Quantum Mechanics in Rigged Hilbert Space Language

by

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To my parents, to my siblings,
and to those who always believed
in me

If you are lucky enough to have lived in
Austin as a young man, then wherever
you go for the rest of your life, it stays
with you, for Austin is a movable feast

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Chapter 1

Introduction

In this chapter, we sketch the contents of this dissertation. These contents will be mostly concerned with the properties of Dirac kets, Lippmann-Schwinger kets, and Gamow vectors.

> Jim looked at the trash, and then looked at me, and back at the trash again. He had got the dream fixed so strong in his head that he couldn't seem to shake it loose and get the facts back into place again, right away. But when he did get the things straightened around, he looked at me steady, without ever smiling, and says:
> "What do dey stan' for? I's gwyne to tell you. When I got all wore out wid work, en wid de callin' for you, en went to sleep, my heart wuz mos' broke bekase you wuz los', en I didn' k'yer no mo' what become er me en de raf'. En when I wake up en fine you back agin, all safe en soun', de tears come en I could a got down on my knees en kiss' yo' foot I's so thankful. En all you wuz thinkin 'bout wuz how you could make a foul uv ole Jim wid a lie. Dat truck dah is *trash*; en trash is what people is dat puts dirt on de head er dey fren's en makes 'em ashamed."
> Then he got up slow, and walked to the wigwam, and went in there, without saying anything but that. But that was enough. It made me feel so mean I could kissed *his* foot to get him to take it back.
> It was fifteen minutes before I could work myself up to go and humble myself to a nigger–but I done it, and I warn't ever sorry for it afterwards, neither. I didn't do him no more mean tricks, and I wouldn't done that one if I'd a knowed it would make him feel that way.
>
> Mark Twain, *The adventures of Huckleberry Finn*

This dissertation is about the description of Dirac kets, Lippmann-Schwinger kets and Gamow vectors in Rigged Hilbert Space language. The Dirac kets are the state vectors associated to any element in the spectrum of an observable. The Lippmann-Schwinger kets are the eigenkets of the Hamiltonian that are relevant in scattering theory. They correspond to the monoenergetic "in" and "out" scattering states. The Gamow vectors are the kets that represent the state vector of a resonance. Our main goal is to show that the Rigged Hilbert Space is the most suitable formalism to describe these kets. Rather than working in an abstract fashion, examples shall be used to illustrate this description. The two examples we shall mainly use are the harmonic oscillator and the square barrier potential.

In this dissertation, no experimental data is discussed. We shall rather focus on the methods, the ideas and principles in terms of which such data can be interpreted and understood. We shall use the Schrödinger equation subject to different boundary conditions as a model for the description of the data. Different boundary conditions upon the Schrödinger equation will yield Dirac kets, Lippmann-Schwinger kets or Gamow vectors. Although such a model involves an idealization, this is probably the best way to understand what these state vectors are.

We should note that the RHS is *not* an interpretation of Quantum Mechanics, but rather the most natural, concise and logic language to formulate such heuristic physical concepts as Dirac kets, Lippmann-Schwinger kets or Gamow vectors.

1.1 A Brief History of the Rigged Hilbert Space

In the late 1920's, Dirac introduced a new mathematical model of Quantum Mechanics based upon a uniquely smooth and elegant abstract algebra of linear operators defined on an infinite dimensional complex vector space equipped with an inner product norm [1]. Dirac's abstract algebraic model of *bras* and *kets* (from the bracket notation for the inner product) proved to be of great heuristic value in the ensuing years, especially in dealing with Hamiltonians whose spectrum is continuous. However, there were serious difficulties in finding a version of linear algebra which could be employed for making the actual numerical calculations.

The Hilbert space (HS) was the first mathematical idealization proposed for Quantum Mechanics [2]. However, as von Neumann explains in the introduction to his book [2], the HS theory and Dirac's formalism are two different things. Although there were attempts to realize the Dirac model in Hilbert space, there was a number of serious problems resulting from the fact that this formalism cannot allocate such things as bras, kets or the Dirac delta function or give a mathematical meaning to the Dirac basis vector expansion, which are essential in any physical formulation of Quantum Mechanics that deals with continuous spectrum. Indeed in his textual presentation [1] Dirac himself states that "*the bra and ket vectors that we now use form a more general space than a Hilbert space*" (see [1], page 40).

In the late 1940's, L. Schwartz gave a precise meaning to the Dirac delta function as a functional over a space of test functions [3]. This led to the development of a new branch of functional analysis, the theory of distributions [3].

About the same time, von Neumann published the theory of direct integral decompositions of a Hilbert space induced by a self-adjoint operator [4] (also valid for more general cases). This spectral theory was closer to classical Fourier analysis, and represented an improvement over former von Neumann's spectral theory [2].

I. Gelfand always thought that von Neumann's spectral theory was not the whole story of the theory of linear operators defined on infinite dimensional vector spaces. Prompted by the theory of distributions, he and his school introduced the Rigged Hilbert Space (RHS). Starting out with this RHS and von Neumann's direct integral decomposition, they were able to prove the so-called Nuclear Spectral Theorem [5] (also known as the Gelfand-Maurin Theorem). This theorem provides a more thorough information on the spectral properties of an operator and treats the continuous and the discrete spectrum on the same footing.

One of the aspects of Dirac's formalism, the continuity of the elements of the algebra of observables, was discussed in the early 1960's in Refs. [6, 7]. If two operators of the algebra of observables satisfy the canonical (Heisenberg) commutation relation, at least one of them cannot be continuous (i.e., bounded) with respect to the Hilbert space topology. In Refs. [6, 7], it is shown that there are subdomains of the Hilbert space that can be endowed with topologies that make those operators continuous; the largest of these subdomains is the Schwartz space.

In the 1960's, some physicists [8, 9, 10] independently realized that the RHS provides a rigorous mathematical rephrasing of all of the aspects of Dirac's formalism. In particular, the Nuclear Spectral Theorem restates Dirac basis vector expansion along with the Dirac bras and kets within a mathematical theory. Later on, other authors came to the same conclusion [11]. Nowadays the RHS is textbook material [12, 13, 14, 15, 16, 17, 18].

During the past few years, the RHS has emerged as the natural mathematical language in the theory of scattering and decay (cf. Refs. [19, 20, 21, 22] and references therein). The RHS has also proved to be very useful in other areas of theoretical physics such as in the construction of generalized spectral decompositions of chaotic maps [23, 24]. In fact, it seems that the RHS is the best known language to deal with scattering and decay in a consistent way. This is the very reason why we are using it here.

The Schrödinger equation is the dynamical equation that governs the behavior of a quantum system. Thus any attempt to show that the RHS contains the mathematical methods needed by Quantum Mechanics should show that the natural framework for the solutions of the Schrödinger equation is the RHS. We recall that none of Refs. [19, 20, 21, 22] took the Schrödinger equation as the dynamical equation. The objective of this dissertation is to obtain the Dirac, Lippmann-Schwinger, and Gamow kets as solutions of the Schrödinger equation subject to different boundary conditions, and to show that these solutions fall in the RHS rather than just in the HS [25, 26, 27].

In the end, the results of this dissertation will allow us to draw a very important conclusion: the RHS is the natural language to deal with scattering and decay.

1.2 Harmonic Oscillator

If the spectrum of an observable is discrete, the mathematical methods of the Hilbert space are sufficient for the purposes of Quantum Mechanics. However, if the spectrum of an observable has a continuous part, the mathematical methods of the Hilbert space are not sufficient, and an extension of these methods is needed.

Physicists use Dirac's bra-ket formalism in order to handle continuous spectra. Four of the most important features of this formalism are:

1. To each element λ of the spectrum of an observable A, there corresponds a ket $|\lambda\rangle$ that is an eigenvector of A with eigenvalue λ,
$$A|\lambda\rangle = \lambda|\lambda\rangle\,. \tag{1.2.1}$$
2. A wave function φ can be expanded by these eigenkets,[1]
$$\varphi = \int_{\text{Spectrum(A)}} d\lambda\, |\lambda\rangle\langle\lambda|\varphi\rangle\,. \tag{1.2.2}$$
3. The eigenkets are normalized according to the following rule:
$$\langle\lambda|\lambda'\rangle = \delta(\lambda - \lambda')\,, \tag{1.2.3}$$
where $\delta(\lambda - \lambda')$ is the Dirac delta function.
4. All algebraic operations such as the commutator of two observables A and B are always well defined,
$$[A, B] = AB - BA\,. \tag{1.2.4}$$

In Quantum Mechanics, observables are assumed to be represented by self-adjoint, linear operators defined on a Hilbert space $\mathcal{H}$. If the operator A associated to an observable is unbounded (which is the most common case in Quantum Mechanics), then A is only defined on a subdomain $\mathcal{D}(A)$ on which A is self-adjoint. In this case, the Hilbert space methods are not sufficient to make sense of (1.2.1)-(1.2.4). The RHS formalism provides the mathematics that are needed to make sense of them.

