mathcal{H}$ . We have  $(U\varphi_n)(x) = F_x(\varphi_n)$  for every  $x$  and the sequence  $\{U\varphi_n\}_n$  converges to  $U\varphi$  in  $L^2(X, \mu)$ . In particular, a subsequence of  $\{U\varphi_n\}$  converges pointwise almost everywhere on  $X$  to  $U\varphi$ . On the other hand, since the maps  $F_x$  are continuous,  $\lim_n F_x(\varphi_n) = \tilde{F}_x(\varphi) = 0$ . This entails that the map  $(U\varphi)(x) = 0$  almost everywhere, that is  $U\varphi = 0$ . Finally, we infer that  $\varphi = 0$ .  $\square$

### 3.2.3 Construction of the representation

Let  $A$  be a linear operator in  $\mathcal{H}$  and suppose that  $\Lambda$  is a dense linear subspace of  $\mathcal{H}$  such that  $\Lambda \subset D(A)$  and  $A\Lambda \subseteq \Lambda$ . Suppose moreover that there exists a hilbertian basis  $\{e_n\}_n$  of  $\mathcal{H}$  contained in  $\Lambda$  such that  $A\Lambda' \subset \Lambda'$  where  $\Lambda' = \text{span}\{e_n : n \in \mathbb{N}\}$ . Let  $\{(F_x, f(x))\}_{x \in X}$  be a measure complete family of antilinear generalized eigenvectors of  $A|_{\Lambda'}$ . Denote by  $\mu$  the corresponding measure. Put  $\overline{F_x}(e_n) = \psi_n(x)$ . It follows from Lemma 3.2.2 that the linear map  $U : \Lambda' \rightarrow \text{span}\{\psi_n(x) : n \in \mathbb{N}\}$  defined by  $U(e_n) = \psi_n(x)$  is bijective. Consider the abstract set  $\mathcal{H} = \{\sum_n c_n \psi_n(x) : \sum_n |c_n|^2 < \infty\}$ . Then  $\mathcal{H}$  may be seen as a Hilbert space, where the scalar product is the completion of

$$(\varphi, \psi) = \int_X \overline{\varphi(x)} \psi(x) d\mu(x), \quad \varphi, \psi \in U\Lambda', \quad (3.1)$$

and the map  $U$  can be extended to a unitary map  $U : \mathcal{H} \rightarrow \mathcal{H}$ . We have  $\overline{F_x} = \delta_x U|_{\Lambda'}$  for every  $x \in X$ , which entails that  $UAU^* \psi(x) = \overline{f(x)} \psi(x)$  for every  $\psi(x) \in U\Lambda'$ . We shall say that the representation  $\mathcal{H}$  is realized with the family of antilinear generalized eigenvectors  $\{(F_x, f(x))\}_{x \in X}$ . Moreover,  $\mathcal{H}$  is the completion of the space of functions  $U\Lambda' = \text{span}\{\psi_n(x) : n \in \mathbb{N}\}$ . Since  $U\Lambda' \subseteq \mathcal{L}^2(X, d\mu)$ , by using classical arguments, we can either suppose that the completion  $\mathcal{H}$  of  $U\Lambda'$  is contained in  $\mathcal{L}^2(X, d\mu)$ , and  $\mathcal{H}$  is a function space (see for instance [47, Proof of Theorem 3.4.1]), or we may suppose that  $\mathcal{H} \setminus U\Lambda' \subseteq L^2(X, d\mu)$ . In particular, in the first case, evaluation maps are defined on  $\mathcal{H}$ , but certainly, they are not in general continuous on  $\mathcal{H}$ . Put  $F_x U^* = |x\rangle$ . Then

$$(\varphi, \psi) = \int_X d\mu F_x U^*(\varphi) \overline{F_x U^*(\psi)} = \int_X d\mu (\varphi|x) \langle x|\psi), \quad \varphi, \psi \in U\Lambda'. \quad (3.2)$$

Hence the notation

$$I|_{U\Lambda'} \equiv \int_X d\mu |x\rangle \langle x|.$$

On the other hand, we may put as a notation,  $\psi(x) = \langle x|\psi\rangle$  for every  $\psi \in \mathcal{H}$ . Then the equality (3.2) has a meaning in  $\mathcal{H}$  and we may also use the notation  $I \equiv \int d\mu |x\rangle \langle x|$  on the space  $\mathcal{H}$ .

Next suppose that we endow  $\Lambda'$  with a metric topology  $\tau$  finer than the one induced by the norm of  $\mathcal{H}$  that makes the maps  $F_x$  continuous and such that  $\Lambda$  coincides with the completion of  $(\Lambda', \tau)$ , then by Lemma 3.2.2, evaluation maps are continuous on  $U\Lambda$  with respect to the topology  $U\tau$  induced by  $\tau$ . On the other hand, observe that for every measurable function  $g : X \rightarrow \mathbb{C}$  which does not vanish,  $(g(x)F_x, f(x))$  is a generalized eigenvector of  $A|_{\Lambda'}$  and the representation realized with respect to the family  $\{g(x)|x\rangle\}_x$  corresponds to a Hilbert space contained in  $L^2(X, |g(x)|^{-2} d\mu)$ .

Finally, we distinguish three particular cases:

(1) All the maps  $F_x$  are continuous with respect to the norm of  $\mathcal{H}$ , hence  $|x\rangle$  can be seen as an element of  $\mathcal{H}$  and evaluation maps are continuous on  $\mathcal{H}$ . That is,  $\mathcal{H}$  is a reproducing kernel Hilbert space (RKHS). Put  $\delta_x = \langle k_x, \cdot \rangle$ ,

then its reproducing kernel is  $K(y, x) = \langle k_y, k_x \rangle$ .

(2) For every  $x$ ,  $F_x$  is continuous with respect to  $\tau$ . Hence evaluation maps are continuous on  $U\Lambda$  with respect to  $U\tau$ .

(3) For every  $x$ ,  $F_x$  is not continuous with respect to  $\tau$ . Hence evaluation maps are not continuous on  $U\Lambda$  with respect to  $U\tau$ .

We shall use the notation  $F_x \equiv |x\rangle$ , when there is no risk of ambiguity.

### 3.2.4 Change of bases formulas

Recall that if  $T : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  is a unitary map, where  $\mathcal{H}_1$  and  $\mathcal{H}_2$  are two finite-dimensional Hilbert spaces of dimension  $n$ , and if  $\{u_i^j\}_i$  is an orthonormal basis of  $\mathcal{H}_j$ , then for every  $u \in \mathcal{H}_1$ , we have

$$|u\rangle = \sum_{k=1}^n \langle u_k^1 | u \rangle |u_k^1\rangle, \quad |u_i^1\rangle = \sum_k \delta_{ik} |u_k^1\rangle.$$

Hence we may write  $I = \sum_{i=0}^n |u_i^1\rangle \langle u_i^1|$  and  $\langle u_i^1 | u_k^1 \rangle = \delta_{ik}$ . On the other hand, we have  $|Tu\rangle = \sum_{i,k} \langle u_k^1 | u \rangle \langle u_i^2 | Tu_k^1 \rangle |u_i^2\rangle$ , hence we have

$$\langle u_i^2 | Tu \rangle = \sum_k \langle u_k^1 | u \rangle \langle u_i^2 | Tu_k^1 \rangle.$$

Analogously, we get

$$\langle u_k^1 | T^{-1}v \rangle = \sum_i \langle u_i^2 | v \rangle \langle u_k^1 | T^{-1}u_i^2 \rangle.$$

In particular, observe that  $\langle u_i^2 | Tu_k^1 \rangle = \overline{\langle u_k^1 | T^{-1}u_i^2 \rangle}$ . In Dirac's formalism, analogous formulas are used for the so called continuous bases, the symbol sum is replaced by the integral [35]. Next we explain a rigorous form. Let  $\mathcal{H}_1, \mathcal{H}_2$  be two infinite dimensional Hilbert spaces, where  $\mathcal{H}_j$  is a closed subspace of  $L^2(X_j, d\mu_j)$ . Suppose that  $\mathcal{H}_j$  is realized with a measure complete family of antilinear generalized eigenvectors  $\{(|x^j\rangle, f^j(x^j))\}_{x \in X_j}$  of the operator  $A_j : \Lambda \rightarrow \Lambda$ , where  $\Lambda$  is a dense linear subspace of  $\mathcal{H}$ . Let  $U_j : \mathcal{H} \rightarrow \mathcal{H}_j$  be the corresponding unitary map, that is,  $U_j A_j U_j^* \psi(\cdot) = \overline{f^j(\cdot)} \psi(\cdot)$ , for  $\psi(\cdot) \in U_j \Lambda$ . Put  $V = U_2 U_1^*$ .

Let  $x, x' \in X_j$ . If the evaluation maps lie in  $\mathcal{H}_j$ , then we may put  $\langle x', x \rangle = K(x', x)$ , the reproducing kernel of  $\mathcal{H}_j$ . In the general case, observe that if we put as in the finite case  $\langle x, x \rangle = 1$  and  $\langle x, x' \rangle = 0$  if  $x \neq x'$ , then the formula  $\psi(\cdot) = \sum_{x' \in X_j} \langle \cdot, x' \rangle \psi(x')$  has a rigorous meaning. Here the sum is trivial. For a general definition of the sum (over an uncountable set) in a normed space see for instance [48, p. 113].

Now for the change of bases formulas between  $(\mathcal{H}_1, \{|x^1\rangle\}_{x^1 \in X_1})$  and  $(\mathcal{H}_2, \{|x^2\rangle\}_{x^2 \in X_2})$ , we can ask the following question:

**Question :** Is there a family of scalars  $\langle x^1, x^2 \rangle$  such that

$$V\Psi(x^2) = \int_{X_1} d\mu_1 \langle x^2, x^1 \rangle \psi(x^1), \quad \psi \in U_1 \Lambda,$$

In other words, is  $V|_{U_1 \Lambda}$  an integral transform? What about  $V^*$  and if  $V^*|_{U_2 \Phi}$  is an integral transform, do we have  $\langle x^2, x^1 \rangle = \overline{\langle x^1, x^2 \rangle}$ ?

Observe that if an integral transform exists between  $(\mathcal{H}_1, \{|x^1\rangle\})$  and  $(\mathcal{H}_2, \{|x^2\rangle\})$ , then we can use it to deduce an integral transform between  $(\mathcal{H}_1, \{g_1(x)|x^1\rangle\})$  and  $(\mathcal{H}_2, \{g_2(x)|x^2\rangle\})$ , where  $g_j : X_j \rightarrow \mathbb{C}$  is a measurable function which does not vanish.

Let  $\{e_n\}_n$  be a Hilbertian basis of  $\mathcal{H}$  contained in  $\Lambda$ . Let  $F \in \overline{\Lambda^*}$ . We shall say that  $F$  is continuous with respect to  $\{e_n\}_n$  if for every  $\varphi \in \Lambda$ ,  $F(\varphi) = \lim_k \sum_{n=0}^k F(e_n)(\varphi|e_n)$ . In this case, we write  $F = \sum F(e_n)|e_n\rangle$ . Next we provide a result which is in the same spirit of the construction of integral transforms described in [49, ch. 5].

**Lemma 3.2.3.** *Suppose that there exists an Hilbertian basis  $\{e_n\}_n$  of  $\mathcal{H}$  contained in  $\Lambda$  such that for every  $x^j$ ,  $|x^j\rangle$  is continuous with respect to  $\{e_n\}_n$ , ( $j = 1, 2$ ). Suppose moreover that for every  $x^2$ , the sum  $\sum_n |(e_n|x^1\rangle \langle x^2|e_n)|$  converges in  $L^2(X_1, d\mu_1)$ . Then for every  $\psi(x^1) \in U_1 \Lambda$*

$$(V\Psi(\cdot))(x^2) = \int_{X_1} d\mu_1(x^1) \langle x^2, x^1 \rangle \psi(x^1),$$

### 3.2. GENERALIZED EIGENVECTORS AND ASSOCIATED REPRESENTATIONS

where  $\langle x^2|x^1 \rangle = \sum_n (e_n|x^1 \rangle \langle x^2|e_n) \in L^2(X_1, d\mu_1)$ .

*Proof.* Fix  $x^2 \in X_2$ . Put  $G_k = \sum_{n=0}^k (e_n|x^2 \rangle |e_n)$ . Then  $G_k \in \Lambda$ . Let  $\psi \in \Lambda$ . Then  $[U_2\psi](x^2) = \langle x^2|\psi \rangle = \lim_k (G_k, \psi) = \lim_k (U_1 G_k, U_1 \psi)$ . Since  $I|_{U_1\Lambda} = \int_{X_1} d\mu_1(x^1)|x^1 \rangle \langle x^1|$ , we get

$$[U_2\psi](x^2) = [V\psi(x^1)](x^2) = \lim_k \int_{X_1} d\mu_1(x^1) (G_k|x^1 \rangle \langle x^1|\psi).$$

On the other hand, it follows from our assumption on the sum that  $\sum_n |(e_n|x^1 \rangle \langle x^2|e_n) \langle x^1|\psi|$  lies in  $L^1(X_1, d\mu_1)$ . Hence we can interchange the integral and the sum in the above equality and we get

$$[V\psi(\cdot)](x^2) = \int_{X_1} d\mu_1(x^1) \langle x^2|x^1 \rangle \langle x^1|\psi),$$

where  $\langle x^2|x^1 \rangle = \sum_n (e_n|x^1 \rangle \langle x^2|e_n)$ , as desired.  $\square$

At this stage, let us mention that Antoine and Grossmann initiated the study of vector spaces with an inner product defined partially, see for instance [7, 50, 23].