On the other hand, one of the key assumptions of Quantum Mechanics is that the quantity
$$(\varphi, A\varphi) \tag{1.2.5}$$
represents the expectation value of the measurement of the observable A in the state φ, and that
$$\Delta_\varphi A = \sqrt{(\varphi, A^2\varphi) - (\varphi, A\varphi)^2} \tag{1.2.6}$$
represents the uncertainty of the measurement of the observable A in the state φ (we assume the wave function φ to be normalized to 1). The expectation value (1.2.5) cannot be

[1] Eq. (1.2.2) is referred to as the Dirac basis vector expansion.

computed for every element of the Hilbert space $\mathcal{H}$, but only for those $\varphi \in \mathcal{H}$ that also belong to $\mathcal{D}(A)$. Similarly, the uncertainty (1.2.6) cannot be computed for every element of $\mathcal{H}$, but just for those $\varphi \in \mathcal{D}(|A|)$ [28]. If we take as physical states those normalizable functions for which physical quantities such as the expectation value (1.2.5) and the uncertainty (1.2.6) can be computed, then it is clear that not every square normalizable function (i.e., every element of $\mathcal{H}$) can represent a physical state. As we shall see, the natural space of physical wave functions is a subspace $\mathbf{\Phi}$ of $\mathcal{H}$, because all physical quantities can be computed for its elements. Further, $\mathbf{\Phi}$ has all the niceties of Dirac's formalism.

For example, let us consider the harmonic oscillator. The algebra of the harmonic oscillator contains the observables position Q and momentum P. These observables are defined as linear operators over the Hilbert space $\mathcal{H}$, and they fulfill the Heisenberg commutation relation:

$$[P, Q] = PQ - QP = -i\hbar I \,. \tag{1.2.7}$$

It is well known that Eq. (1.2.7) implies that either P or Q is an unbounded operator. This implies that either P or Q cannot be defined on the whole Hilbert space—they are, in fact, defined on certain dense subdomains $\mathcal{D}(P)$ and $\mathcal{D}(Q)$ on which P and Q are self-adjoint. Therefore, the expression $PQ - QP$ is not defined on the whole Hilbert space. Moreover, since $\mathcal{D}(P)$ and $\mathcal{D}(Q)$ do not remain stable under the action of P and Q, the expression $PQ - QP$ is only defined on those $\varphi \in \mathcal{H}$ such that $\varphi \in \mathcal{D}(Q)$, $\varphi \in \mathcal{D}(P)$, $P\varphi \in \mathcal{D}(Q)$ and $Q\varphi \in \mathcal{D}(P)$. Therefore, the Heisenberg commutation relation (1.2.7) is not defined on the whole of $\mathcal{H}$, but only on a subspace of it. We recall that Eq. (1.2.7) leads to the Heisenberg uncertainty relation:

$$\Delta_\varphi P \; \Delta_\varphi Q \geq \frac{\hbar}{2} \,. \tag{1.2.8}$$

Now, if we want the expectation values of H, P and Q,

$$(\varphi, A\varphi) \,, \quad A = H, P, Q \,, \tag{1.2.9}$$

the uncertainties of H, P and Q,

$$\Delta_\varphi A \,, \quad A = H, P, Q \,, \tag{1.2.10}$$

and the Heisenberg uncertainty relation (1.2.8) to be well defined, then the square normalizable wave function φ must be not only in $\mathcal{H}$, but also in $\mathcal{D}(P)$, $\mathcal{D}(Q)$, $\mathcal{D}(H)$, $\mathcal{D}(|P|)$, $\mathcal{D}(|Q|)$, $\mathcal{D}(|H|)$.

Hence, a subdomain $\mathbf{\Phi}$ of $\mathcal{H}$ where all of the physical quantities (1.2.7)-(1.2.10) can be computed is needed. Clearly, $\mathbf{\Phi}$ should be stable under the action of P, Q and H. It seems that the best candidate for $\mathbf{\Phi}$ is given by the intersection of the domains of all the powers of P, Q and H,

$$\mathbf{\Phi} = \bigcap_{\substack{n=0 \\ A=P,Q,H}}^{\infty} \mathcal{D}(A^n) \,. \tag{1.2.11}$$

The space in Eq. (1.2.11) is the maximal invariant subspace of the algebra of the harmonic oscillator. On $\mathbf{\Phi}$, all physical quantities such as expectation values and uncertainties can be

computed. Algebraic relations such as the Heisenberg commutation relation are well defined on $\mathbf{\Phi}$. In particular, the Heisenberg uncertainty principle is well defined on $\mathbf{\Phi}$.

The spectrum of the Hamiltonian of the harmonic oscillator is discrete, and its eigenvectors are square normalizable (actually, they are elements of $\mathbf{\Phi}$). This means that, as far as the eigenvectors of H are concerned, there is no need to go beyond the Hilbert space $\mathcal{H}$. However, the spectrum of the position and momentum observables is continuous, and coincides with the set of real numbers. Following the prescription (1.2.1), we associate an eigenvector $|p\rangle$ to each of the elements p of the (continuous) spectrum of P,

$$P|p\rangle = p|p\rangle\,, \quad -\infty < p < +\infty\,. \tag{1.2.12}$$

According to (1.2.2), a wave function can be expanded by these eigenkets,

$$\varphi = \int_{-\infty}^{+\infty} dp\, |p\rangle\langle p|\varphi\rangle\,. \tag{1.2.13}$$

Obviously, the kets $|p\rangle$ are not in the Hilbert space—a larger linear space is needed to accommodate them. It happens that those $|p\rangle$ acquire meaning as antilinear functionals over the space $\mathbf{\Phi}$. That is, $|p\rangle \in \mathbf{\Phi}^\times$, where $\mathbf{\Phi}^\times$ represents the set of antilinear functionals over the space $\mathbf{\Phi}$. Similar considerations hold for the position operator Q,

$$Q|x\rangle = x|x\rangle\,, \quad |x\rangle \in \mathbf{\Phi}^\times\,, \quad -\infty < x < +\infty\,. \tag{1.2.14}$$

$$\varphi = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|\varphi\rangle\,, \quad \varphi \in \mathbf{\Phi}\,. \tag{1.2.15}$$

In this way, the Gelfand triplet

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \tag{1.2.16}$$

of the harmonic oscillator arises in a natural way. The Hilbert space $\mathcal{H}$ comes from the requirement that the wave functions must be square normalizable. The subspace $\mathbf{\Phi}$ is the set of physical wave functions, i.e., the wave functions on which any expectation value, any uncertainty and any commutator can be computed. The dual space $\mathbf{\Phi}^\times$ contains the eigenkets associated to the continuous spectrum of the observables of the algebra. These eigenkets are defined as functionals over the space $\mathbf{\Phi}$, and they can be used to expand any $\varphi \in \mathbf{\Phi}$ as in Eq. (1.2.13) or Eq. (1.2.15).

These ideas will be elaborated in Chapter 3, where the Rigged Hilbert Space of the harmonic oscillator is constructed.[2] The harmonic oscillator will be studied from a different point of view to that used in textbooks on Quantum Mechanics. The standard approach to the harmonic oscillator is to start out with the (position) Schrödinger realization of the algebra of operators, i.e., one takes for granted the well-known differential expressions for Q, P and H. From these expressions one derives, for instance, the Heisenberg commutation

[2] Chapter 3 is a substantial improvement of and an extension to Ref. [29].

relation. One can also derive that the Hamiltonian has a countable number of eigenvalues whose corresponding eigenvectors are given by the Hermite polynomials. The above prescriptions of Dirac's formalism are also assumed, although it is not mentioned that the Hilbert space mathematics cannot incorporate them. In this dissertation, we shall not take for granted the position realization of the algebra of the harmonic oscillator, but rather derive this realization from algebraic assumptions. We shall just assume some algebraic relations to be fulfilled by the operators P, Q and H, namely the Heisenberg commutation relation

$$[P, Q] = PQ - QP = -i\hbar I \,, \tag{1.2.17}$$

and the expression of H in terms of P and Q,

$$H = \frac{1}{2\mu} P^2 + \frac{\mu\omega^2}{2} Q^2 \,. \tag{1.2.18}$$

We shall make an additional essential assumption: the existence of an eigenvector ϕ_0 of the energy operator,

$$H\phi_0 = 1/2\, \hbar\omega\, \phi_0 \,. \tag{1.2.19}$$

From this algebraic starting point, we shall derive first that H possesses a countable number of eigenvalues $\hbar w(n + 1/2)$, $n = 0, 1, 2, \ldots$, corresponding to some eigenvectors ϕ_n. The linear space spanned by the ϕ_n will be called Ψ. This linear space will be equipped with two different topologies: the usual Hilbert space topology, which generates the Hilbert space $\mathcal{H}$ from Ψ, and a stronger, nuclear topology, which generates the space $\mathbf{\Phi}$ from Ψ. This nuclear topology will make the elements of the algebra continuous operators. Once $\mathbf{\Phi}$ is constructed, we shall construct $\mathbf{\Phi}^\times$ and therewith the Rigged Hilbert Space of the harmonic oscillator:

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \,. \tag{1.2.20}$$

The eigenkets $|p\rangle$ and $|x\rangle$ will be continuous antilinear functionals over $\mathbf{\Phi}$, i.e., they will be elements of $\mathbf{\Phi}^\times$. The eigenket equations $Q|x\rangle = x|x\rangle$, $P|p\rangle = p|p\rangle$ will find their mathematical setting as functional equations over $\mathbf{\Phi}$. The statement of the Gelfand-Maurin Theorem will be given, which will guarantee the existence of a complete set of generalized eigenvectors of the position and momentum operators. It will be shown that this theorem is the mathematical statement that justifies the heuristic Dirac basis vector expansions (1.2.13) and (1.2.15). We shall derive the Schrödinger representation of the harmonic oscillator. In this representation, the standard expressions for P, Q and H in terms of differential operators will be obtained. The position realization of the RHS (1.2.20) by spaces of functions and distributions will be also obtained. The space $\mathbf{\Phi}$ will be realized by the Schwartz space $\mathcal{S}(\mathbb{R})$, and $\mathbf{\Phi}^\times$ will be realized by the space of tempered distributions $\mathcal{S}(\mathbb{R})^\times$. Thus the position realization of the RHS (1.2.20) will read

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{S}(\mathbb{R})^\times \,. \tag{1.2.21}$$

The eigenvectors ϕ_n of H will be realized by the Hermite polynomials.

Therefore, we shall give a proper mathematical framework for the operations that the physics of the harmonic oscillator seems to need, and we will throw light onto the problem of how the Schrödinger realization of the algebra of operators of the harmonic oscillator can be singled out. The important point is that this realization, which is introduced *ad hoc* in the literature, can be derived from proper algebraic assumptions within the RHS formalism.

1.3 A Rigged Hilbert Space of the Square Barrier Potential

The fundamental equation of Quantum Mechanics is the Schrödinger equation. Thus, showing that the RHS contains the mathematical methods needed by Quantum Mechanics is tantamount to showing that the natural framework for the solutions of the Schrödinger equation is the RHS. To show this, we shall use the example of the square barrier potential [25, 26].

The time dependent Schrödinger equation reads as

$$i\hbar\frac{\partial}{\partial t}\varphi(t) = H\varphi(t)\,, \tag{1.3.1}$$

where H denotes the Hamiltonian, and $\varphi(t)$ denotes the value of the wave function φ at time t. Dirac's formalism solves this equation formally as follows: for each energy E in the spectrum $\mathrm{Sp}(H)$ of the Hamiltonian, there exists a ket $|E\rangle$ that is an eigenvector of H,

$$H|E\rangle = E|E\rangle\,, \quad E \in \mathrm{Sp}(H)\,. \tag{1.3.2}$$

These eigenkets form a complete basis system that expands any wave function φ as

$$\varphi = \int dE\,|E\rangle\langle E|\varphi\rangle \equiv \int dE\,\varphi(E)|E\rangle\,. \tag{1.3.3}$$

The time dependent solution of Eq. (1.3.1) is obtained by Fourier-transforming the time independent solution of Eq. (1.3.3),

$$\varphi(t) = \int dE\,e^{-iEt/\hbar}\,\varphi(E)\,. \tag{1.3.4}$$

If the spectrum of the Hamiltonian has a continuous part, and if the energy E belongs to this continuous part of the spectrum, then the corresponding eigenket $|E\rangle$ that solves Eq. (1.3.2) is not square integrable, i.e., $|E\rangle$ is not an element of the Hilbert space. As in the case of the harmonic oscillator, the Hilbert space cannot handle these non-normalizable kets, whereas the RHS formalism can.

The main shortcoming of the RHS formalism is that it does not provide a prescription to construct the spaces $\mathbf{\Phi}$, $\mathbf{\Phi}^\times$, or the eigenkets $|E\rangle$. The general statement of the Nuclear Spectral Theorem [5] just assures the existence of the eigenkets $|E\rangle$, and assumes the spaces $\mathbf{\Phi}$, $\mathbf{\Phi}^\times$ to be given beforehand. Therefore, a systematic procedure to construct the RHS

of Schrödinger Hamiltonians is needed. The fourth chapter of this dissertation provides this systematic procedure [25, 26]. In order to make things clear, we shall illustrate this procedure through the square barrier potential, although the same method can be applied to a large class of potentials.

The procedure to construct the RHS of the square barrier potential is as follows. First, we write down the time independent Schrödinger equation in the radial position representation:

$$\langle r|H|E\rangle \equiv h\langle r|E\rangle = E\langle r|E\rangle \,, \tag{1.3.5}$$

where h is the following Schrödinger differential operator:

$$h \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) \,, \tag{1.3.6}$$

and

$$V(r) = \begin{cases} 0 & 0 < r < a \\ V_0 & a < r < b \\ 0 & b < r < \infty \end{cases} \tag{1.3.7}$$

is the square barrier potential. By applying the Sturm-Liouville theory (Weyl theory) [30] to the time independent Schrödinger equation (1.3.5), we obtain a domain $\mathcal{D}(H)$ on which the differential operator h is self-adjoint. This domain induces the self-adjoint Hamiltonian H. The next step is to compute the Green functions (i.e., the resolvent) of H, the spectrum of H (which in our example is $[0, \infty)$), and the unitary operator U that diagonalizes H. The operator U allows us to obtain the energy representation of the Hilbert space and the direct integral decomposition induced by the Hamiltonian. The direct integral decomposition is not enough for the purposes of Quantum Mechanics. The reasons why the direct integral decomposition (i.e., the Hilbert space methods) is not enough for the purposes of Quantum Mechanics are the same as in the case of the harmonic oscillator:

(i) The expectation values and the uncertainties of the Hamiltonian in any physical wave function should be well defined.

(ii) Algebraic operations should be well defined. Since $\mathcal{D}(H)$ is not stable under the action of H, the powers of H are not well defined on all of the elements of $\mathcal{H}$. Hence, a subdomain $\mathbf{\Phi}$ included in $\mathcal{D}(H)$ that remains stable under the action of H and all of its powers is needed,

$$H^n : \mathbf{\Phi} \longmapsto \mathbf{\Phi} \,, \quad n = 0, 1, 2, \ldots \tag{1.3.8}$$

(Obviously, if Eq. (1.3.8) holds, then the expectation values and the uncertainties of H in any φ of $\mathbf{\Phi}$ are well defined.)