#### 3.2.5 The spectral theorem and generalized eigenvectors

The nuclear spectral theorem asserts that any unitary or self-adjoint operator of the RHS  $\Phi \subset \mathcal{H} \subset \Phi^\times$  admits a complete family of continuous generalized eigenvectors (see the proof in [8] and a revised and corrected version in [43]). Next we provide an elementary construction of a complete family of algebraic generalized eigenvectors for unitary or self-adjoint operators which are cyclic in a Hilbert space. In the case of a RHS  $\Phi \subset \mathcal{H} \subset \Phi^\times$ , our construction is suitable for cyclic unitary or self-adjoint operators having a cyclic vector lying in  $\Phi$ . Observe that this is the case for many physical operators (see the next chapter).

**Theorem 3.2.1.** *Let  $A$  be a cyclic linear operator in  $\mathcal{H}$ . Suppose that there exists a set  $X \subseteq \mathbb{C}$ , a positive measure  $\mu$  on  $X$  and a unitary map  $U : \mathcal{H} \rightarrow L^2(X, d\mu)$  such that  $UAU^*(\psi(x)) = x\psi(x)$  for every  $\psi(x) \in UD(A)$ . Let  $\varphi$  be a cyclic vector of  $A$  and put  $\Lambda = \text{span}\{A^n\varphi : n \in \mathbb{N}\}$ . Then there exists a complete family  $\{F_x\}_{x \in X}$  of generalized eigenvectors of  $A|_\Lambda$  such that  $(U\psi)(x) = F_x(\psi)$  for every  $\psi \in \Lambda$  and  $x \in X$ .*

*Proof.* The linear operator  $UAU^*$  is cyclic and it is easy to see that  $U\varphi$  is a cyclic vector. Hence  $L^2(X, \mu) = \text{span}\{x^n(U\varphi)(x) : n \in \mathbb{N}\}$ . This entails that for every non-negligible subset  $Y$  of  $X$ , we must have  $U\varphi|_Y \neq 0$ . Hence we can choose a true function,  $\psi_0 : X \rightarrow \mathbb{C}$  representative of  $U\varphi$  such that  $\psi_0(x) \neq 0$  for every  $x \in X$ . Consider the functions  $\psi_n : X \rightarrow \mathbb{C}$  defined by  $\psi_n(x) = x^n\psi_0(x)$ . We have  $UAU^*(\psi_n(x)) = \psi_{n+1}(x)$ . We distinguish two cases, either  $\mathcal{H}$  is infinite-dimensional, hence the set  $\{A^k\varphi : k \in \mathbb{N}\}$  is linearly independent; or  $\mathcal{H}$  has finite dimension, hence there exists  $N \in \mathbb{N}$  such that  $\{A^k\varphi : 0 \leq k \leq N\}$  is a basis of  $\mathcal{H}$  and  $\dim \mathcal{H} = N + 1$ . For every  $x \in X$ , consider the linear form  $F_x \in \Lambda^*$  defined by  $F_x(A^n\varphi) = \psi_n(x)$ . Then  $F_x \neq 0$  and  $F_x A|_\Lambda = xF_x$ . Next let us show that the family  $\{F_x\}_{x \in X}$  is complete. Let  $\psi = \sum_{n=0}^l c_n A^n \varphi \in \Lambda$ , where  $l \in \mathbb{N}$  and suppose that  $F_x(\psi) = 0$  for every  $x \in X$ . Since  $\psi_0$  does not vanish on  $X$ , we infer that  $\sum c_n x^n = 0$  for every  $x \in X$ . Consider the complex polynomial  $P = \sum_{k=0}^l c_k X^k$ . Either  $P = 0$ , or it has at most  $l$  roots. Suppose for a moment that  $P \neq 0$  and has degree  $l$ . Then  $X$  must be finite, with cardinality at most  $l$ . This implies that  $\dim \mathcal{H} \leq l$ . On the other hand,  $N \geq l$ , that is  $\dim \mathcal{H} \geq l + 1$ , a contradiction. This completes the proof.  $\square$

**Remark 3.2.1.** *Using the notations of the above proposition, let  $N \in \mathbb{N} \cup \{\infty\}$  be maximal such that  $\{A^n\varphi\}_{0 \leq n \leq N}$  is linearly independent. Then it is easy to see that the norm defined on  $\Lambda$  by  $\|\sum_{n=0}^N c_n A^n \varphi\| = \sum |c_n| (n+1)^n$  makes all the functionals  $F_x$  continuous.*

For the general case of a self-adjoint operator, we have the following : using the notations in Section 2.3.7, we denote by  $\Lambda = \Lambda(\{\varphi^j\}_j)$  the linear span of  $A^k\varphi^j$ , where  $k \in \mathbb{N}$  and  $j \in J$  and let  $\pi_j : \Lambda \rightarrow \text{span}\{A^k\varphi^j : k \in \mathbb{N}\}$  be the natural projection. .

**Theorem 3.2.2.** *Let  $A$  be a self-adjoint linear operator in  $\mathcal{H}$  and let  $\Phi$  be a dense linear subspace of  $\mathcal{H}$  such that  $A\Phi \subseteq \Phi$ . Let  $U : \mathcal{H} \rightarrow \mathcal{K} = \int_X^\oplus H_x d\mu(x)$  be the direct integral representation associated to  $A$ , such that  $UAU^*\psi(x) = x\psi(x)$  for every  $\psi(x) \in UD(A)$ . Then there exists a dense linear subspace  $\Lambda$  of  $\mathcal{H}$  with  $\Lambda \subseteq \Phi$ ,  $A\Lambda \subseteq \Lambda$ , and a family  $\{F_x\}_{x \in \sigma(A)}$  of generalized eigenvectors of  $A|_\Lambda$  such that  $(U\psi)(x) = (F_x(\pi_{i_1}\psi), \dots, F_x(\pi_{i_{n(x)}}\psi))$  for every  $\psi \in \Lambda$ . Moreover, for every  $x$  and  $j \in J_x$ ,  $F_x\pi_j$  is a generalized eigenvector of  $A|_\Lambda$  and the family  $\{F_x\pi_j : x \in \sigma(A), j \in J_x\}$  is complete.*

*Proof.* Since  $\Phi$  is dense in  $\mathcal{H}$ , it contains a spectral basis  $\{\varphi^j\}_{j \in J}$ , where  $J \subseteq \mathbb{N}$ . Consider the representation of  $\mathcal{H}$  defined by  $\mathcal{H}_1 = \oplus_{j \in J} L^2(X_j, d\mu)$  where  $X_j \subseteq \sigma(A)$ ,  $L^2(X_j, d\mu)$  is associated to  $\varphi^j$  as described above. As in the proof of Theorem 3.2.1, for every  $j$ , choose a true function  $\varphi_0^j(x) : X_j \rightarrow \mathbb{C}$  which does not vanish and such that  $\varphi_0^j(x) = \varphi^j(x)$  in  $L^2(X_j, d\mu)$ . Fix  $x \in \sigma(A)$  and  $j$ . Consider the linear functional  $F_x$  defined on  $\Lambda = \Lambda(\{\varphi^j\}_j)$  by  $F_x(A^k\varphi_j) = 0$  if  $x \notin X_j$  and  $F_x(A^k\varphi_j) = x^k\varphi_0^j(x)$  if  $x \in X_j$ . Since the family  $\{A^k\varphi^j : k \in \mathbb{N}, j \in J\}$  is linearly independent, then  $F_x$  is well defined. Fix  $j \in J$  and let  $\psi \in \text{span}\{A^k\varphi^j : k \in \mathbb{N}\}$ . Then  $(U^j\psi)(x) = F_x(\psi)$  for every  $x \in X_j$ . Let  $\psi \in \Lambda$ , then  $\psi = \sum_j \pi_j\psi$ , and

$$(U\psi)(x) = (F_x(\pi_{i_1}\psi), \dots, F_x(\pi_{i_{n(x)}}\psi)).$$

Next let us check that the family  $\{F_x\pi_j\}_{x,j}$  is complete. Let  $\psi \in \Lambda$  and suppose that  $F_x\pi_j\psi = 0$  for every  $x$  and  $j$ . Then, by the above result, for every  $j$ ,  $\pi_j\psi = 0$ . Thus,  $\psi = 0$  as desired.  $\square$

### 3.3 True vectors for a self-adjoint operator

Let  $A$  be a self-adjoint operator in a Hilbert space  $\mathcal{H}$ . We shall see that there exist spectral bases based on polynomials of  $A$  instead of the resolvent. Let  $\psi \in \mathcal{H}$ . Remark that  $P_\psi^A$  has finite moments if and only if  $\psi \in D^\infty(A)$ . In this case, we have

$$\int_{\mathbb{R}} \lambda^n dP_\psi^A = \langle \psi, A^n \psi \rangle, \quad (n \in \mathbb{N}).$$

Put  $\Lambda_\psi = \text{span}\{P^A(\Lambda)\psi : \Lambda \text{ interval}\}$ , so that  $\mathcal{H}_\psi = \overline{\Lambda_\psi}$ . Suppose next that  $\psi \in D^\infty(A)$  and set  $\mathcal{T}\Lambda_\psi = \text{span}\{A^n\psi : n \in \mathbb{N}\}$ . We shall say that  $\psi$  is a true vector for  $A$  if  $\mathcal{H}_\psi = \overline{\mathcal{T}\Lambda_\psi}$ . Hence  $\psi$  is a true vector for  $A$  if and only if polynomials are dense in  $L^2(\mathbb{R}, P_\psi^A)$ . If moreover the moment sequence  $\{\langle \psi, A^n \psi \rangle\}_n$  is determinate, we shall say that  $\psi$  is a fundamental vector for  $A$ . In this case,  $P_\psi^A$  is the unique associated moment measure. Now suppose that the sequence  $\{\langle \psi, A^n \psi \rangle\}_n$  is positive definite. This is equivalent to the fact that the family  $\{A^n\psi : n \in \mathbb{N}\}$  is linearly independent. Then the family  $\{\langle \psi, A^n \psi \rangle\}_n$  is determinate if and only if the operator  $A|_{\mathcal{T}\Lambda_\psi}$  is essentially self-adjoint. On the other hand, if  $\{\langle \psi, A^n \psi \rangle\}_n$  is not determinate, then  $A|_{\mathcal{H}_\psi}$  has a singular spectrum.

Remark that via Theorem 2.3.9, every cyclic self-adjoint operator  $A$  has a true vector  $\psi$  which is a cyclic vector. In particular, every self-adjoint operator  $A$  admits a spectral basis formed by true vectors. If moreover  $A$  has absolutely continuous spectrum, then it admits a spectral basis formed by fundamental vectors.

Observe that if  $\mu_1$  and  $\mu_2$  are two positive regular Borel measures with finite moments and  $U : L^2(\mathbb{R}, d\mu_1) \rightarrow L^2(\mathbb{R}, d\mu_2)$  is a unitary map such that  $UQU^* = Q$ , then it may be that  $\mu_1$  is determinate but  $\mu_2$  is not. Next we provide an elementary concrete example.

**Example 3.3.1.** *Consider the pair of operators  $(P_s, Q)$  in the one dimensional Schrödinger representation  $\mathcal{H}_s = L^2(\mathbb{R}, dx)$ , where  $P_s$  is the momentum operator. Both  $P_s$  and  $Q$  are cyclic, a common fundamental cyclic vector is the Hermite function  $h_0 = e^{-x^2/2}$ . More generally, observe that if  $\psi$  is a true vector for  $P_s$ , then  $\text{supp } \psi = \text{supp } \mathcal{F}\psi = \mathbb{R}$ . In particular,  $\psi$  and  $\mathcal{F}\psi$  are cyclic vectors for  $Q$ . On the other hand, elements of  $\mathcal{C}_c^\infty(\mathbb{R})$  are cyclic vectors for  $P_s$  but are not true vectors. Fix  $g \in \mathcal{C}_c^\infty(\mathbb{R})$ , then  $P_g^{P_s} = |\hat{g}(x)|^2 dx$ . Since  $\hat{h}_0 = h_0$ , then  $P_{h_0}^{P_s} = e^{-x^2} dx$ . With no loss of generality, we suppose that  $\hat{g}(x) \neq 0$  for every  $x$ . Let  $V : L^2(\mathbb{R}, e^{-x^2} dx) \rightarrow L^2(\mathbb{R}, |\hat{g}(x)|^2 dx)$  be the unitary map defined by  $Vf = e^{-x^2/2}(\hat{g}(x))^{-1}f(x)$  for every  $f \in \mathcal{C}[X]$ , then 1 is a fundamental vector for  $Q$  in  $L^2(\mathbb{R}, e^{-x^2} dx)$ , while polynomials are not dense in  $L^2(\mathbb{R}, |\hat{g}(x)|^2 dx)$ .*

### 3.3. TRUE VECTORS FOR A SELF-ADJOINT OPERATOR

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**Remark 3.3.1.** 1. A true cyclic vector  $\varphi$  for  $Q$  in  $L^2(\mathbb{R}, d\mu)$  do necessarily satisfy  $\text{supp}(\mu) \subset \text{supp}(\varphi)$ .

2. Recall that in the case of a finite Borel measure  $\mu$ , the constant function  $x \mapsto 1$  is a cyclic vector for  $Q$  in  $L^2(\mathbb{R}, d\mu)$ . However, it is not a true cyclic vector in general. Indeed, this is equivalent to the fact that polynomials are dense in  $L^2(\mathbb{R}, d\mu)$  which is not always the case. It is however the case for example if  $d\mu$  is finite and with a distribution function which decays faster than polynomials at infinity (the Gaussian measure  $d\mu = e^{-x^2} dx$  for example). This is the case in particular if  $d\mu$  is finite and compactly supported.