(iii) For each $E \in \mathrm{Sp}(H)$, there is a Dirac ket $|E\rangle$ such that the eigenequation (1.3.2) and the Dirac basis vector expansion (1.3.3) hold. The kets $|E\rangle$ are defined in terms of the

eigenfunctions $\langle r|E\rangle$ of (1.3.5) as

$$\begin{aligned} |E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\langle r|E\rangle dr\,. \end{aligned} \tag{1.3.9}$$

After realizing that the Hilbert space is not sufficient to account for (*i*)-(*iii*), we construct the RHS

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \tag{1.3.10}$$

of the square barrier potential. This RHS accounts for (*i*)-(*iii*), because of the following reasons:

(**1**) The space $\mathbf{\Phi}$ is stable under the action of H (this will give (1.3.8)). On the space $\mathbf{\Phi}$, all algebraic operations involving the Hamiltonian H are well defined. In particular, the expectation values of the Hamiltonian in any element of $\mathbf{\Phi}$ are well defined. The elements of $\mathbf{\Phi}$ are represented by well-behaved functions, in contrast to the elements of the Hilbert space, which are represented by sets of equivalent functions that can vary arbitrarily on any set of zero Lebesgue measure. As in the example of the harmonic oscillator, we conclude that not every element of the Hilbert space can be a physically acceptable wave function—only the elements of $\mathbf{\Phi}$ fulfill all the conditions to be a wave function.

(**2**) The ket $|E\rangle$, as defined by (1.3.9), is a well-defined antilinear functional on $\mathbf{\Phi}$, i.e., $|E\rangle \in \mathbf{\Phi}^\times$. In the energy representation, $|E\rangle$ acts as the antilinear Schwartz delta functional. Moreover, $|E\rangle$ is an eigenvector of H as in Eq. (1.3.2). To see this, we have to recall that in RHS language, Eq. (1.3.2) means that

$$\langle H\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi \in \mathbf{\Phi}\,. \tag{1.3.11}$$

The action of H can be extended to the kets $|E\rangle$ in $\mathbf{\Phi}^\times$ as follows:

$$\langle\varphi|H^\times|E\rangle = \langle H\varphi|E\rangle\,, \quad \forall\varphi \in \mathbf{\Phi}\,. \tag{1.3.12}$$

Because H is continuous on $\mathbf{\Phi}$, the operator $H^\times$ is a uniquely defined extension of H. Using the definition (1.3.12), we rewrite Eq. (1.3.11) as

$$\langle\varphi|H^\times|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi \in \mathbf{\Phi}\,. \tag{1.3.13}$$

Omitting the arbitrary φ in this equation leads to

$$H^\times|E\rangle = E|E\rangle\,, \tag{1.3.14}$$

which is the same as Eq. (1.3.2). (Note that in Eq. (1.3.14) we have denoted the action of the Hamiltonian on the ket $|E\rangle$ by $H^\times$ and not just by H. We shall use this notation in order to stress that the Hamiltonian is acting on vectors that lie outside the Hilbert space.)

(**3**) Any element of $\mathbf{\Phi}$ can be expanded in terms of the eigenkets $|E\rangle$ as in Eq. (1.3.3).

From (**1**)-(**3**) it follows that, when continuous spectrum is present, the natural framework for the solutions of the Schrödinger equation is the Rigged Hilbert Space rather than just the Hilbert space.

1.4 Scattering off the Square Barrier Potential

The above procedure to construct RHSs of Schrödinger Hamiltonians also shows that the RHS can incorporate boundary conditions imposed upon the Schrödinger equation:

$$\boxed{\begin{array}{c}\text{Schrödinger equation}\\ + \\ \text{boundary conditions}\end{array}} \longrightarrow \mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times}.$$

The Hilbert space $\mathcal{H}$ is needed to incorporate the requirement that the wave functions are square integrable. Moreover, $\mathcal{H}$ singles out the scalar product used to compute probability amplitudes. The space $\mathbf{\Phi}^{\times}$ is needed to incorporate the Dirac kets associated with the eigenfunctions of the time independent Schrödinger equation subject to boundary conditions. The space $\mathbf{\Phi}$ is needed to incorporate the wave functions on which the Dirac kets act as continuous antilinear functionals and for which all the algebraic operations and all the expectation values are well defined.

We are now going to see that the RHS formalism is also able to incorporate the boundary conditions of a scattering system. In essence, the RHS can accommodate the Lippmann-Schwinger equation.[3] To illustrate this, we shall use the example of scattering off the square barrier potential.

Loosely speaking, we send a beam of prepared initial in-states φ^{in} towards the square barrier potential. After the collision takes place, φ^{in} becomes φ^{out}. We then measure the probability to find a final out-state ψ^{out}. The amplitude of this probability is given by

$$(\psi^{out}, \varphi^{out}) = (\psi^{out}, S\varphi^{in}), \tag{1.4.1}$$

where S is the S-matrix. The canonical understanding is that the initial in-state φ^{in} and the final out-state ψ^{out} are asymptotic forms of the so-called in-state φ^{+} and out-state ψ^{-} in the remote past and in the distant future, respectively. In terms of these, the probability amplitude (1.4.1) reads

$$(\psi^{-}, \varphi^{+}). \tag{1.4.2}$$

The asymptotic states φ^{in} and ψ^{out} are related to the "exact" states φ^{+} and ψ^{-} by the Møller operators,

$$\Omega_{+}\varphi^{in} = \varphi^{+}, \tag{1.4.3a}$$
$$\Omega_{-}\psi^{out} = \psi^{-}. \tag{1.4.3b}$$

It is customary to split up the (total) Hamiltonian H into the free Hamiltonian H_0 and the potential V,

$$H = H_0 + V. \tag{1.4.4}$$

[3] For a mathematical approach to the Lippmann-Schwinger equation in terms of RHSs of Hardy functions see Ref. [31].

The potential V is interpreted as the interaction between the components of the initial prepared states, for instance, the interaction between the in-going beam and the target. The initial in-state φ^{in} and the final out-state ψ^{out} evolve under the influence of the free Hamiltonian H_0, whereas the in-state φ^+ and the out-state ψ^- evolve under the influence of the (total) Hamiltonian H.

Therefore, the dynamics of a scattering system is governed by the Schrödinger equation subject to certain boundary conditions. These boundary conditions specify what is "in" and what is "out." The Lippmann-Schwinger equation for the in- and out-kets $|E^\pm\rangle$ has those "in" and "out" boundary conditions built into it,[4]

$$|E^\pm\rangle = |E\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|E^\pm\rangle\,. \tag{1.4.5}$$

Eq. (1.4.5) is an integral equation, and is equivalent to the Schrödinger equation

$$H^\times|E^\pm\rangle = E|E^\pm\rangle \tag{1.4.6}$$

subject to certain boundary conditions. The most important of these boundary conditions is built into the "infinitesimal imaginary parts" $\pm i\epsilon$, which characterize what is "in" $(+i\epsilon)$ and what is "out" $(-i\epsilon)$. We then say that the $|E^\pm\rangle$ are eigenvectors of the Hamiltonian whose corresponding eigenvalues have an "infinitesimal imaginary part."

Needless to say, the Lippmann-Schwinger kets $|E^\pm\rangle$ are, mathematically speaking, defined as antilinear functionals. The in-ket $|E^+\rangle$ acts on the in-states φ^+, while the out-ket $|E^-\rangle$ acts on the out-states ψ^-. Since the eigenvalues of the kets $|E^\pm\rangle$ have an "infinitesimal imaginary part," the wave functions $\langle\varphi^+|E^+\rangle$ and $\langle\psi^-|E^-\rangle$ should have meaning not only for real energies, but also for energies with an "infinitesimal imaginary part." Mathematically this means that the wave functions $\langle\varphi^+|E^+\rangle$ and $\langle\psi^-|E^-\rangle$ should be the boundary values of analytic functions of the (complex) variable E. The analytical properties satisfied by the in-ket $|E^+\rangle$ (or, equivalently, by the wave function $\langle\varphi^+|E^+\rangle$) are different to those satisfied by the out-ket $|E^-\rangle$ (or, equivalently, by the wave function $\langle\psi^-|E^-\rangle$). In incorporating these two different types of boundary conditions into the RHS framework, we will end up constructing two different RHSs. One RHS corresponds to the in-states φ^+,

$$\mathbf{\Phi}_- \subset \mathcal{H} \subset \mathbf{\Phi}_-^\times\,, \tag{1.4.7}$$

while the other RHS corresponds to the out-states ψ^-,

$$\mathbf{\Phi}_+ \subset \mathcal{H} \subset \mathbf{\Phi}_+^\times\,. \tag{1.4.8}$$

The Lippmann-Schwinger kets belong to the dual spaces of these RHSs,

$$|E^\pm\rangle \in \mathbf{\Phi}_\mp^\times\,. \tag{1.4.9}$$

[4]In Eq. (1.4.5), the symbol $|E\rangle$ denotes an eigenket of the free Hamiltonian H_0, not the eigenket of the total Hamiltonian of Eq. (1.3.9).

The wave functions φ^+ are usually called in-states, whereas the wave functions ψ^- are called out-states. Occasionally, we shall call the ψ^- observables (or out-observables), because they are determined by the registration apparatus. In order to grasp the meaning of this terminology, let us consider the matrix element (ψ^-, φ^+). This scalar product is the amplitude of the probability to observe the out-state ψ^- in the in-state φ^+,

$$\mathcal{P}_{\varphi^+\to\psi^-} = |(\psi^-, \varphi^+)|^2 \,. \tag{1.4.10}$$

Since ψ^- is determined by the property that we want to measure, it stands to reason that we call it observable and denote it by a specific symbol. In order to stress the distinction between states and observables, the probability (1.4.10) may be written as

$$\mathcal{P}_{\varphi^+\to\psi^-} = \mathrm{Tr}(P_{\psi^-} W_{\varphi^+}) \,, \tag{1.4.11}$$

where Tr stands for trace and

$$W_{\varphi^+} \equiv |\varphi^+\rangle\langle\varphi^+| \,, \tag{1.4.12}$$

$$P_{\psi^-} \equiv |\psi^-\rangle\langle\psi^-| \,. \tag{1.4.13}$$

The Lippmann-Schwinger equation will be studied in Chapter 5 within the example of the square barrier potential. We shall first write Eq. (1.4.5) in the radial position representation,

$$\langle r|E^\pm\rangle = \langle r|E\rangle + \langle r|\frac{1}{E - H_0 \pm i\epsilon} V|E^\pm\rangle \,. \tag{1.4.14}$$

Next, we shall obtain the Lippmann-Schwinger eigenfunctions $\langle r|E^\pm\rangle$. The continuation of these eigenfunctions to complex values of the energy, that we denote by $\langle r|(E \pm i\epsilon)^\pm\rangle$, will be used to define the action of the Lippmann-Schwinger kets:

$$\langle\varphi^+|E^+\rangle := \lim_{\epsilon\to 0}\int_0^\infty dr\, \langle\varphi^+|r\rangle\langle r|(E + i\epsilon)^+\rangle \,, \quad \varphi^+ \in \mathbf{\Phi}_- \,, \tag{1.4.15a}$$

$$\langle\psi^-|E^-\rangle := \lim_{\epsilon\to 0}\int_0^\infty dr\, \langle\psi^-|r\rangle\langle r|(E - i\epsilon)^-\rangle \,, \quad \psi^- \in \mathbf{\Phi}_+ \,. \tag{1.4.15b}$$

This definition needs a comment. The action of the Lippmann-Schwinger kets is defined as the limits in Eq. (1.4.15) in order to keep track of the $\pm i\epsilon$ boundary conditions. The $\pm i\epsilon$ boundary conditions just mean that we are approaching the cut (i.e., the spectrum of H) either from above ($+i\epsilon$) or from below ($-i\epsilon$). Therefore, the action of the Lippmann-Schwinger kets $|E^\pm\rangle$ should be viewed as the limit of the integrals in Eq. (1.4.15) when ϵ tends to 0.

The conditions under which the ket (1.4.15a) is well defined are in general different to those under which (1.4.15b) is well defined. Since these conditions determine the space of wave functions on which the kets act, the space $\mathbf{\Phi}_-$ on which the in-ket $|E^+\rangle$ acts is different

from the space $\mathbf{\Phi}_+$ on which the out-ket $|E^-\rangle$ acts. Although the precise form of the spaces $\mathbf{\Phi}_\pm$ will not be given, we shall provide a list of necessary conditions that must be satisfied by the elements of $\mathbf{\Phi}_\pm$. For the sake of definiteness, we shall assume sometimes that those spaces are, in the energy representation, subspaces of spaces of Hardy class (see also [31]).

Once the Lippmann-Schwinger kets are constructed, the complex basis vector expansions of the states φ^+ and of the observables ψ^- follow:

$$\varphi^+ = \int_0^\infty dE\, |E^+\rangle\langle^+E|\varphi^+\rangle\,, \tag{1.4.16a}$$

$$\psi^- = \int_0^\infty dE\, |E^-\rangle\langle^-E|\psi^-\rangle\,. \tag{1.4.16b}$$

We will also construct the Møller operators and the S-matrix, and express the matrix element (1.4.2) in terms of the in- and out-Lippmann-Schwinger kets,

$$(\psi^-, \varphi^+) = \int_0^\infty dE\, \langle\psi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle\,. \tag{1.4.17}$$

This expression will be used later to derive the complex basis vector expansion generated by the Gamow vectors.

We remark that the RHS (1.3.10) was called *a* RHS of the square barrier potential and not *the* RHS of the square barrier potential, because different boundary conditions upon the Schrödinger equation yield different RHSs for the same potential. The space $\mathbf{\Phi}$ of Eq. (1.3.10) is neither $\mathbf{\Phi}_+$ nor $\mathbf{\Phi}_-$, because $\mathbf{\Phi}$ incorporates neither the "in" nor the "out" boundary conditions of the scattering off the square barrier potential [32].

1.5 The Gamow Vectors of the Square Barrier Potential Resonances

The Gamow vectors are the state vectors of resonances. They are defined as eigenvectors of the Hamiltonian with a complex eigenvalue. The description of the Gamow vectors, impossible in the Hilbert space, can be accomplished within the RHS formulation of Quantum Mechanics.

Experimentally, resonances often appear as peaks in the cross section whose shape resemble the well-known Breit-Wigner distribution. The Breit-Wigner distribution has two characteristic parameters: the energy E_R at which the distribution reaches its maximum, and its width Γ_R at half-maximum. The inverse of Γ_R is the lifetime of the decaying state [33]. The peak of the cross section with Breit-Wigner shape is related to a first-order pole of the S-matrix in the energy representation $S(E)$ at the complex number $z_R = E_R - i\Gamma_R/2$. The theoretical expression of the cross section in terms of $S(E)$ fits the shape of the experimental cross section in the neighborhood of E_R. This is why the first-order pole of the S-matrix is often taken as the theoretical definition of a resonance.

Although a resonance has a finite lifetime, it is otherwise assigned all the properties that are also attributed to stable particles, like angular momentum, charge, spin, parity and other particle labels. For example, consider [34] the bombardment of stable Pb^{206} nuclei by a beam of α particles whose energy is peaked around 5.4 MeV. The cross section for α+Pb^{206} scattering has an incredibly sharp resonance whose width is of the order of 10^{-18} eV. For times (after the α+Pb^{206} scattering has taken place) much less than 138 days, there will be nuclei in the target that have all the chemical and physical properties associated with the atomic numbers $Z = 84$, $A = 210$, and we call these nuclei Po^{210}. The probability to find Po^{210} is not stationary, however, but decreases exponentially with a characteristic decay time of 138 days. For times short compared to 138 days, Po^{210} is to all intends an atomic nucleus. In fact, we include it (and the rest of unstable nuclei) in the periodic table of elements along with the stable nuclei.

In particle physics the situation is the same (cf. for instance [35]). Unstable particles are listed along with the stable ones in the Particle Data Table [36] and attributed values for the mass, the spin and the width (or lifetime). Thus, stable particles differ from the unstable ones by the value of their width, which is zero in the case of stable particles and different from zero in the case of unstable ones. Hence, phenomenologically, unstable particles are not less fundamental than the stable ones, which are, according to current experimental evidence, only the proton, the electron, the photon, the neutrinos and possibly the graviton.

Theoretically, stable and unstable particles are usually treated on a different footing. The reason is that an unstable particle, unlike a stable one, cannot be described within the Hilbert space formalism. However, there are some theoretical models that treat stable and unstable particles on the same footing. For instance, in the eightfold way of Gell-Mann and Ne'eman [37] many multiplets contain both stable and unstable particles—no fundamental distinction between stable and unstable particles is made.

Because resonances are particles with a finite lifetime—not just peaks in the cross section—a state vector description for resonances is needed. The Gamow vectors are the natural state vectors of resonances [27]. The description of resonances by Gamow vectors allows us to interpret them as autonomous experimentally decaying physical systems.