## CASE STUDIES

### 4.1 The algebra of the Harmonic oscillator

We describe in this section the number representation and the associated RHS. Let  $\Psi$  be a complex linear space and let  $P, Q : \Psi \rightarrow \Psi$  be linear operators satisfying the canonical commutation rule (CCR), that is  $[P, Q] = -i\hbar I$ . Put

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}Q^2, \quad a = \sqrt{\frac{m\omega}{2\hbar}}Q + \frac{i}{\sqrt{2m\omega\hbar}}P,$$

$$a_+ = \sqrt{\frac{m\omega}{2\hbar}}Q - \frac{i}{\sqrt{2m\omega\hbar}}P, \quad N = a_+a.$$

The following properties, which are well known, are easy to prove

**Lemma 4.1.1.** (1)  $H = \hbar\omega(N + \frac{1}{2}I) = \frac{\hbar\omega}{2}(a_+a + aa_+)$ ,  $[a, a_+] = I$  and  $[a, (a_+)^n] = n(a_+)^{n-1}$ .

(2) If  $\alpha$  is an eigenvalue of  $N$  and  $v$  is an  $\alpha$ -eigenvector, then  $Na_+v = (\alpha + 1)a_+v$  and  $Nav = (\alpha - 1)av$ .

**Remark 4.1.1.** Suppose that a scalar product is defined on  $\Psi$ . Then  $P$  and  $Q$  are symmetric if and only if  $a_+^* = a$ .

Next we state the basic properties of irreducible algebraic representations of the Heisenberg algebra generated by  $I, P, Q$ , such that the Hamiltonian has a minimal real eigenvalue. This is slightly more general than [14] (see also [33]), since we do not suppose that  $\Psi$  is endowed with a scalar product  $(\cdot, \cdot)$ . We provide a proof for completeness.

**Theorem 4.1.1.** Suppose that  $H$  admits a minimal real eigenvalue  $\lambda$ . Let  $u$  be a  $\lambda$ -eigenvector and suppose that  $\Psi$  coincides with the minimal complex linear subspace containing  $u$  and invariant under  $P$  and  $Q$ . Then

(1)  $\lambda = \frac{\omega\hbar}{2}$  and 0 is the minimal eigenvalue of  $N$ . Set  $\varphi_0 = u$  and for every  $k \geq 1$ , set  $\varphi_k := (a_+)^k \varphi_0$ . Then  $\varphi_k \neq 0$  and  $N\varphi_k = k\varphi_k$ .

(2)  $\Psi$  coincides with  $\text{span}\{\varphi_0, \varphi_1, \dots\}$  and  $\sigma(N, \Psi) = \mathbb{N}$ .

(3) There exists a unique scalar product  $(\cdot, \cdot)$  on  $\Psi$  for which  $P$  and  $Q$  are symmetric and  $\|\varphi_0\| = 1$ . In this case, the states  $\{\varphi_k\}_k$  are orthogonal.

(4) For all  $k \geq 0$  let  $\phi_k = \frac{1}{\sqrt{k!}}\varphi_k$ . Then the family  $\{\phi_k\}_k$  is an orthonormal basis of  $\Psi$ . Moreover,  $a\phi_0 = 0$  and we have

$$a_+\phi_k = \sqrt{k+1}\phi_{k+1}, \quad a\phi_l = \sqrt{l}\phi_{l-1}, \quad N\phi_k = k\phi_k, \quad k \in \mathbb{N}, l \in \mathbb{N}^*.$$

#### 4.1. THE ALGEBRA OF THE HARMONIC OSCILLATOR

*Proof.* For (1), let  $\alpha$  be the corresponding minimal real eigenvalue of  $N$ . Then,  $\alpha - 1$  is not an eigenvalue of  $N$  and it follows from Lemma 4.1.1 that  $au = 0$ . Therefore  $\alpha u = Nu = 0$ , hence  $\alpha = 0$ . Now for the second assertion it is easy to check, using once again Lemma 4.1.1, that for every  $k$ ,  $N\varphi_k = k\varphi_k$ . Suppose that for some  $k \geq 0$ ,  $\varphi_k \neq 0$ , then since

$$\varphi_k = [a, a_+] \varphi_k = a\varphi_{k+1} - N\varphi_k = a\varphi_{k+1} - k\varphi_k,$$

we infer that  $\varphi_{k+1} \neq 0$ . Thus by induction,  $\varphi_k \neq 0$  for all  $k \geq 0$ .

Next to prove (2), set  $V = \text{span}\{\varphi_0, \varphi_1, \dots\}$ . Then  $V \subseteq \Psi$  and  $u \in V$ . On the other hand, we show by induction on  $k$  that  $a\varphi_k = k\varphi_{k-1}$  for every  $k \geq 1$ . Thus  $V$  is invariant under  $a$  and  $a_+$ , hence it is invariant under  $P$  and  $Q$ . Moreover we get  $V = \Psi$ . For the second assertion, we already know that  $\mathbb{N} \subset \sigma(N, \Psi)$ . If  $\lambda \notin \mathbb{N}$ , we check easily that  $N - \lambda$  is bijective and hence  $\lambda \notin \sigma(N, \Psi)$ .

For (3), suppose that there is a scalar product  $(\cdot, \cdot)$  on  $\Psi$  for which  $P$  and  $Q$  are symmetric. We have for every  $k \in \mathbb{N}$  and  $l \in \mathbb{N}^*$ ,

$$(\varphi_{k+1}, \varphi_l) = (\varphi_k, a\varphi_l) = \frac{l}{k+1} (a\varphi_{k+1}, \varphi_{l-1}) = \frac{l}{k+1} (\varphi_{k+1}, \varphi_l).$$

Moreover,  $(a_+\varphi_k, \varphi_0) = 0 = (\varphi_{k+1}, \varphi_0)$ . Thus, the family  $\{\varphi_k\}_k$  is orthogonal. On the other hand, we have

$$(a_+\varphi_k, \varphi_{k+1}) = (\varphi_{k+1}, \varphi_{k+1}), \quad (\varphi_k, a\varphi_{k+1}) = (k+1)(\varphi_k, \varphi_k).$$

Hence we must have  $(\varphi_{k+1}, \varphi_{k+1}) = (k+1)(\varphi_k, \varphi_k)$ . Suppose that  $\|\varphi_0\| = 1$ . Then, by induction, we see that  $\|\varphi_{k+1}\| = \sqrt{k+1}\|\varphi_k\|$  for all  $k \geq 0$ . Finally, it is clear that the formulas

$$(\varphi_k, \varphi_l) = \delta_{kl}\|\varphi_k\|^2, \quad \|\varphi_{k+1}\| = \sqrt{k+1}\|\varphi_k\|, \quad \|\varphi_0\| = 1,$$

define a scalar product on  $\Psi$  for which  $a_+^* = a$ .

For (4), we prove easily that the family  $\{\varphi_k\}$  is orthonormal and the last assertion is easy to check.  $\square$

**Remark 4.1.2.** *It is easy to see (from the proof) that the condition  $H$  admits a minimal real eigenvalue in the above theorem may be replaced by the condition there exists  $u \in \Psi \setminus \{0\}$  such that  $au = 0$ .*

From now on, we suppose that  $\Psi$  is endowed with the scalar product described in the above theorem. Denote by  $\mathcal{H}$  the Hilbert space completion of  $(\Psi, (\cdot, \cdot))$ . We shall use the notation  $\varphi_n = |n\rangle$ .

Let us now turn to the algebraic relation of symmetry between  $P$  and  $Q$ . Put  $|-1\rangle = 0$ . Then we have for every  $n \in \mathbb{N}$

$$Q|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle), \quad (4.1)$$

$$P|n\rangle = -i\sqrt{\frac{\hbar m\omega}{2}} (\sqrt{n}|n-1\rangle - \sqrt{n+1}|n+1\rangle). \quad (4.2)$$

Put  $\{n\rangle = i^n|n\rangle$ . Then

$$P\{n\rangle = \sqrt{\frac{\hbar m\omega}{2}} (\sqrt{n}\{n-1\rangle + \sqrt{n+1}\{n+1\rangle).$$

That is, if  $c = \frac{1}{m\omega}$ , then  $M(cP, \{\{n\rangle\}_n) = M(Q, \{|n\rangle\}_n)$ . Analogously, if  $c' = -m\omega$ , then  $M(c'Q, \{\{n\rangle\}_n) = M(P, \{|n\rangle\}_n)$ . Let  $\Gamma: \mathcal{H} \rightarrow \mathcal{H}$  be the unitary operator that satisfies  $\Gamma(|n\rangle) = \{n\rangle$ , then  $c\Gamma^*P\Gamma = Q$ .

Now for completeness, we provide an elementary proof of the fact that the operators  $P, Q, H$  are essentially self-adjoint.

**Proposition 4.1.1.** *The operators  $P, Q, H: \Psi \subset \mathcal{H} \rightarrow \mathcal{H}$  are essentially self-adjoint.*

*Proof.* Let us first calculate  $N^*$ . Let  $\psi = \sum_0^\infty c_k|k\rangle \in D(N^*)$  and put  $\eta = N^*\psi = \sum_0^\infty d_k|k\rangle$ . Then it follows from the equality  $(\eta, n) = (\psi|N|n)$  for every  $|n\rangle$  that  $d_n = nc_n$ . Hence

$$D(N^*) = \left\{ \sum_0^\infty c_k|k\rangle \in \mathcal{H} : \sum_0^\infty k^2|c_k|^2 < \infty \right\}, \quad N^* \sum_0^\infty c_k|k\rangle = \sum_0^\infty kc_k|k\rangle.$$

Now it is clear that  $N^*$  coincides with the closure  $N$  of  $\mathcal{H}$ , hence  $N$  is essentially self-adjoint.

Next, for  $Q$ , we assume that  $\frac{\hbar}{2m\omega} = 1$ . Let  $\psi = \sum_0^\infty c_k |k\rangle \in D(Q^*)$  and put  $\eta = Q^* \psi$ . Put  $c_{-1} = 0$ . It follows from equation (4.1) that

$$(\eta, n) = (\psi | Q | n) = \sqrt{n} \bar{c}_{n-1} + \sqrt{n+1} \bar{c}_{n+1} \quad (n \geq 1), \quad (\psi | Q | 0) = c_1.$$

Hence

$$\eta = \sum_0^\infty (n | \eta) | n \rangle = \sum_0^\infty (\sqrt{n} c_{n-1} + \sqrt{n+1} c_{n+1}) | n \rangle.$$

Observe that

$$\sum_0^k c_n Q | n \rangle = \sum_0^{k-1} [\sqrt{n} c_{n-1} + \sqrt{n+1} c_{n+1}] | n \rangle + \sqrt{k} c_{k-1} | k \rangle + \sqrt{k+1} c_k | k+1 \rangle.$$

On the other hand, since  $\sum_n |c_n|^2 < \infty$ , we can choose a subsequence  $\{c_{n_k}\}_k$  of  $\{c_n\}_n$  such that  $\lim_k \sqrt{n_k} c_{n_k-1} = 0$ . But  $\sum_n |\sqrt{n} c_{n-1} + \sqrt{n+1} c_{n+1}|^2 < \infty$ , hence

$$\lim_k \sqrt{n_k + 1} c_{n_k} = 0.$$

This entails that  $\lim_k \sum_0^{n_k} c_n Q | n \rangle = \eta$  in  $\mathcal{H}$ . That is,  $D(\bar{Q}) = D(Q^*)$  and  $Q$  is essentially self-adjoint. Finally,  $P = c^{-1} \Gamma Q \Gamma^*$  is essentially self adjoint.  $\square$

Since  $H$  is essentially self-adjoint, it follows from [51, Theorem 5] that the realization of the (CCR) associated to  $\Psi$  is integrable (see also [52]).

Next we endow the linear space  $\Psi$  with a topology that makes all the powers of  $H$  continuous. Let  $\tau$  be the topology defined on  $\Psi$  by the family of scalar products  $\{\langle \cdot, \cdot \rangle_n\}_{n \in \mathbb{N}^*}$  where for every  $n$ , the norm  $\|\cdot\|_n$  associated to  $\langle \cdot, \cdot \rangle_n$  is defined by  $\|\varphi\|_n = \|(N+I)^{n/2} \varphi\|$  for every  $\varphi \in \Psi$ . Then it is easy to see that  $N, a_+$  and  $a$  are continuous on  $\Psi$  and if  $S \in \{N, a, a_+\}$ , then

$$\|S\varphi\|_n \leq \|\varphi\|_{n+2}, \quad (n \in \mathbb{N}^*),$$

Denote by  $\Phi$  the completion of  $\Psi$  with respect to the topology  $\tau$ , then

$$\Phi = \left\{ \sum_n c_n |n\rangle \in \mathcal{H} : \sum_n c_n (N+I)^{k/2} |n\rangle \in \mathcal{H}, \forall k \in \mathbb{N} \right\}. \quad (4.3)$$

In particular, the  $\tau$  topology defines a metric on  $\Phi$  [8]. Denote by  $\mathcal{A}(\Psi)$  the unital associative complex algebra of operators on  $\Psi$  generated by  $a, a_+$  and the relation  $[a, a_+] = I$ . Then  $\mathcal{A}(\Psi)$  is the first Weyl algebra (also called the Heisenberg-Weyl algebra), it was introduced by Weyl and a systematic study was initiated in [53]. Clearly, every element  $A \in \mathcal{A}(\Psi)$  can be extended to a continuous operator on  $\Phi$ . Moreover, if  $A$  is symmetric, its extension remains symmetric. Denote by  $\mathcal{A}(\Phi)$  the algebra formed by all those extensions. We shall keep the same notations for  $A \in \mathcal{A}(\Psi)$  and its continuous extension, and we shall write the symbol  $\mathcal{A}$  for either  $\mathcal{A}(\Phi)$  or  $\mathcal{A}(\Psi)$ , when there is no risk of ambiguity.

Denote by  $\|\cdot\|_0 = \|\cdot\|$  the initial norm of  $\Psi$ . Then  $\|\cdot\|_n \leq \|\cdot\|_m$  for all  $n \leq m$  in  $\mathbb{N}$ . For every  $n$ , denote by  $\Phi_n$  the completion of  $\Phi$  with respect to  $\|\cdot\|_n$ . It is easy to see that

$$\Phi_n = \left\{ \sum_k c_k \phi_k \in \mathcal{H} : \sum_k |c_k|^2 (k+1)^n < \infty \right\} \text{ and } \Phi = \bigcap_{n \in \mathbb{N}} \Phi_n.$$

The assumption of nuclearity is crucial in the proof of the nuclear spectral theorem, see the proofs of the theorem in [8, 43]. As it was pointed out by Roberts [13, p. 107], it is not difficult to prove nuclearity for this system. Though we shall not use explicitly the nuclear spectral theorem, we provide here an elementary proof of the nuclearity of  $\Phi$ . Indeed, we have a stronger property

**Lemma 4.1.2.** *Let  $n, m \in \mathbb{N}^*$  such that  $m \leq n$  and let  $i : \Phi_n \rightarrow \Phi_m$  be the natural injection. Then if  $n - m > 2$ ,  $i$  is a trace-class operator. In particular,  $\Phi$  is nuclear.*

## 4.2. EIGENSTATES OF THE HAMILTONIAN IN FUNCTION SPACES

*Proof.* Let  $\varphi = \sum_{j=0}^{\infty} c_j |j\rangle$  be an element of  $\Phi_n$ . For all  $j \geq 0$ , put  $\lambda_j = \frac{1}{(j+1)^{\frac{n-m}{2}}}$ . Then  $\varphi = \sum_{j=0}^{\infty} \lambda_j (j+1)^{\frac{m}{2}} c_j |j\rangle_m$  and  $(k|\varphi)_n = (k+1)^{\frac{m}{2}} c_k$  for every  $k \in \mathbb{N}$ . This entails that  $\varphi = \sum_{j=0}^{\infty} \lambda_j (j|\varphi)_n |j\rangle_m$ . Now it is clear that if  $n-m > 2$ ,  $i$  is of trace-class.  $\square$

Let  $\Phi^\times$  be the topological antidual space of  $\Phi$ . It is now easy to conclude that  $\Phi \subset \mathcal{H} \subset \Phi^\times$  is a RHS [8].

## 4.2 Eigenstates of the Hamiltonian in function spaces

Next we pursue our study of the algebra of the quantum harmonic oscillator, and we see how the three other fundamental representations (position, momentum and Bargmann-Fock) arise naturally, using fundamental operators of the system and their generalized eigenvectors. The three spaces are spaces of functions, associated to pairs  $(A, B)$  of operators in the first Weyl algebra that satisfy  $[A, B] = I$ ,  $A\psi(x) = x\psi(x)$  and  $B\psi(x) = -\frac{d\psi(x)}{dx}$ . At this stage, a natural question presents itself: Are there other important examples of representations overlooked? In other words, can we, by using the generalized eigenvectors and associated representations, find new important representations physically? From our study, it seems that the first step to finding an answer is the characterization of  $A \in \mathcal{A}$  that admits a pair  $B$  such that  $[A, B] = I$ ? This condition was partially investigated in [54]. The authors here showed that in this case the centralizer of  $A$  is  $\mathbb{C}[A]$ . Other necessary conditions were given in [55]. But it seems that this question is still open [56].

Let  $z \in \mathbb{C}$ . It is easy to see that  $|0\rangle \notin (Q-z)\Psi$  and  $(Q-z)\Psi + \mathbb{C}|0\rangle = \Psi$ . Hence  $z$  is a generalized eigenvalue and the associated space of generalized eigenvectors has dimension one. With respect to the Hilbert space  $\mathcal{H}$ , Hermite polynomials correspond to the algebraic generalized eigenvectors of  $Q$  and  $P$ . Indeed, more exactly every solution  $|F\rangle$  of the equation  $Q^\times F = zF$  in  $\overline{\Psi^*}$  is defined by the relations  $FQ|n\rangle = zF|n\rangle$  for every  $n$ . By solving the associated recurrence relations, see for instance [57] or [14], we get

$$(n, F_z) = \frac{1}{\sqrt{2^n n!}} (0|F_z) H_n(\sqrt{m\omega/\hbar} z). \quad (4.4)$$

On the other hand, for  $G \in \overline{\Psi^*}$ ,

$$P^\times G = zG \Leftrightarrow G\Gamma Q = czG\Gamma \Leftrightarrow G = F_{cz}\Gamma^*.$$

Thus every solution of the equation  $P^\times G = zG$  in  $\overline{\Psi^*}$  is defined by

$$(n, G_z) = \frac{i^n}{\sqrt{2^n n!}} (0|G_z) H_n(\sqrt{1/\hbar m \omega} z).$$

Next we use properties of Hermite polynomials to show the continuity of  $F_x$  and  $G_x$ , for  $x \in \mathbb{R}$ .

**Lemma 4.2.1.** *Let  $x \in \mathbb{R}$  and let  $|F\rangle$  be the element of  $\overline{\Psi^*}$  defined by  $(n|F) = \frac{1}{\sqrt{2^n n!}} H_n(x)$ . Then  $|F\rangle$  is continuous for the topology induced by the norm  $\|\cdot\|_n$ , for every  $n \in \mathbb{N}^*$ . In particular  $F \in \Psi^\times$ .*

*Proof.* First observe that if  $|F\rangle$  is continuous for  $\|\cdot\|_n$  and  $n \leq m$ , then  $|F\rangle$  is continuous for  $\|\cdot\|_m$ . Let  $\varphi = \sum_{n=0}^l c_n |n\rangle$  be an element of  $\Psi$  and let  $k \in \mathbb{N}^*$ . Then

$$(\varphi|F) = \sum_{n=0}^l \overline{c_n} (n+1)^{k/2} \frac{1}{\sqrt{2^n n!} (n+1)^k} H_n(x).$$

Thus

$$\begin{aligned} |(\varphi|F)| &\leq \left[ \sum_{n=0}^l |c_n|^2 (n+1)^k \right]^{1/2} \left[ \sum_{n=0}^l \frac{1}{2^n n! (n+1)^k} H_n(x)^2 \right]^{1/2} \\ &\leq \|\varphi\|_k \left[ \sum_{n=0}^{\infty} \frac{1}{2^n n! (n+1)^k} H_n(x)^2 \right]^{1/2}, \end{aligned}$$

where the convergence of the second series can be deduced by using for instance the following inequality (see [?])

$$H_n^2(x) \leq \frac{C e^{x^2} 2^n n!}{\sqrt{2n+1-x^2}}, \quad |x| < \sqrt{2n+1}.$$

for some positive constant  $C$ . □

Thus, for every  $x \in \mathbb{R}$ , by considering the continuous extensions, we may suppose that  $F_x$  and  $G_x$  lie in  $\Phi^\times$ . Moreover, observe that  $F_x$  and  $G_x$  are continuous with respect to  $\{|n\rangle\}_n$ . In particular, we shall write

$$\begin{aligned} |F_x\rangle &= \sum_{n=0}^{\infty} \frac{1}{\sqrt{2^n n!}} (0|F_x\rangle H_n(\sqrt{m\omega/\hbar} x)|n\rangle, \\ |G_x\rangle &= \sum_{n=0}^{\infty} \frac{i^n}{\sqrt{2^n n!}} (0|G_x\rangle H_n(\sqrt{1/\hbar m\omega} x)|n\rangle. \end{aligned}$$

**Proposition 4.2.1.** *Suppose that the map  $x \mapsto (0|F_x\rangle$  is continuous on  $\mathbb{R}$ , then the family  $\{F_x\}_{x \in \mathbb{R}}$  is strongly continuous. Analogously, if the map  $x \mapsto (0|G_x\rangle$  is continuous on  $\mathbb{R}$ , then the family  $\{G_x\}_{x \in \mathbb{R}}$  is strongly continuous.*

*Proof.* Put  $f(x) = (0|F_x\rangle$  for every  $x \in \mathbb{R}$ . Let  $\{x_n\}_n$  be a sequence of real numbers converging to  $x \in \mathbb{R}$  and let  $\phi = \sum_n c_n |n\rangle \in \Phi$ . Put  $\alpha = \sqrt{m\omega/\hbar}$ . Then, since the map  $f$  is continuous, we get

$$\lim_k (\phi|F_{x_k}\rangle = f(x) \lim_k \lim_N \sum_{n=0}^N \frac{c_n}{\sqrt{2^n n!}} H_n(\alpha x_k).$$

But the series  $\sum_n \frac{c_n}{\sqrt{2^n n!}} H_n(\alpha x)$  converges uniformly in a neighborhood of  $x$ , thus

$$\lim_k (\phi|F_{x_k}\rangle = f(x) \lim_N \lim_k \sum_{n=0}^N \frac{c_n}{\sqrt{2^n n!}} H_n(\alpha x_k) = (\phi|F_x\rangle,$$

as desired. □

Now from the well known orthogonality relation satisfied by Hermite polynomials, we deduce the following relation for every  $\alpha \in \mathbb{R}$

$$\frac{\alpha}{2^n n! \sqrt{\pi}} \int_{\mathbb{R}} H_n(\alpha x) H_m(\alpha x) e^{-\alpha^2 x^2} dx = \delta_{nm}, \quad \forall n \in \mathbb{N}. \quad (4.5)$$

Put  $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ . Next observe that for every function  $g : \mathbb{R} \rightarrow \mathbb{C}$  which does not vanish, the family  $\{g(x)|F_x\rangle\}_{x \in \mathbb{R}}$  is measure-complete with respect to the measure

$$d\mu = \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2} |g(x)|^{-2} dx.$$

Hence it is complete by Proposition 3.2 and the family  $\{g(x)\langle F_x|n\rangle\}_{x \in \mathbb{R}}$  is orthonormal. By using the well known fact that Hermite functions constitute an orthogonal basis of  $L^2(\mathbb{R}, dx)$ , we conclude that  $\{\frac{g(x)}{\sqrt{2^n n!}} H_n(\alpha x)\}$  is an orthonormal basis of  $L^2(\mathbb{R}, d\mu)$ .

Next we see that Hermite functions are associated to the pairs of operators  $(Q, P)$  and  $(P, Q)$ .

**Proposition 4.2.2.** *Let  $\mathcal{H}$  be a Hilbert space, and let  $U : \mathcal{H} \rightarrow \mathcal{H}$  be unitary such that  $U\Psi$  is a space of  $\mathcal{C}^\infty$ -functions on  $\mathbb{R}$ . Then  $UQU^*\psi(x) = x\psi(x)$  and  $UPU^*\psi(x) = -i\hbar\psi'(x)$  for every  $\psi(x) \in U\Psi$  if and only if there exists  $\lambda \in \mathbb{C}$  such that*

$$U|n\rangle = \lambda \frac{1}{\sqrt{2^n n!}} h_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right).$$

Moreover, for  $\lambda = (m\omega/\hbar\pi)^{1/4}$ , the representation  $\mathcal{H}$  is isomorphic to  $L^2(\mathbb{R}, dx)$ .

## 4.2. EIGENSTATES OF THE HAMILTONIAN IN FUNCTION SPACES

*Proof.* Suppose that  $UQU^*\psi(x) = x\psi(x)$  and  $UPU^*\psi(x) = -i\hbar\psi'(x)$  for every  $\psi(x) \in U\Psi$ . Let  $x \in \mathbb{R}$ . It follows from Lemma 3.2.1 and the equality (4.4) that

$$\delta_x U|n\rangle = \frac{1}{\sqrt{2^n n!}} f(x) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right),$$

where  $f : X \rightarrow \mathbb{C}$  is a map which does not vanish. Put  $U|n\rangle = \psi_n$ . Then  $\psi_0(x) = f(x)$ ,  $\psi_1(x) = \sqrt{\frac{2m\omega}{\hbar}} x f(x)$ , and  $UPU^*\psi_0(x) = im\omega x f(x)$ . On the other hand, observe that

$$UPU^*\psi_0(x) = -i\hbar\psi_0'(x) \Leftrightarrow -i\hbar f'(x) = im\omega x f(x).$$

Hence there exists  $\lambda \in \mathbb{C}$  such that  $f(x) = \lambda e^{-\frac{m\omega}{2\hbar} x^2}$ . Now for the converse, it is enough to calculate  $UPU^*\psi_n(x)$  for every  $n$ . With no loss of generality, we may put  $\lambda = 1$ . Recall the following recurrence formula satisfied by Hermite functions [58, p. 187]

$$h_n'(x) = nh_{n-1}(x) - \frac{1}{2}h_{n+1}(x).$$

Substituting  $h_n$  with its expression in terms of  $\psi_n$  gives

$$-i\hbar\psi_n'(x) = -i\sqrt{\frac{\hbar m\omega}{2}} (\sqrt{n} \psi_{n-1}(x) - \sqrt{n+1} \psi_{n+1}(x)),$$

as desired.

Now for the last assertion, we apply once again the fact that Hermite functions form an orthogonal basis of  $L^2(\mathbb{R}, dx)$ . Since the vector  $U|n\rangle$  must be unitary, we use equation (4.5) and we deduce the exact value of  $\lambda$ .  $\square$

Denote by  $U : \mathcal{H} \rightarrow L^2(\mathbb{R}, dx)$  the unitary map between the number representation and position space which is described in the above proposition. By using the induced topology from  $\Phi$ , and the fact that Hermite functions lie in the Schwartz space  $\mathcal{S}(\mathbb{R})$ , we check easily that  $U\Phi$  coincides with  $\mathcal{S}(\mathbb{R})$ . Now we may use the position representation to check that  $\sigma(\bar{Q}, \mathcal{H}) = \sigma(U\bar{Q}U^*, L^2(\mathbb{R}, dx)) = \mathbb{R}$ . A detailed study can be found in [38, p. 54], or we can check it directly. Indeed, observe first observe that

$$D(U\bar{Q}U^*) = \{\psi(x) \in L^2(\mathbb{R}, dx) : x\psi(x) \in L^2(\mathbb{R}, dx)\}.$$

On the other hand, let  $\lambda \in \mathbb{R}$  and set  $\theta_n(x) = \sqrt{n/2} \mathbb{1}_{[\lambda-1/n, \lambda+1/n]}$ , then  $\|\theta_n\|_2 = 1$ , while  $\lim_n \|(U\bar{Q}U^* - \lambda)\theta_n\|_2 = 0$ . Hence  $(U\bar{Q}U^* - \lambda)^{-1}$  cannot be bounded. Consider the trivial (true) function  $\varepsilon_\lambda$  defined on  $\mathbb{R}$  by  $\varepsilon_\lambda(\lambda) = 1$  and  $\varepsilon_\lambda(x) = 0$  if  $x \neq \lambda$ . It is clear that  $\varepsilon_\lambda$  is a  $\lambda$ -eigenvector of the operator  $\psi(x) \mapsto x\psi(x)$  defined on the linear space of functions on  $\mathbb{R}$ . Moreover, observe that the family of maps  $\{\sqrt{2/n} \theta_n(x)\}_n$  converges simply to  $\varepsilon_\lambda$ . Finally, let  $z \in \mathbb{C} \setminus \mathbb{R}$ . It is well known and easy to see that by basic distribution theory,  $F_z U^*$  cannot be a tempered distribution. Thus, the functional  $F_z$  is not continuous on  $\Phi$ .