The energy eigenfunction with complex eigenvalue was originally introduced by Gamow in his paper on α-decay of atomic nuclei [38], and used thereafter by a number of authors (see for example, Refs. [39, 40, 41, 42, 43] and references therein). The real part of the complex eigenvalue is associated with the energy of the resonance, and the imaginary part is associated with the inverse of the lifetime. The Gamow eigenfunctions have an exponentially decaying time evolution, in accordance with the exponential law observed in α decay of radioactive nuclei [44, 45, 46, 47]. The Gamow eigenfunctions are obtained as solutions of the Schrödinger equation subject to the purely outgoing boundary condition. This condition was introduced by Siegert [48].

Gamow's treatment is merely heuristic though, and it cannot be made rigorous in the Hilbert space theory, because self-adjoint operators on a Hilbert space can only have real eigenvalues. Recall however that Dirac's bra-ket formulation of Quantum Mechanics was also heuristic and without mathematical justification until the RHS formulation of Quantum

Mechanics was suggested [8, 9, 10]. During the past few years, it has become clear that the RHS mathematics also asserts the legitimacy of Gamow's proposition (cf. Refs. [19, 20, 21, 22] and references therein). In RHS language, the Gamow vectors are eigenvectors of the dual extension of the self-adjoint Hamiltonian. This extension can surely have complex eigenvalues.[5]

A complementary approach to resonances started with Breit and Wigner, who described a resonance by means of the Breit-Wigner distribution [50]. (Curiously enough, this distribution had been independently introduced five years earlier by Fock [51].) Now, if a vector is to obey the exponential decay law and also to correspond to the Breit-Wigner distribution, then this distribution must be nonzero over the full energy real line (see Ref. [52] and references therein). Because the spectrum of the Hamiltonian is bounded from below, say $[0, \infty)$, the Breit-Wigner distribution then has to be defined also at energies that do not belong to the physical spectrum [52]. This seems to imply that the exponential decay law is incompatible with the Breit-Wigner distribution, because the Breit-Wigner distribution leads to the exponential law only when is defined over the full energy real line $(-\infty, \infty)$ rather than just over the physical spectrum $[0, \infty)$. However, it has been shown that even though the spectrum of the Hamiltonian is $[0, \infty)$, the Breit-Wigner distribution can be defined on the full energy real line by means of RHSs of Hardy functions [20], and hence the Breit-Wigner distribution yields the exponential law. The essential ingredient to do so is the so-called van Winter's theorem [53]. This theorem allows us to piece together the physical spectrum, which coincides with $[0, \infty)$, and the support of the Breit-Wigner distribution, which coincides with $(-\infty, \infty)$.

Thus, there are two ways of describing a resonance: the Gamow vectors, which are eigensolutions of the Schrödinger equation subject to a purely outgoing boundary condition, and the Breit-Wigner distribution, which arises from the resonance pole of the S-matrix. It is the major goal of this dissertation to show that the energy representation of the Gamow vectors is given by the Breit-Wigner distribution. The square barrier potential will be used to illustrate this point.

The Gamow vectors of the square barrier potential will be constructed in Chapter 6. The Gamow eigenkets will be defined as the solutions of a homogeneous integral equation of the Lippmann-Schwinger type. If we denote the Gamow ket associated to the complex energy $z_R = E_R - i\Gamma_R/2$ by $|z_R^-\rangle$, then $|z_R^-\rangle$ satisfies the following integral equation:

$$|z_R^-\rangle = \frac{1}{z_R - H_0 + i0} V |z_R^-\rangle \,. \tag{1.5.1}$$

This equation was introduced (in a different language) by A. Mondragón[6] *et al.* in Ref. [40]. It is well known that the poles of a scattering system come in pairs, i.e., if $z_R = E_R - i\Gamma_R/2$

[5] Eigenvectors of the dual extension of self-adjoint operators with complex eigenvalues in the RHS were systematically studied for the first time in the reduction of SO(2,1) with respect to its noncompact subgroup [49].

[6] I am indebted to Prof. Alfonso Mondragón for his careful and patient explanations on Eq. (1.5.1).

is a pole of the S-matrix, then $z_R^* = E_R + i\Gamma_R/2$ is also a pole of the S-matrix. The Gamow vector associated to the pole z_R^* is denoted by $|z_R^{*+}\rangle$, and satisfies the following integral equation:

$$|z_R^{*+}\rangle = \frac{1}{z_R^* - H_0 - i0} V |z_R^{*+}\rangle \,. \tag{1.5.2}$$

In Chapter 6, we will solve the integral equations (1.5.1) and (1.5.2) in the radial position representation. In this representation, these integral equations are equivalent to the time independent Schrödinger equation subject to a purely outgoing boundary condition. The resonance spectrum is then singled out by this purely outgoing boundary condition. As we shall see, this is the same resonance spectrum as that defined by the poles of the S-matrix [27]. The Gamow kets will be shown to be generalized eigenvectors of the Hamiltonian with complex eigenvalues:

$$H^\times |z_R^-\rangle = z_R |z_R^-\rangle \,, \qquad |z_R^-\rangle \in \mathbf{\Phi}_+^\times \,, \tag{1.5.3a}$$

$$H^\times |z_R^{*+}\rangle = z_R^* |z_R^{*+}\rangle \,, \qquad |z_R^{*+}\rangle \in \mathbf{\Phi}_-^\times \,. \tag{1.5.3b}$$

Next, we shall compute the energy representation of these Gamow vectors. We shall consider two energy representations. One energy representation will be associated to the physical spectrum, which is $[0, \infty)$ in our example. The other energy representation will be associated to the support of the Breit-Wigner distribution, which is $(-\infty, \infty)$. We will show that the $[0, \infty)$-energy representation of the Gamow vectors is the complex delta function, and that its $(-\infty, \infty)$-energy representation is given by the Breit-Wigner distribution.

Once the Gamow kets are constructed, we shall see that their time evolution is governed by a semigroup [20]. More precisely, we shall see that the time evolution of $|z_R^-\rangle$ can be defined only for *positive* values of time, whereas the time evolution of $|z_R^{*+}\rangle$ can be defined only for *negative* values of time:

$$e^{-iH^\times t/\hbar} |z_R^-\rangle = e^{-iz_R t/\hbar} |z_R^-\rangle = e^{-iE_R t/\hbar} e^{-\Gamma_R t/(2\hbar)} |z_R^-\rangle \,, \qquad \text{for } t > 0 \text{ only} \,, \tag{1.5.4a}$$

$$e^{-iH^\times t/\hbar} |z_R^{*+}\rangle = e^{-iz_R^* t/\hbar} |z_R^{*+}\rangle = e^{-iE_R t/\hbar} e^{\Gamma_R t/(2\hbar)} |z_R^{*+}\rangle \,, \qquad \text{for } t < 0 \text{ only} \,. \tag{1.5.4b}$$

Therefore, the Gamow vectors that we shall construct have all the properties that are demanded from a resonance state:

1. They are eigenvectors of the (dual extension of the self-adjoint) Hamiltonian with complex eigenvalues. These eigenvalues are also poles of the S-matrix.

2. They correspond to the Breit-Wigner amplitude in the $(-\infty, +\infty)$-energy representation.

3. Their time evolution is governed by a semigroup, and obeys the exponential decay law.

The Gamow vectors will be used also as basis vectors. The expansion generated by the Gamow vectors will be called the complex basis vector expansion. We shall see that

the Gamow vectors do not form a complete basis system. An additional set of Dirac kets corresponding to the energies that lie in the negative real axis of the second sheet of the Riemann surface will be added to complete them. As we shall see, the expansion of an in-state $\varphi^+ \in \mathbf{\Phi}_-$ reads

$$\varphi^+ = \int_0^{-\infty} |E^-\rangle S(E) \langle^+ E|\varphi^+\rangle dE - 2\pi i \sum_{n=0}^{\infty} r_n |z_n^-\rangle \langle^+ z_n|\varphi^+\rangle \,, \tag{1.5.5}$$

where $z_n = E_n - i\Gamma_n/2$ represents the n-th resonance energy of the square barrier potential, and r_n represents the residue of the S-matrix $S(E)$ at z_n. In Eq. (1.5.5), the infinite sum contains the resonances contribution, whereas the integral is associated to the background.