Analogously to the position space, we obtain the following characterization of the momentum space

**Proposition 4.2.3.** *Let  $\mathcal{H}$  be a Hilbert space, and let  $U : \mathcal{H} \rightarrow \mathcal{H}$  be unitary such that  $U\Psi$  is a space of  $\mathcal{C}^\infty$ -functions on  $\mathbb{R}$ . Then  $UPU^*\psi(x) = x\psi(x)$  and  $UQU^*\psi(x) = i\hbar\psi'(x)$  for every  $\psi(x) \in U\Psi$  if and only if there exists  $\lambda \in \mathbb{C}$  such that*

$$U|n\rangle = \lambda \frac{(-i)^n}{\sqrt{2^n n!}} h_n\left(\sqrt{1/\hbar m\omega} x\right).$$

Moreover, for  $\lambda = (1/\hbar m\omega\pi)^{1/4}$ , the representation  $\mathcal{H}$  is isomorphic to  $L^2(\mathbb{R}, dx)$ .

Put

$$|x\rangle = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \sum_n \frac{1}{\sqrt{2^n n!}} h_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) |n\rangle,$$

and

$$|p\rangle = \left(\frac{1}{\hbar m \omega \pi}\right)^{1/4} \sum_n \frac{i^n}{\sqrt{2^n n!}} h_n(1/\sqrt{\hbar m \omega} x) |n\rangle.$$

To find  $\langle p, x \rangle$ , one may use the fact that  $\mathcal{F}(h_n(x)) = (-i)^n h_n(p)$  (see for instance [?]), where  $\mathcal{F}$  is the unitary map defined on  $L^2(\mathbb{R}, dx)$  as a completion of the Fourier transform on the Schwartz space

$$\mathcal{F}\{f\}(p) = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{-ipx} f(x) dx, \quad f \in \mathcal{S}(\mathbb{R}).$$

By rescaling, one gets the desired formulas (see [14]). Here we shall use Lemma 3.2.3. Observe that all the maps  $|x\rangle$  and  $|p\rangle$  are continuous with respect to the basis  $\{|n\rangle\}_n$ , and it follows from Mehler's formula for Hermite polynomials that

$$\sum_n \langle e_n | x \rangle \langle p | e_n \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} = \langle p, x \rangle.$$

Arguing analogously, we show that  $\langle x, p \rangle = \overline{\langle p, x \rangle}$ .

The canonical coherent states, eigenvectors of the annihilation operator are well known and easy to compute. If  $z \in \mathbb{C}$ , every solution  $B_z$  of the equation  $a_+^\times B = zB$  in  $\Psi^*$  has the form  $B_z = \sum_{n=0}^{\infty} \langle 0 | B_z \rangle \frac{z^n}{\sqrt{n!}} |n\rangle$ , and  $B_z \in \mathcal{H}$ . It is well known that  $\{\frac{z^n}{\sqrt{n!}}\}_n$  is an orthonormal family with respect to the measure  $e^{-|z|^2} dz$ , the closed subspace of  $L^2(\mathbb{C}, e^{-|z|^2} dz)$  generated by this family is the Bargmann-Fock space

$$\mathcal{F} = \{\psi : \mathbb{C} \rightarrow \mathbb{C}, \quad \psi \text{ is analytic and } \int |\psi(z)|^2 e^{-|z|^2} dz < \infty\},$$

In particular, the family  $\{B_z\}_{z \in \mathbb{C}}$  is measure-complete. By Section 3.2, for every measurable map  $g : \mathbb{C} \rightarrow \mathbb{C}$  which does not vanish, we can associate a representation to the family of generalized eigenvectors  $\{g(z)|B_z\rangle\}_{z \in \mathbb{C}}$ . Next we see that to get a unitary representation associated to the pair  $(a, a^+)$ , the map  $g$  must be a constant. In particular, the representation must be isomorphic to  $\mathcal{F}$ .

**Proposition 4.2.4.** *Let  $\mathcal{H}$  be a Hilbert space and let  $U : \mathcal{H} \rightarrow \mathcal{H}$  be unitary such that  $U\Psi$  is a space of holomorphic functions on  $\mathbb{C}$ . Then  $Ua^+U^*\psi(z) = z\psi(z)$  and  $UaU^*\psi(z) = \partial_z\psi(z)$  for every  $\psi(z) \in U\Psi$  if and only if there exists  $\lambda \in \mathbb{C}$  such that*

$$(U|n\rangle)(z) = \lambda \frac{z^n}{\sqrt{n!}}.$$

Furthermore,  $\mathcal{H}$  can be seen as a RKHS, its reproducing kernel is  $K(z', z) = \lambda e^{\bar{z}'z}$  and for  $\lambda = 1$ , the representation  $\mathcal{H}$  is isomorphic to  $\mathcal{F}$ .

*Proof.* Put  $\psi_n(z) = (U|n\rangle)(z)$ . Since  $Ua^+U^*\psi(z) = z\psi(z)$  for every  $\psi(z) \in U\Psi$ , by Lemma 3.2.1,  $\delta_z$  is a generalized eigenvector for  $a^+$  with respect to  $z$ , that is,  $\delta_z = B_{\bar{z}}$ . Hence  $\psi_n(z) = \langle B_{\bar{z}} | n \rangle = \langle B_{\bar{z}} | 0 \rangle \frac{z^n}{\sqrt{n!}}$ . On the other hand, it follows from the equality  $UaU^*\psi_0 = \partial_z\psi_0 = 0$  that  $\partial_z \langle B_{\bar{z}} | 0 \rangle = 0$  for all  $z \in \mathbb{C}$ . Thus the map  $z \mapsto \langle B_{\bar{z}} | 0 \rangle$  is a constant  $\lambda$ . The converse is immediate. Now it is clear that we can assume that the completion  $\mathcal{H}$  of  $U\Psi$  is constructed with holomorphic functions.

For the rest of the proof, we suppose that  $\lambda = 1$ . To get the reproducing kernel, we use the fact that evaluation maps are continuous with respect to the norm on  $U\Phi$ . Hence for every  $\psi(\cdot) \in U\Phi$ ,

$$\delta_z \psi(\cdot) = \delta_z \left( \sum_n \langle \psi_n(\cdot), \psi(\cdot) \rangle \psi_n(\cdot) \right) = \sum_n \langle \psi_n(\cdot), \psi(\cdot) \rangle \frac{z^n}{\sqrt{n!}}.$$

Hence  $\delta_z = \langle \sum_n \frac{\bar{z}^n}{\sqrt{n!}} \psi_n(\cdot), \cdot \rangle$ . This implies that  $K(z, z') = \sum_n \frac{\bar{z}^n}{\sqrt{n!}} \psi_n(z')$ , as desired. The rest of the proof is immediate.  $\square$

### 4.3. DIAGONALIZING THE FREE HAMILTONIAN BY USING ALGEBRAIC GENERALIZED EIGENVECTORS

Put  $|z\rangle = \sum_n \frac{z^n}{\sqrt{n!}}|n\rangle$ . Then  $|z\rangle \in \Phi$  and the generalized eigenvector  $|x\rangle$  is well defined on  $|\bar{z}\rangle$ . Moreover, we have

$$\langle \bar{z}|x\rangle = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-m\omega x^2/2\hbar} \sum_n \frac{1}{n!} \left(\frac{z}{\sqrt{2}}\right)^n H_n(\sqrt{m\omega/\hbar} x)$$

By using the exponential generating function of the Hermite polynomials, we get

$$\langle \bar{z}|x\rangle = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp(\sqrt{2m\omega/\hbar}xz - \frac{1}{2}(z^2 + m\omega/\hbar x^2)).$$

Now it follows from Lemma 3.2.3 that the unitary map corresponding to the change from position space to  $\mathcal{F}$  is given by

$$\Upsilon : L^2(\mathbb{R}, dx) \rightarrow \mathcal{F}, \quad \Upsilon(\psi(x))(z) = \int_{\mathbb{R}} dx \langle \bar{z}, x \rangle \psi(x).$$

This corresponds to the well known Bargmann transform [59].

On the other hand, since  $a|0\rangle = 0$ , there is no Hilbert space  $\mathcal{H}$ , completion of a space of functions and unitary map  $U : \mathcal{H} \rightarrow \mathcal{H}$  such that  $UaU^*\psi(x) = x\psi(x)$ . This can be also deduced from the fact that the operator  $a$  does not admit an algebraic generalized eigenvector.

## 4.3 Diagonalizing The free Hamiltonian by using algebraic generalized eigenvectors

### 4.3.1 The Hilbert spaces $\mathcal{H}_a, \mathcal{H}_s, \mathcal{H}_b$ and $\iota : \mathcal{H}_b \rightarrow \mathcal{H}_s$

Denote by  $(\mathcal{H}_a, P_a, Q_a)$  the Heisenberg representation of quantum states for a point particle of mass  $m$  moving on the real line under the potential  $\frac{1}{2}m\omega^2 x^2$ , where  $\mathcal{H}_a = l^2(\mathbb{N})$ ,  $P_a$  is the momentum operator and  $Q_a$  is the position operator, both are self-adjoint. Let  $\{\phi_n : n \in \mathbb{N}\}$  be the Hilbertian basis of  $\mathcal{H}_a$  formed by the eigenvectors of the Hamiltonian  $\frac{1}{2m}P_a^2 + \frac{m\omega^2}{2}Q_a^2$ , then for every  $n \in \mathbb{N}$  we have (see for instance [60, 61])

$$Q_a \phi_n = \sqrt{\frac{\hbar}{2m\omega}} \left( \sqrt{n} \phi_{n-1} + \sqrt{n+1} \phi_{n+1} \right), \quad (4.6)$$

$$P_a \phi_n = -i\sqrt{\frac{\hbar m\omega}{2}} \left( \sqrt{n} \phi_{n-1} - \sqrt{n+1} \phi_{n+1} \right). \quad (4.7)$$

Let  $(\mathcal{H}_s, P_s, Q_s)$  be Schrödinger's representation for the particle, then

$$\mathcal{H}_s = L^2(\mathbb{R}, dx), \quad Q_s \psi(x) = x\psi(x), \quad P_s = -\mathcal{F} Q_s \mathcal{F}^{-1}, \quad (\psi \in D_{Q_s}).$$

Denote by  $D_s$  the domain of definition of  $P_s^2$  and by  $U_0$  the unitary map which connects the two representations and diagonalizes  $Q_a$ ,

$$U_0 : \mathcal{H}_a \rightarrow \mathcal{H}_s, \quad \phi_n \mapsto \left(\frac{m\omega}{\hbar}\right)^{1/4} \frac{1}{\pi^{1/4} \sqrt{2^n n!}} h_n \left( \sqrt{\frac{m\omega}{\hbar}} x \right).$$

In particular, we have

$$Q_s = U_0 Q_a U_0^{-1}, \quad P_s = U_0 P_a U_0^{-1}.$$

Next let  $\mathcal{H}_b = L^2((0, \infty), dx)$  and  $P_b^2 = -\hbar^2 \frac{d^2}{dx^2}$ , the self-adjoint operator in  $\mathcal{H}_b$  with domain

$$D_b = \{f \in AC(0, \infty) : f' \in AC(0, \infty), f, f'' \in L^2(0, \infty), f(0) = 0\}.$$

Put  $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ ,  $\beta' = \sqrt{\frac{\hbar m\omega}{2}}$ . Consider the normalized hermite functions of  $\mathcal{H}_s$

$$\tilde{h}_n(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}\sqrt{2^n n!}} h_n(\alpha x) = U_0 \phi_n,$$

and put  $\check{h}_n(x) = \chi_{(0,\infty)}(x)\tilde{h}_n(x)$ . The family  $\{\sqrt{2}\check{h}_{2n+1}\}_{n \in \mathbb{N}}$  forms an orthonormal basis of  $\mathcal{H}_b$ . We consider the following extension of elements of  $\mathcal{H}_b$

$$\iota : \mathcal{H}_b \rightarrow \mathcal{H}_s, \quad \sum_n \alpha_n \check{h}_{2n+1} \mapsto \sum_n \alpha_n \tilde{h}_{2n+1}.$$

Then  $\iota$  is linear and for every  $f \in \mathcal{H}_b$ , we have  $\|f\|_{\mathcal{H}_b} = \frac{1}{\sqrt{2}}\|\iota(f)\|_{\mathcal{H}_s}$ . Denote by  $\mathcal{H}_s^o$  (resp.  $\mathcal{H}_s^e$ ) the odd (resp. even) part of  $\mathcal{H}_s$ . Then

$$\mathcal{H}_s^o = \overline{\text{span}\{\tilde{h}_{2n+1}(x) : n \in \mathbb{N}\}}, \quad \mathcal{H}_s^e = \overline{\text{span}\{\tilde{h}_{2n}(x) : n \in \mathbb{N}\}},$$

and the map

$$\iota' : \mathcal{H}_b \rightarrow \mathcal{H}_s^o, \quad \psi \mapsto \frac{1}{\sqrt{2}}\iota(\psi),$$

is unitary. Put  $\Psi_a = \text{span}\{\phi_n : n \in \mathbb{N}\}$ ,  $\Psi_s = \text{span}\{\check{h}_n : n \in \mathbb{N}\}$  and  $\Psi_b = \text{span}\{\tilde{h}_n : n \in \mathbb{N}\}$ . Then  $\Psi_s = U_0\Psi_a$ . Since for every  $n \in \mathbb{N}$  we have

$$P_a^2 \phi_n = -\beta'^2(\sqrt{n(n-1)}\phi_{n-2} - (2n+1)\phi_n + \sqrt{(n+1)(n+2)}\phi_{n+2}),$$

where  $\phi_{-2} = 0$ , then

$$M(P_a^2 |_{\Psi_a}, \{\phi_n\}_n) = M(P_s^2 |_{\Psi_s}, \{\check{h}_n\}_n) = M(P_b^2 |_{\Psi_b}, \{\tilde{h}_n\}_n) \quad (4.8)$$

In particular, observe that  $\iota'P_b^2\iota'^{-1} = P_s^2 |_{\mathcal{H}_s^o}$ .