As we said above, the Gamow vectors have a semigroup time evolution. This semigroup time evolution expresses the time asymmetry built into a decaying process. Some authors such as Fonda *et al.* [52], Cohen-Tannoudji *et al.* [54], or Goldberger and Watson [55] have called this time asymmetry the *irreversibility* of a decaying process. In recent years, many authors using various languages have claimed that time asymmetry is a feature of the time evolution of any closed quantum systems (not just of a resonance process). For instance, Gell-Mann and Hartle have introduced the time asymmetry of closed quantum systems in terms of *decoherence histories* [56]. Haag uses the concept of *event* [57]. Bohm, Antoniou, and Kielanowski use the *preparation-registration* arrow of time [58]. Although we shall not discuss time asymmetry in this dissertation, we would like to mention that, for this author, the time asymmetry of a closed quantum system is built into the propagators (for more on this see Ref. [32], where the arrow of time of Quantum Electrodynamics is discussed).

1.6 Time Reversal

We shall also study how the time asymmetry of the resonances behaves under the action of the time reversal operator [59]. In order to do it, we shall apply the time reversal operator to the Gamow vectors. Essentially, we will show in Chapter 7 that the so-called "growing" Gamow vector is really the time reversed of the so-called "decaying" Gamow vector [60]. We shall also study more exotic possibilities, which are based on the work by Wigner.

When constructing projective representations of the Poincaré group extended by time reversal and parity, Wigner [61, 62] found that there are four possibilities. Three of these possibilities imply a doubling of the space supporting the representation. Later on, J. F. Cariñena and M. Santander[7] studied the projective representations of the Galilei group extended by time inversion and parity [63]. They also found four possibilities for the case with mass. As in the relativistic case, the standard case does not yield a doubling of the space that supports the representation, whereas the other three possibilities do yield a doubling.

Based on the work by Wigner [61, 62], Bohm has tried to find a meaning to the doubling of spaces [64]. In Chapter 7, we shall construct this doubling explicitly for one of the non-standard time reversal operators in the nonrelativistic domain.

[7] I thank Professor M. Santander for making me aware of his paper with Professor J. F. Cariñena and for his explanations on it.

1.7 Synopsis

The organization of this dissertation is as follows:

In Chapter 2, we review the mathematical methods of the Rigged Hilbert Space. The algebraic structures (linear spaces), the topological structures (topological spaces), and their combinations (linear topological spaces) are introduced in a pedestrian way. The countably Hilbert spaces, which are the class of linear topological spaces almost exclusively used in Quantum Mechanics, are studied in more detail. At the end of Chapter 2, the Hilbert space mathematical methods used in this dissertation are presented.

In Chapter 3, we construct the RHS of the harmonic oscillator.[8] This system is studied from a different point of view to that used in Quantum Mechanics textbooks. Instead of assuming that the position and momentum operators are given by the multiplication and derivative operators, we shall make three simple algebraic assumptions: the Heisenberg commutation relation, the expression of the Hamiltonian in terms of the position and momentum operators, and the existence of an eigenvector of the Hamiltonian. From these algebraic assumptions, we shall construct the RHS of the harmonic oscillator and the Schrödinger representation of the algebra of the harmonic oscillator.

In Chapter 4, we construct a RHS of the square barrier Hamiltonian by means of the Sturm-Liouville theory. This theory provides the direct integral decomposition of the Hilbert space. From this direct integral decomposition, we shall construct the RHS.

In Chapter 5, we turn to the description of the Lippmann-Schwinger equation within the RHS formalism. First, the Lippmann-Schwinger eigenfunctions will be computed. We shall define the Lippmann-Schwinger eigenkets in terms of the Lippmann-Schwinger eigenfunctions and see that they are defined on different spaces of wave functions. The Lippmann-Schwinger kets will be used as basis vectors to expand the wave functions. As well, the Møller operators and the S-matrix are explicitly constructed.

In Chapter 6, we construct the Gamow vectors of the square barrier resonances. First, we compute the resonance energies as poles of the S-matrix. The integral equation of A. Mondragón *et al.* for the Gamow vectors will be translated into the RHS language. The Gamow eigenfunctions in the position representation are obtained as the solutions of the time independent Schrödinger equation subject to the purely outgoing boundary condition. These eigensolutions will be associated to certain eigenfunctionals (Gamow kets). The $[0, \infty)$-energy representation of the Gamow eigenfunction will be related to the complex delta function, and the $(-\infty, \infty)$-energy representation of the Gamow eigenfunction will be related to the Breit-Wigner amplitude. The semigroup time evolution of the Gamow vectors will also be computed. The Gamow vectors will be used as basis vectors. We shall see that the Gamow vectors do not form a complete basis—an additional set of kets needs to be added in order to obtain a complete basis. The time asymmetry of the purely outgoing boundary condition will be disclosed. To finish the chapter, we shall elaborate on the exponential decay law of the Gamow vectors.

In Chapter 7, we study the behavior of resonances under the time reversal operation. We

[8] This chapter is a substantial improvement of and an extension to Ref. [29].

shall study the standard time reversal operator and also a non-standard one, which yields a doubling of the RHS.

Chapter 2

Mathematical Framework of Quantum Mechanics

In this chapter, we review the mathematical methods of the Rigged Hilbert Space. The algebraic structures (linear spaces), the topological structures (topological spaces), and their combinations (linear topological spaces) are introduced in a pedestrian way. The countably Hilbert spaces, which are the class of linear topological spaces almost exclusively used in Quantum Mechanics, are studied in more detail. At the end of this chapter, the Hilbert space mathematical methods used in this dissertation are presented.

> They rushed down the street together, digging everything in the early way they had, which later became so much sadder and perceptive and blank. But then they danced down the streets like dingledodies, and I shambled after as I've been doing all my life after people who interest me, because the only people for me are the mad ones, the ones who are mad to live, mad to talk, mad to be saved, desirous of everything at the same time, the ones who never yawn or say a commonplace thing, but burn, burn, burn like fabulous yellow roman candles exploding like spiders across the stars and in the middle you see the blue centerlight pop and everybody goes "Awww!".
>
> Jack Kerouac, *On the road*

2.1 Linear Spaces

2.1.1 Introduction

There are some major principles in Quantum Mechanics that seem to come from experimental data. Among them, there are the *linear superposition principle* and the *probabilistic nature* of Quantum Mechanics. These two principles suggest that the mathematical idealization of Quantum Mechanics should include a linear space Ψ with a scalar product $(\,\cdot\,,\,\cdot\,)$ defined on it. Then $(\Psi, (\,\cdot\,,\,\cdot\,))$ will be our primary mathematical object.

2.1.2 Linear Spaces and Scalar Product

A linear space $\mathbf{\Phi}$ is a set of elements $\varphi, \psi, \phi, \ldots$ which is assigned an algebraic structure that is a generalization of certain aspects of the three-dimensional real space $\mathbb{R}^3$. The elements, also called *vectors*, are defined to obey rules which are well-known properties of vectors in $\mathbb{R}^3$. The vector spaces which we use are in general not three-dimensional, but can have any dimension N, often infinite, and are defined, in general, over the complex numbers $\mathbb{C}$ rather than over the real numbers $\mathbb{R}$. There are two algebraic operations, the addition of vectors and the multiplication of a vector by a scalar. The rules for these operations that define the vector space are similar to those in $\mathbb{R}^3$.