### 4.3.2 A basis of generalized eigenvectors of $P_a^2 |_{\Psi_a}$

Let  $z \in \mathbb{C}$  and let  $F_z \in \Psi_a^*$ . Then  $F_z$  is a solution of the eigenvalue equation  $(P_a^2)^\circ F_z = zF_z$  if and only if

$$(z - 3\beta'^2)F_z\phi_1 = -\sqrt{6}\beta'^2 F_z\phi_3, \quad (z - \beta'^2)F_z\phi_0 = -\sqrt{2}\beta'^2 F_z\phi_2,$$

and for every  $n \geq 2$

$$(z - \beta'^2(2n+1))F_z\phi_n = -\beta'^2[\sqrt{n(n-1)}F_z\phi_{n-2} + \sqrt{(n+2)(n+1)}F_z\phi_{n+2}].$$

In particular, for  $z \in \mathbb{C}$  fixed, the space of  $z$ -generalized eigenvectors has dimension 2, a basis is  $\{F_z^1, F_z^2\}$ , where

$$F_z^1(\phi_{2n+1}) = 0, \quad F_z^1(\phi_0) = 1, \quad (4.9)$$

$$F_z^2(\phi_{2n}) = 0, \quad F_z^2(\phi_1) = 1. \quad (4.10)$$

Put

$$P_n(z) = F_{-\beta'^2 z}^1(\phi_{2n}), \quad Q_n(z) = F_{-\beta'^2 z}^2(\phi_{2n+1}),$$

for all  $n \in \mathbb{N}$  and  $P_0(z) = Q_0(z) = 1$ , so that  $\{P_n(z)\}_n$  and  $\{Q_n(z)\}_n$  are two families of polynomial functions with  $\deg P_n = \deg Q_n = n$  satisfying :

$$(z - c_n)P_n(z) = d_{n-1}P_{n-1}(z) + d_n P_{n+1}(z) \quad \forall n \geq 0 \quad P_{-1} \equiv 0.$$

#### 4.3. DIAGONALIZING THE FREE HAMILTONIAN BY USING ALGEBRAIC GENERALIZED EIGENVECTORS

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$$(z - c'_n)Q_n(z) = d'_{n-1}Q_{n-1}(z) + d'_nQ_{n+1}(z) \quad \forall n \geq 0 \quad Q_{-1} \equiv 0.$$

where  $c_n, d_n, c'_n$  and  $d'_n$  are given by :

$$c_n = -(4n+1), \quad d_n = \sqrt{(2n+1)(2n+2)},$$

and

$$c'_n = -(4n+3), \quad d'_n = \sqrt{(2n+2)(2n+3)}.$$

Now by the basic theory of moments there exists a unique measure  $\sigma_1$  (resp.  $\sigma_2$ ) on  $\mathbb{R}$  such that  $\{P_n(x)\}$  (resp.  $\{Q_n(x)\}$ ) is an orthonormal basis of  $L^2(\mathbb{R}, d\sigma_1)$  (resp.  $L^2(\mathbb{R}, d\sigma_2)$ ) (see for instance [39]).

#### 4.3.3 Generalized Laguerre polynomials and the measures $\sigma_1, \sigma_2$

The space of linear generalized eigenvectors of  $P_a |_{\Psi_a}$  has dimension one and is generated by  $(R_z, z)$  with [14]

$$R_z(\phi_n) = \frac{(-i)^n}{\sqrt{2^n n!}} H_n(\gamma z), \quad R_z(\phi_0) = 1, \quad (n \in \mathbb{N}^*, \gamma = (\hbar m \omega)^{-1/2}).$$

Since  $(P_a^\circ)^\circ = (P_a^\circ)^2$ , fixing a branch cut for  $\sqrt{\cdot}$ , we see that, for every  $z \in \mathbb{C}$  with  $z \neq 0$ , the relations

$$G_z^1 = R_{\sqrt{z}}, \quad G_z^2 = R_{-\sqrt{z}}$$

define two linearly independent solutions of the generalized eigenvalue equation  $(P_a^\circ)^\circ F_z = z F_z$ . Thus for every fixed  $z \in \mathbb{C}$  with  $z \neq 0$ , every solution  $F_z$  above is of the form

$$F_z = C_1 G_z^1 + C_2 G_z^2, \quad C_1, C_2 \in \mathbb{C}.$$

But  $H_n(-z) = (-1)^n H_n(z)$  for every  $z \in \mathbb{C}$ , hence,

$$F_z(\phi_n) = \frac{(-i)^n}{\sqrt{2^n n!}} [C_1 + (-1)^n C_2] H_n(\gamma \sqrt{z}), \quad (z \in \mathbb{C}, z \neq 0).$$

By using the defining relations (4.9), we infer that

$$F_z^1(\phi_{2n}) = \frac{(-1)^n}{2^n \sqrt{(2n)!}} H_{2n}(\gamma \sqrt{z}).$$

On the other hand, by using the relations (4.10), we infer that

$$F_z^2(\phi_{2n+1}) = \frac{(-1)^n H_{2n+1}(\gamma \sqrt{z})}{2^{n+1} \sqrt{(2n+1)!} \gamma \sqrt{z}}.$$

Next let  $\lambda \in \mathbb{R}^+$  with  $\lambda \neq 0$ .

Hence

$$F_\lambda^1(\phi_{2n}) = \frac{2^n n!}{\sqrt{(2n)!}} L_n^{(-1/2)}(\gamma^2 \lambda), \quad F_\lambda^2(\phi_{2n+1}) = \frac{2^n n!}{\sqrt{(2n+1)!}} L_n^{(1/2)}(\gamma^2 \lambda).$$

Or, the  $L_n^{(\alpha)}(\lambda)$ 's are orthogonal with respect to the weight function  $\lambda^\alpha e^{-\lambda}$  on the half line  $(0, \infty)$  and

$$\int_0^\infty (L_n^{(\alpha)}(\lambda))^2 \lambda^\alpha e^{-\lambda} d\lambda = \frac{\Gamma(\alpha + n + 1)}{n!}.$$

Thus

$$\frac{\sqrt{n!}}{\sqrt{\Gamma(n+1/2)}} L_n^{(-1/2)}(\gamma^2 \lambda) = \pi^{-1/4} F_\lambda^1(\phi_{2n}),$$

and

$$\frac{\sqrt{n!}}{\sqrt{\Gamma(n+3/2)}} L_n^{(1/2)}(\gamma^2 \lambda) = \pi^{-1/4} \sqrt{2} F_\lambda^2(\phi_{2n+1}).$$

Put

$$\begin{aligned} \psi_{2n}(\lambda) &= F_\lambda^1(\phi_{2n}) = \frac{\pi^{1/4} \sqrt{n!}}{\sqrt{\Gamma(n+1/2)}} L_n^{(-1/2)}(\gamma^2 \lambda), \\ \psi_{2n+1}(\lambda) &= F_\lambda^2(\phi_{2n+1}) = \frac{\pi^{1/4} \sqrt{n!}}{\sqrt{2} \sqrt{\Gamma(n+3/2)}} L_n^{(1/2)}(\gamma^2 \lambda). \end{aligned}$$

Set

$$d\sigma_1(\lambda) = \chi_{(0,\infty)} \frac{\gamma}{\sqrt{\pi\lambda}} e^{-\gamma^2 \lambda} d\lambda, \quad d\sigma_2(\lambda) = \chi_{(0,\infty)} \frac{2\gamma^3 \sqrt{\lambda}}{\sqrt{\pi}} e^{-\gamma^2 \lambda} d\lambda.$$

Then  $\{\psi_{2n}(\lambda)\}_n$  is an orthonormal basis of  $L^2(\mathbb{R}^+, d\sigma_1)$ , while  $\{\psi_{2n+1}(\lambda)\}_n$  is an orthonormal basis of  $L^2(\mathbb{R}^+, d\sigma_2)$ .

### 4.3.4 Diagonalizing $P_s^2$ and $P_b^2$

It is now clear that  $\tilde{h}_0$  and  $\tilde{h}_1$  are fundamental vectors for  $P_s^2$ . Moreover,

$$(\mathcal{H}_s)_{\tilde{h}_0} = \mathcal{H}_s^e, \quad P_{\tilde{h}_0}^{P_s^2} = \sigma_1 \quad \text{and} \quad (\mathcal{H}_s)_{\tilde{h}_1} = \mathcal{H}_s^o, \quad P_{\tilde{h}_1}^{P_s^2} = \sigma_2.$$

In particular,  $P_s^2|_{\Psi_s \cap \mathcal{H}_s^o}$  and  $P_s^2|_{\Psi_s \cap \mathcal{H}_s^e}$  are essentially self adjoint. Thus the unitary map  $U_s : \mathcal{H}_s \rightarrow L^2(\mathbb{R}^+, d\sigma_1) \oplus L^2(\mathbb{R}^+, d\sigma_2)$  defined by  $U_s(\tilde{h}_{2n}) = \psi_{2n}$  and  $U_s(\tilde{h}_{2n+1}) = \psi_{2n+1}$  diagonalizes  $P_s^2$  with respect to the spectral basis  $\{\tilde{h}_0, \tilde{h}_1\}$ . More exactly,

$$U_s P_s^2 U_s^{-1} \psi(\lambda) = \lambda \psi(\lambda), \quad \psi \in U_s D_s.$$

The corresponding spectral decomposition of  $P_b^2$  is realized by the unitary map  $U_b = U_s \iota' : \mathcal{H}_b \rightarrow L^2((0, \infty), \sigma_2(\lambda))$ . Hence

$$U_b(\sqrt{2}\tilde{h}_{2n+1}) = \psi_{2n+1}(\lambda) = F_\lambda^2(\phi_{2n+1}), \quad n \in \mathbb{N}.$$

Moreover, we infer that  $U_b P_b^2 U_b^{-1} f(\lambda) = \lambda f(\lambda)$  for every  $f \in U_b D_b$ . Put  $F_\lambda^{2,b}(\sqrt{2}\tilde{h}_{2n+1}) = \psi_{2n+1}(\lambda)$ . Then  $F_\lambda^{2,b} = F_\lambda^2 U_0^{-1} \iota'$ .

## 4.4 A RHS construction based on the extension $\iota : \mathcal{H}_b \rightarrow \mathcal{H}_s$

### 4.4.1 The construction

We shall use the classical RHS construction

$$\Phi_s \subset \mathcal{H}_s \subset \Phi_s^\times,$$

where  $\Phi_s$  coincides with the Schwartz space (see for instance [14, 60, 61, 13]). Its locally convex topology  $\tau_s$ , defined by the family of scalar products  $\{(\cdot, \cdot)_n\}_n$  corresponds to the initial topology with respect to the maps  $I, (P_s^2 + Q_s^2) : \Psi_s \rightarrow (\Psi_s, \|\cdot\|_{\mathcal{H}_s})$ . It makes continuous the operators  $P_s, Q_s : (\Psi_s, \tau) \rightarrow (\Psi_s, \tau)$ . The RHS for  $P_b^2$  in

#### 4.4. A RHS CONSTRUCTION BASED ON THE EXTENSION $\iota : \mathcal{H}_B \rightarrow \mathcal{H}_S$

$\mathcal{H}_b$  will be inherited from  $\Phi_S \cap \mathcal{H}_S^0$ , by using the extension map  $\iota : \mathcal{H}_B \rightarrow \mathcal{H}_S$ . Next we describe this construction. For  $\psi = \sum_k c_k \check{h}_{2k+1}$  and  $\varphi = \sum_k d_k \check{h}_{2k+1}$  in  $\Psi_b$ , put

$$\langle \psi, \varphi \rangle_n = \frac{1}{2} (\iota(\psi), \iota(\varphi))_n = \frac{1}{2} \sum_k (2k+2)^n \overline{c_k} d_k, \quad n \in \mathbb{N}.$$

Set  $\langle \psi, \psi \rangle_n^{1/2} \equiv \|\psi\|_n$ . Then  $\|\psi\|_0 = \|\psi\|_{\mathcal{H}_b}$  and  $\|\cdot\|_n \leq \|\cdot\|_{n+1}$  for every  $n$ . Let  $\Phi_{b,n}$  be the completion of  $(\Psi_b, \langle \cdot, \cdot \rangle_n)$  and set  $\Phi_b = \bigcap_n \Phi_{b,n}$ . Then  $\Phi_b$  is a countably Hilbert space. Observe that for every  $n$ ,

$$\|\check{h}_{2s+1}\|_n = \sqrt{2^{n-1}} (s+1)^{n/2}.$$

Put

$$\check{h}_{2s+1}^n = \frac{\check{h}_{2s+1}}{\sqrt{2^{n-1}} (s+1)^n}.$$

Then  $\{\check{h}_{2s+1}^n\}$  is an orthonormal basis of  $\Phi_{b,n}$ . Moreover, for every  $n \in \mathbb{N}$  and  $k \geq 3$ , the map  $\iota_{n+k,n} : \Phi_{b,n+k} \rightarrow \Phi_{b,n}$  is nuclear. Indeed, we check easily that

$$\iota_{n+k,n} = \sum_s \frac{1}{(2s+2)^{k/2}} \langle \check{h}_{2s+1}^{n+k}, \cdot \rangle_{n+k} \check{h}_{2s+1}^n.$$

Thus,  $\Phi_b$  is a RHS. On the other hand, since  $P_b^2|_{\Psi_b}$  is essentially self-adjoint, we infer that  $\Phi_b$  is a RHS for  $P_b^2$ . In short,  $\Phi_b = \iota'^{-1}(\Phi_S \cap \mathcal{H}_S^0)$  and  $\Phi_S \cap \mathcal{H}_S^0$  is a RHS for  $P_S^2|_{\mathcal{H}_S^0}$ .

Observe that contrary to known constructions (see [62, 13, 8, 63]), the fundamental vector  $\check{h}_1$  belongs to  $\Phi_b$  but  $\Phi_b$  is not invariant under  $Q$ . This is not surprising since  $\mathcal{H}_b$  is not a Hilbert space for the pair  $(P, Q)$  (in the usual sense) because  $P|_{\mathcal{C}_c^\infty(\mathbb{R}^+)}$  does not admit a self-adjoint extension. In Section 4.4.4, we shall see that calculations may be conducted in  $\Phi_S$  by using the extension map  $\iota$ .

#### 4.4.2 Continuity and strong continuity of generalized eigenvectors

To use Dirac's notations on  $\Phi_S$  and  $\Phi_b$ , we need continuity, and strong continuity of generalized eigenvectors.

In  $\Phi_a$ , set  $\|\sum_k c_k \phi_k\|_{n,a}^2 = \|\sum_k c_k \check{h}_k\|_{n,s}^2 = \sum_k (k+1)^n |c_k|^2$ . Then

**Lemma 4.4.1.** *Let  $\lambda \in \mathbb{R}^+$ . The map  $F_\lambda^2$  (resp.  $F_\lambda^{2,b}$ ) is continuous for the norm  $\|\cdot\|_{n,a}$  (resp.  $\|\cdot\|_n$ ) for every  $n \neq 0$ . Let us keep the same notation for the extension by continuity of  $F_\lambda^2$  (resp.  $F_\lambda^{2,b}$ ) to  $\Phi_S$  (resp.  $\Phi_b$ ). Then, the family of generalized eigenvectors  $\{F_\lambda^2\}_{\lambda \in \mathbb{R}^+}$ , (resp.  $\{F_\lambda^{2,b}\}_{\lambda \in \mathbb{R}^+}$ ) is strongly continuous.*

*Proof.* Let  $\lambda > 0$  and let  $\varphi = \sum_{k=0}^l c_k \phi_k$  be an element of  $\Psi_a$ , where  $l \in \mathbb{N}$ . Then we have

$$F_\lambda^2(\varphi) = \sum_k \frac{(-1)^k c_{2k+1} H_{2k+1}(\gamma\sqrt{\lambda})}{2^{k+1} \sqrt{(2k+1)!} \gamma\sqrt{\lambda}}. \quad (4.11)$$

Thus for  $n \neq 0$ , we infer that

$$|F_\lambda^2(\varphi)| \leq \|\varphi\|_{n,a} \left[ \sum_{k=0}^{\infty} \frac{H_{2k+1}(\gamma\sqrt{\lambda})^2}{2^{2k+2} (2k+1)! (2k+2)^n \gamma^2 \lambda} \right]^{\frac{1}{2}}, \quad (4.12)$$

where the convergence of the second series can be deduced from the following inequality [?]

$$H_k^2(\gamma\sqrt{\lambda}) \leq \frac{C e^{\gamma^2 \lambda} 2^k k!}{\sqrt{2k+1} - \lambda^2}, \quad |\lambda| \leq \sqrt{2k+1}, \quad (4.13)$$

for some positive constant  $C$ . We have thereby shown that  $F_\lambda^2$  is continuous on  $\Psi_a$ , hence it can be extended to a continuous map  $F_\lambda^2 : \Phi_a \rightarrow \mathbb{C}$ .

Next let  $(\lambda_l)_l$  be a sequence of elements of  $\mathbb{R}_+^*$  such that  $\lambda_l \rightarrow \lambda$  and suppose that  $\varphi = \sum_k c_k \phi_k \in \Phi_a$ . Observe that equations (4.11)-(4.13) hold true for  $\varphi$  and  $\lambda_l$ . It follows from (4.12) and (4.13) that the r.h.s. of (4.11) converges uniformly in a neighborhood of  $\lambda$ . In particular, the family  $\{F_\lambda^2\}_{\lambda>0}$  is strongly continuous on  $\Phi_a$ .

Now let  $\{\lambda_l\}_l$  be a sequence converging to 0. We use (4.12) and (4.13) to see that the sequence of functions  $\{F_{\lambda_l}^2(\varphi)\}_l$  converges uniformly in a neighborhood of  $\varphi$ . Set  $S\varphi = \lim_l F_{\lambda_l} \varphi$ . Then  $S$  is linear and continuous on  $\Phi_a$ . Moreover,  $SP_a^2\varphi = 0$  for every  $\varphi \in \Phi_a$ ,  $S\phi_1 = 1$  and  $S\phi_{2k} = 0$  for every  $k$ . Thus  $S|_{\Psi_a} = F_0^2$  as desired.

Finally, for  $F_\lambda^{2,b}$ , the desired properties follow from the equality  $F_\lambda^{2,b} = F_\lambda^2 U_0^{-1} \iota'$  for every  $\lambda \geq 0$ .  $\square$

### 4.4.3 Diagonalizing via the regular solution:

Let  $\lambda \in (0, \infty)$ , let  $\chi(\lambda, x)$  be a solution of  $-\hbar^2 \frac{d^2}{dx^2} f = \lambda f$ . Put  $\Upsilon_\lambda f = \int_0^\infty \chi(\lambda, x) f(x) dx$  for every  $f \in \mathcal{C}_c^\infty(0, \infty)$ . Then  $\Upsilon_\lambda$  is a generalized eigenvector for  $(P_b^2|_{\mathcal{C}_c^\infty(0, \infty)}, \lambda)$ .

Suppose from now on that  $\chi(0) = 0$  ( $\chi(x) = c \sin(\sqrt{\lambda}x, c \in \mathbb{C})$ ). It is well known that  $\Upsilon_\lambda$  can be extended to a bounded map on  $\mathcal{H}_b$ , which corresponds to the Fourier sine transform. Moreover, for every  $f \in D_b$ , we have  $\Upsilon_\lambda P_b^2 f = \lambda \Upsilon_\lambda f$ . Next consider the map  $L_\lambda : \Psi_s \rightarrow \mathbb{C}$  defined by

$$L_\lambda(f) = \int_{-\infty}^{+\infty} \sin(\sqrt{\lambda}x) f(x) dx.$$

Then it is easy to check that  $L_\lambda(P_s^2|_{\Psi_s}) = \lambda L_\lambda$  and  $L_\lambda(\tilde{h}_{2n}) = 0$  for every  $n$ . Hence there exists  $g(\lambda) \in \mathbb{C}$  such that  $L_\lambda U_0 = g(\lambda) F_\lambda^2$ . But

$$U_0(\phi_1) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} h_1(\alpha x), \quad \text{and} \quad L_\lambda(h_1(\alpha x)) = \frac{2\sqrt{2\pi\lambda}}{\alpha^2} e^{-\frac{\lambda}{2\alpha^2}}.$$

Thus,

$$g(\lambda) = L_\lambda U_0(\phi_1) = \frac{2\pi^{1/4}}{\alpha^{3/2}}, \quad \sqrt{\lambda} e^{-\frac{\lambda}{2\alpha^2}}$$

That is,

$$L_\lambda U_0 = 2\pi^{1/4} \left(\frac{m\omega}{\hbar}\right)^{-3/4} \sqrt{\lambda} e^{-\frac{\lambda\hbar}{2m\omega}} F_\lambda^2.$$

Put  $d\sigma_s(\lambda) = g(\lambda)^{-2} d\sigma_2(\lambda)$ , then the unitary map  $V : \mathcal{H}_s^o \rightarrow L^2(\mathbb{R}, d\sigma_s(\lambda))$ , which satisfies  $Vf = L_\lambda f$  for every  $f \in \Psi_s \cap \mathcal{H}_s^{\text{odd}}$  satisfies  $VP_s^2 V^{-1} \psi(\lambda) = \lambda \psi(\lambda)$  for every  $\psi \in V(D_s \cap \mathcal{H}_s^o)$ . Put

$$d\sigma(\lambda) = 2d\sigma_s(\lambda) = \chi_{(0, \infty)} \frac{1}{\pi\hbar^3 \sqrt{\lambda}} e^{\frac{\hbar^2-1}{\hbar m\omega} \lambda} dx.$$

By using the unitary map  $V\iota'$ , we infer that the map

$$U : \mathcal{H}_b \rightarrow L^2(\mathbb{R}, d\sigma(\lambda)), \quad f(x) \mapsto \int_0^{+\infty} \sin(\sqrt{\lambda}x) f(x) dx,$$

is unitary and satisfies  $UP_b^2 U^{-1} \psi(\lambda) = \lambda \psi(\lambda)$  for every  $\psi \in UD_b$ .

We argue analogously for  $\lambda = 0$ . Consider

$$L_0 : U_0 \Psi \rightarrow \mathbb{C}, \quad f(x) \mapsto \int_{-\infty}^{+\infty} x f(x) dx.$$

Then

$$L_\lambda^0(h_1(\alpha x)) = 2\sqrt{2\pi}\alpha^{-2}, \quad L_0(\tilde{h}_{2n}) = 0, \quad \forall n \in \mathbb{N}.$$

Hence we get

$$L_0^1 U_0 = 2\alpha^{-3/2} \pi^{1/4} F_0^2.$$

#### 4.4.4 Calculations from $\Phi_b$ to $\Phi_s$

By using the unitary correspondance  $\iota'$ , we deduce the following relations

**Proposition 4.4.1.** *Let  $g \in \mathcal{H}_b$ . Then  $P_g^{P_b^2} = \frac{1}{2}P_{1g}^{P_b^2}$  and for every bounded measurable map  $f : \mathbb{R} \rightarrow \mathbb{C}$ ,  $\iota f(P_b^2) = f(P_s^2)\iota$ . In particular, for every  $z \in \mathbb{C} \setminus \mathbb{R}$  and  $t \in \mathbb{R}$ , we have*

$$\iota(P_b^2 - z)^{-1} = (P_s^2 - z)^{-1}\iota, \quad \iota e^{-itP_b^2} = e^{-itP_s^2}\iota.$$

**Remark 4.4.1.** *Consider the extension map*

$$\zeta : \mathcal{H}_b \rightarrow \mathcal{H}_s, \quad \sum_n \alpha_n \check{h}_{2n} \mapsto \sum_n \alpha_n \tilde{h}_{2n}.$$

Let  $z \in \mathbb{C} \setminus \mathbb{R}$  and let  $k = \sqrt{z}$  with  $\text{Im } k > 0$ . Then by using the two linearly independent solutions  $e^{ikx}$  and  $e^{-ikx}$  of the homogeneous equation  $-u'' - zu = 0$ , we show that for every  $g \in \mathcal{H}_b$ ,

$$[(P_s^2 - z)^{-1}\zeta - \zeta(P_b^2 - z)^{-1}]g = -4ike^{ikx} \int_x^{+\infty} e^{iky}g(y)dy, \quad x \in (0, +\infty).$$

Indeed, the extension map  $\zeta$  corresponds to the boundary-value condition  $f'(0) = 0$ .

### 4.5 A similar RHS construction for the square barrier potential

The RHS construction for  $P_b^2$  can be generalized to many differential operators. Moreover, the method of construction may be adapted to different boundary conditions. Next we shall focus on the square barrier potential. Let  $V_0$  be a positive real constant and let  $a, b \in \mathbb{R}$  with  $0 < a < b$ . Consider the formal differential operator  $H$  defined by

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \chi_{(a,b)}V_0.$$

Let  $A_b$  be the restriction of  $H$  in  $\mathcal{H}_b$  defined by

$$D(A_b) = \{f \in \mathcal{H}_b : f, f' \in AC(0, \infty), f(0) = 0, f'' \in \mathcal{H}_b\}.$$

Then  $A_b^* = A_b$ . It is known and straightforward to check that  $\sigma(A_b) = \mathbb{R}^+$ . Next let

$$H_1 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x),$$

where

$$V(x) = \begin{cases} \chi_{(a,b)}V_0 & \text{if } x > 0 \\ \chi_{(-b,-a)}V_0 & \text{if } x < 0. \end{cases}$$

Denote by  $A_s$  the self-adjoint operator in  $\mathcal{H}_s$  which is a restriction of  $H_1$ , with domain the Sobolev space

$$D(A_s) = \{f \in \mathcal{H}_s : f, f' \in AC(\mathbb{R}), f'' \in \mathcal{H}_s\}.$$

One can check that  $\mathcal{H}_s^0$  reduces  $A_s$  and  $\iota'A_b\iota'^{-1} = A_s|_{\mathcal{H}_s^0}$ .

$$D^\infty(A_b) = \{f \in \mathcal{C}^\infty(\mathbb{R}^+) : f^{(n)}(0) = f^{(n)}(a) = f^{(n)}(b) = 0, f^{(n)} \in \mathcal{H}_b, \forall n \in \mathbb{N}\}.$$

As in Section 4.4.4, we see that  $P_g^{A_b} = \frac{1}{2}P_{1g}^{A_b}$  and for every bounded measurable map  $f : \mathbb{R} \rightarrow \mathbb{C}$ ,  $\iota f(A_b) = f(A_s)\iota$ . Next we recall and describe the standard construction of a RHS for  $A_s$  [8, 13]. Consider the following dense subspace of  $\mathcal{H}_s$

$$\Psi_s^{\text{sb}} = \{f \in \mathcal{C}_c^\infty(\mathbb{R}) : f^{(n)}(\pm a) = f^{(n)}(\pm b) = 0, n \in \mathbb{N}\}.$$

Then  $\Psi_s^{\text{sb}} \subset \Phi_s$ , it is invariant under  $P_s$ ,  $Q_s$  and under multiplication by the functions  $\chi_{(a,b)}$  and  $\chi_{(-b,-a)}$ . Let  $\tau$  be the topology of  $\Phi_s$ , then  $\tau|_{\Psi_s^{\text{sb}}}$  makes the maps  $I, A_s$  and  $Q$  continuous. Denote by  $\Phi_s^{\text{sb}}$  the completion of  $(\Psi_s^{\text{sb}}, \tau)$ , then we may write

$$\Phi_s^{\text{sb}} = \{f \in D^\infty(A_s) : \int_{-\infty}^{+\infty} |x^n A_s^m f(x)|^2 dx < \infty, (n, m \in \mathbb{N})\}.$$

It follows from the basic theory of singular Sturm-Liouville operators that  $(A_s|_{\Phi_s^{\text{sb}}})^* = A_s$ . In particular, we infer that  $A_s|_{\Phi_s^{\text{sb}}}$  is essentially self-adjoint.

Now for  $A_b$ , observe first that  $\Phi_s^{\text{sb}} \cap \mathcal{H}_s^0$  is a RHS in  $\mathcal{H}_s^0$ . Moreover,  $\mathcal{H}_s^0$  reduces  $A_s$  and  $\Phi_s^{\text{sb}} \cap \mathcal{H}_s^0$  is a RHS for  $A_s|_{\mathcal{H}_s^0}$ . Put  $\Phi_b^{\text{sb}} = \iota'^{-1}(\Phi_s^{\text{sb}} \cap \mathcal{H}_s^0)$ . Since  $\iota'$  is unitary, we infer that  $\Phi_b^{\text{sb}}$  is a RHS construction for  $A_b$ . Observe that  $\Phi_b^{\text{sb}}$  is different from the standard constructions [64, 8, 13], and is not invariant under  $Q$ . In particular, there are functions  $f_\varepsilon \in \Phi_b^{\text{sb}}$  such that  $f_\varepsilon(x) = \check{h}_1(x)$  for every  $x \in \mathbb{R}^+$  with  $\inf\{|x-a|, |x-b|\} > \varepsilon$ .

## 4.6 Algebraic manipulations

Let  $A$  be a self-adjoint operator in  $\mathcal{H}$  and let  $\{\psi_n\}_{n \in \mathbb{N}}$  a Hilbertian basis of  $\mathcal{H}$ . Put  $\Lambda = \text{span}\{\psi_n : n \in \mathbb{N}\}$  and suppose that  $A\Lambda \subset \Lambda$ . The next result, though elementary, emphasizes the importance of the case where the space of algebraic generalized eigenvectors of  $A|_\Lambda$  has dimension one, since in this case, it may characterize the spectral representation in a general sense.

**Lemma 4.6.1.** *Let  $L : \mathcal{H} \rightarrow L^2(\mathbb{R}, \sigma(\lambda))$  be a linear map. Suppose that for every  $\varphi \in \Lambda$ ,  $L\varphi$  is a continuous function and  $(LA\varphi)(\lambda) = \lambda(L\varphi)(\lambda)$ . Then for every  $\lambda \in \text{supp}(\sigma) \setminus \mathcal{L}(L\Lambda)$ , the linear map  $\delta_\lambda L$  is a generalized eigenvector for  $(A|_\Lambda, \lambda)$ .*

*Proof.* Straightforward. □

It is clear that if  $A$  is cyclic and  $\psi$  is a true cyclic vector for  $A$ , then for  $\Lambda = \text{span}\{A^n \psi : n \in \mathbb{N}\}$ , the space of generalized eigenvectors of  $A|_\Lambda$  has dimension one. Next we shall look closely at two examples of  $\Lambda$  in  $\mathcal{H}_b$ , constructed by using two observables. In both cases  $\Lambda$  is a dense linear subspace of  $\mathcal{H}_b$ , having a countable Hamel basis.

### 4.6.1 The free Hamiltonian and the position observable in $\mathcal{H}_b$

Denote by  $\Lambda$  the minimal linear subspace of  $\Psi_b$  which contains  $\check{h}_1$  and is invariant under  $Q$ . Then  $\Lambda \subset D_b$  but it is not invariant under  $P_b^2$ . Let  $\lambda \in \mathbb{R}$ . Next we shall calculate the dimension of

$$\mathcal{E}_\lambda = \{F \in \Psi_b^* : FP_b^2|_\Lambda = \lambda F|_\Lambda\}.$$

It follows from (4.8) that we can work in  $\Psi_a$  instead of  $\Psi_b$ . Moreover, the relations (4.6) and (4.7) entail that

$$\Lambda = \text{span}\{\phi_{2n+1} : n \in \mathbb{N}\} + \text{span}\{\phi_{2n} + \alpha_n \phi_{2n+2} : n \in \mathbb{N}\}, \quad \alpha_n = \sqrt{\frac{(2n+2)}{2n+1}}.$$

First, observe that there exists a unique linear map  $G_\lambda \in \mathcal{E}_\lambda$  such that  $G_\lambda(\phi_0) = G_\lambda(\phi_1) = 0$  and  $G_\lambda(\phi_2) = 1$ . On the other hand, observe that if  $F : \Psi_a \rightarrow \mathbb{C}$  is a linear map satisfying  $FP_a^2\psi = \lambda F\psi$  for every  $\psi \in \Lambda$  and  $F\psi_k = 0$  for  $k = 0, 1, 2$ , then  $F = 0$ .

**Lemma 4.6.2.**  $\mathcal{E}_\lambda$  has dimension 3 and  $\mathcal{E}_\lambda = \text{span}\{F_\lambda^1, F_\lambda^2, G_\lambda\}$ .

*Proof.* It is clear that  $F_\lambda^1$  and  $F_\lambda^2$  lie in  $\mathcal{E}_\lambda$ . Next let  $F \in \mathcal{E}_\lambda$  and put  $\gamma_j = F\phi_j$  for  $j = 0, 1, 2$ . We claim that

$$F = \gamma_0 F_\lambda^1 + \gamma_1 F_\lambda^2 + (\gamma_2 - \gamma_0 F_\lambda^1 \phi_2) G_\lambda.$$

## 4.6. ALGEBRAIC MANIPULATIONS

To prove the claim put

$$\Lambda_1 = \text{span}\{\phi_{2n+1} : n \in \mathbb{N}\}, \quad \Lambda_2 = \text{span}\{\phi_{2n} : n \in \mathbb{N}\}$$

Recall that  $P^2\Lambda_j \subset \Lambda_j$  for  $j = 1, 2$ . It follows from our former computations in Section ?? that  $F|_{\Lambda_1} \in \text{span}\{F_\lambda^2\}$ , hence  $F|_{\Lambda_1} = \gamma_1 F_\lambda^2$ . On the other hand, it is easy to check that

$$(F - \gamma_0 F_\lambda^1 - \gamma_1 F_\lambda^2 - (\gamma_2 - \gamma_0 F_\lambda^1 \phi_2) G_\lambda) \phi_j = 0, \quad j = 0, 1, 2$$

Hence we can conclude.  $\square$

The above result provides, in our opinion, additional support for calculations in  $\Phi_s$  and  $\mathcal{H}_s$  instead of  $\Phi_b$  and  $\mathcal{H}_b$  by using the extension map  $\iota$ .

### 4.6.2 The SBP and the free Hamiltonian in $\mathcal{H}_b$

Fix  $f \in D^\infty(A_b)$ . Then  $\chi_{(a,b)} f \in D^\infty(A_b)$ . Denote by  $\Lambda$  the minimal linear subspace of  $\mathcal{H}_b$  which contains  $f$  and is invariant under  $A_b$  and  $P_b^2$ . Then  $\Lambda = \Lambda_1 + \Lambda_2$ , where

$$\Lambda_1 = \text{span}\{f^{(2n)} : n \in \mathbb{N}\}, \quad \Lambda_2 = \text{span}\{\chi_{(a,b)} f^{(2n)} : n \in \mathbb{N}\}$$

It is clear that  $A_b \Lambda_2 \subset \Lambda_2$ . In particular, observe that if  $f$  is a true cyclic vector for  $A_b$ , then  $\Lambda$  is dense in  $\mathcal{H}_b$ . Next we conclude with the following result on the dimension of the space of generalized eigenvectors of  $A_b|_\Lambda$ .

**Proposition 4.6.1.** *Suppose that  $f$  is a true cyclic vector of  $A_b$ . Then for every  $z \in \mathbb{C}$ , the space of solutions  $S_z \in \Lambda^*$  of the eigenvalue equation  $S_z A_b|_\Lambda = z S_z$  is two dimensional and the family  $\{S_z^1, S_z^2\}$  defined by*

$$S_z^1(\chi_{(a,b)} f) = 1, \quad S_z^1(f) = 0, \quad S_z^1 A_b|_\Lambda = z S_z^1 \tag{4.14}$$

$$S_z^2(\chi_{(a,b)} f) = 0, \quad S_z^2(f) = 1, \quad S_z^2 A_b|_\Lambda = z S_z^2 \tag{4.15}$$

forms a basis.

*Proof.* First of all observe that since  $f$  is a true cyclic vector of  $A_b$ , the family  $\{f, \chi_{(a,b)} f\}$  is linearly independent. Next Let  $G$  be a generalized eigenvector of  $A_b|_\Lambda$ . Since  $A_b \Lambda_2 \subset \Lambda_2$ , it is easy to see that  $G|_{\Lambda_2}$  is completely determined by  $G(\chi_{(a,b)} f)$ . Now an induction argument shows that  $G$  is completely determined by  $G(f)$  and  $G(\chi_{(a,b)} f)$ . In particular,  $S_z^1$  and  $S_z^2$  are well defined by the relations (4.14) and (4.15), and

$$G = G(\chi_{(a,b)} f) S_z^1 + G(f) S_z^2.$$

$\square$

Observe that  $\check{h}_1 \in D(A_b)$  but  $A_b \check{h}_1 \notin D(A_b)$ . If we want to keep track of Hermite functions it is legitimate to question whether the abstract model for the SBP can be refined so that  $\check{h}_1$  (or a slight modification) belongs to  $D^\infty(A_b)$ .

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## Résumé

Les vecteurs propres généralisés sont des outils clés dans la théorie des triplets de Gelfand. Soit  $\mathcal{H}$  un espace de Hilbert et soit  $\Phi$  un sous-espace dense de  $\mathcal{H}$ . Soit  $A : D(A) \rightarrow \mathcal{H}$  un opérateur linéaire non-borné à domaine dense défini sur  $\mathcal{H}$  tel que  $\Phi \subset D(A)$  et  $A\Phi \subset \Phi$ . Les vecteurs propres généralisés de  $A$  sont les vecteurs propres du dual algébrique de  $A : \Phi \rightarrow \Phi$ . Dans le cas où  $\Phi$  est muni d'une topologie  $\tau$  plus fine que celle induite par celle de  $\mathcal{H}$ , les vecteurs propres généralisés qui sont  $\tau$ -continus peuvent être d'un grand intérêt. Nous discutons des conditions qui garantissent l'existence d'une représentation associée aux vecteurs propres généralisés de  $A$ . A titre d'application, nous passons en revue et affinons l'étude de Böhm sur l'algèbre de l'oscillateur harmonique quantique. Nous discutons également des constructions canoniques de triplets de Gelfand. Nous nous concentrons sur les opérateurs cycliques autoadjoints et utilisons l'Hamiltonien libre unidimensionnel sur la demi-droite comme modèle. Nous proposons une construction non-standard qui peut être généralisée à de nombreux systèmes quantiques. Notre construction est motivée par le théorème d'unicité de Stone-von Neumann.

**Mots-clés :** Triplet de Gelfand; nucléarité; représentation; opérateur autoadjoint cyclique; théorème d'unicité de Stone-von Neumann.

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## Abstract

Generalized eigenvectors are key tools in the theory of rigged Hilbert spaces. Let  $\mathcal{H}$  be a Hilbert space and let  $\Phi$  be a dense subspace of  $\mathcal{H}$ . Let  $A$  be a densely defined linear operator in  $\mathcal{H}$  such that  $\Phi \subset D(A)$  and  $A\Phi \subset \Phi$ . The generalized eigenvectors of  $A$  are the eigenvectors of the algebraic dual of  $A : \Phi \rightarrow \Phi$ . In the case where  $\Phi$  is endowed with a topology  $\tau$  finer than the norm topology inherited from  $\mathcal{H}$ , generalized eigenvectors that are  $\tau$ -continuous may be of great interest. We discuss conditions which ensure the existence of representations associated to generalized eigenvectors of  $A$ . As an application, we review and refine Böhm's study of the algebra of quantum harmonic oscillator. We also discuss canonical rigged Hilbert space constructions. We focus on cyclic selfadjoint operators and use the one-dimensional free Hamiltonian on the half line as a model. We propose a nonstandard construction that can be generalized to many quantum systems. Our construction is motivated by the Stone von-Neumann uniqueness theorem.

**Keywords:** Rigged Hilbert space; nuclearity; representation; cyclic selfadjoint operators; Stone-von Neumann uniqueness theorem.