Definition A *linear space* (also called *vector space*) $\mathbf{\Phi}$ over the complex numbers $\mathbb{C}$ is a set of elements φ, ψ, $\phi, \ldots$ for which the sum $\varphi + \psi$ of any two elements φ, ψ and the multiplication by a complex number $\lambda \in \mathbb{C}$, $\lambda\psi$, are defined and are elements of $\mathbf{\Phi}$, and have the following properties

$$\text{(VS1)} \quad \varphi + \psi = \psi + \varphi\,, \quad \forall \varphi, \psi \in \mathbf{\Phi}\,; \tag{2.1.1}$$

$$\text{(VS2)} \quad (\phi + \psi) + \varphi = \phi + (\psi + \varphi)\,, \quad \forall \phi, \psi, \varphi \in \mathbf{\Phi}\,; \tag{2.1.2}$$

$$\text{(VS3)} \quad \text{There exists a } 0 \in \mathbf{\Phi} \text{ such that } 0 + \varphi = \varphi\,, \quad \forall \varphi \in \mathbf{\Phi}\,; \tag{2.1.3}$$

$$\text{(VS4)} \quad \forall\, \varphi \in \mathbf{\Phi} \text{ there exists } \psi \in \mathbf{\Phi} \text{ such that } \varphi + \psi = 0 \text{ (we write } \psi \equiv -\varphi)\,; \tag{2.1.4}$$

$$\text{(VS5)} \quad (\lambda\mu)\varphi = \lambda(\mu\varphi)\,, \quad \forall \lambda, \mu \in \mathbb{C}\,,\ \forall \varphi \in \mathbf{\Phi}\,; \tag{2.1.5}$$

$$\text{(VS6)} \quad (\lambda + \mu)\varphi = \lambda\varphi + \mu\varphi\,, \quad \forall \lambda, \mu \in \mathbb{C}\,,\ \forall \varphi \in \mathbf{\Phi}\,; \tag{2.1.6}$$

$$\text{(VS7)} \quad \lambda(\varphi + \psi) = \lambda\varphi + \lambda\psi\,, \quad \forall \lambda \in \mathbb{C}\,,\ \forall \varphi, \psi \in \mathbf{\Phi}\,; \tag{2.1.7}$$

$$\text{(VS8)} \quad 1\varphi = \varphi\,, \quad \forall \varphi \in \mathbf{\Phi}\,. \tag{2.1.8}$$

From these, it follows that the zero element is unique and that, for each φ in $\mathbf{\Phi}$, the element $-\varphi$ is unique; moreover, $0\varphi = 0$ and $(-1)\varphi = -\varphi$ for all φ in $\mathbf{\Phi}$ and $\lambda 0 = 0$ for all λ in $\mathbb{C}$. A linear space over the field of real numbers can be described in exactly the same way with the word "real" substituted for the word "complex." The spaces that we shall use in Quantum Mechanics will have additional properties besides (2.1.1)-(2.1.8).

A subset S in a linear space $\mathbf{\Phi}$ is called a *subspace* of $\mathbf{\Phi}$ if S is a linear space under the same definitions of the operations of addition and multiplication by a number inherited from $\mathbf{\Phi}$, i.e., if it follows from $\varphi, \psi \in S$ and $\alpha \in \mathbb{C}$ that $\alpha\varphi \in S$ and $\varphi + \psi \in S$.

An expression of the form $\lambda_1\varphi_1 + \lambda_2\varphi_2 + \cdots + \lambda_n\varphi_n$, where the λ's are in $\mathbb{C}$ and the φ's in $\mathbf{\Phi}$, is called a *linear combination* of the vectors $\varphi_1, \varphi_2, \ldots, \varphi_n$. The vectors $\varphi_1, \varphi_2, \ldots, \varphi_n$ are said to be *linearly dependent* if there exist numbers $\alpha_1, \alpha_2, \ldots, \alpha_n$, not all zero, for which $\alpha_1\varphi_1 + \alpha_2\varphi_2 + \cdots + \alpha_n\varphi_n = 0$. If the equation $\alpha_1\varphi_1 + \alpha_2\varphi_2 + \cdots + \alpha_n\varphi_n = 0$ holds only for $\alpha_1 = \alpha_2 = \cdots = \alpha_n = 0$, then the vectors $\varphi_1, \varphi_2, \ldots, \varphi_n$ are called *linearly independent*. A space $\mathbf{\Phi}$ is said to be *finite dimensional* or, more precisely, *n-dimensional* if there are n and not more than n linearly independent vectors in $\mathbf{\Phi}$. If the number of linearly independent vectors in $\mathbf{\Phi}$ is arbitrarily large, then $\mathbf{\Phi}$ is said to be *infinite-dimensional*. Every system of n linearly independent vectors in an n-dimensional space $\mathbf{\Phi}$ is called a basis for $\mathbf{\Phi}$.

If $\varphi_1, \varphi_2, \ldots, \varphi_n$ is a basis for an n-dimensional space $\mathbf{\Phi}$ and φ is an arbitrary vector in $\mathbf{\Phi}$, then $\varphi, \varphi_1, \varphi_2, \ldots, \varphi_n$ are linearly dependent, so that

$$\alpha\varphi + \alpha_1\varphi_1 + \alpha_2\varphi_2 + \cdots + \alpha_n\varphi_n = 0\,, \tag{2.1.9}$$

for some $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ not all zero. Then $\alpha \neq 0$, for otherwise we should have

$$\alpha_1\varphi_1 + \alpha_2\varphi_2 + \cdots + \alpha_n\varphi_n = 0\,, \tag{2.1.10}$$

where $\alpha_1, \alpha_2, \ldots, \alpha_n$ are not all zero, which contradicts the supposition that the vectors $\varphi_1, \ldots, \varphi_n$ are linearly independent. But, if $\alpha \neq 0$, it follows from (2.1.9) that

$$\varphi = \xi_1\varphi_1 + \xi_2\varphi_2 + \cdots + \xi_n\varphi_n\,, \tag{2.1.11}$$

where $\xi_i = -\alpha_i/\alpha$. This representation of the element φ is unique. Thus, every vector φ in an n-dimensional space $\mathbf{\Phi}$ can be uniquely represented in the form (2.1.11), where $\varphi_1, \ldots, \varphi_n$ is a basis for $\mathbf{\Phi}$. The numbers $\xi_1, \ldots, \xi_n$ are called the *coordinates* of the vector φ relative to the basis $\varphi_1, \ldots, \varphi_n$. Notice that when the vectors are added, their corresponding coordinates relative to a fixed basis are added and, when a vector is multiplied by any number, all the coordinates are multiplied by that number.

Clearly the vectors $\vec{a}, \vec{b}, \ldots$ in the three-dimensional space $\mathbb{R}^3$ fulfill the relations (2.1.1)-(2.1.8). The set of complex infinitely differentiable continuous functions which vanish rapidly at infinity (called the *Schwartz space*) also fulfills these relations. One often says that the abstract vector space structure defined by the above rules is *realized* by other mathematical objects, if these objects appear to us more "real" than the "abstract" vectors. Thus if one feels more familiar with functions one may prefer the "realization" of $\mathbf{\Phi}$ by a space of functions over the space $\mathbf{\Phi}$ itself.

In physics, the abstract mathematical objects are realized by objects with a physical interpretation. Thus, a physicist's realization of a linear space is not by other more familiar or more interesting mathematical objects, but by physical objects. In particular, in quantum physics, the elements of the space $\mathbf{\Phi}$ will be the mathematical images of pure physical states which will be called state vectors. Thus, a vector structure is "realized" by a concrete space whose elements are interpreted as the physical states of a quantum system.

For the purposes of Quantum Mechanics, a linear space is a set with very little mathematical structure. We will equip it with another structure by defining a scalar product. This notion is again a generalization of the dot product in $\mathbb{R}^3$.

Definition A linear space is called *a scalar product space* (or *Euclidean space* or *pre-Hilbert space*) if for each pair of vectors $\varphi, \psi \in \mathbf{\Phi}$ we can define a complex number (φ, ψ) satisfying the following properties:

$$\text{(SP1)} \quad (\varphi, \psi) = \overline{(\psi, \varphi)} \quad \forall \varphi\,, \psi \in \mathbf{\Phi} \text{ (the overline denotes complex conjugation)}\,, \tag{2.1.12}$$

$$\text{(SP2)} \quad (\varphi, \alpha\psi_1 + \beta\psi_2) = \alpha(\varphi, \psi_1) + \beta(\varphi, \psi_2)\,, \quad \forall\, \varphi, \psi_1, \psi_2 \in \mathbf{\Phi}\,, \forall\, \alpha, \beta \in \mathbb{C}\,, \tag{2.1.13}$$

$$\text{(SP3)} \quad (\varphi, \varphi) \geq 0\,, \text{ and } (\varphi, \varphi) = 0 \text{ iff } \varphi = 0\,. \tag{2.1.14}$$

This function is called a *scalar product* and (φ, ψ) is called the scalar product of the elements φ and ψ.

The usual scalar product in $\mathbb{R}^3$, $(\vec{a}, \vec{b}) = \vec{a} \cdot \vec{b}$ clearly fulfills the conditions (2.1.12)-(2.1.14) with all numbers being real instead of complex.

As in $\mathbb{R}^3$, one calls two vectors φ and ψ *orthogonal* if

$$(\varphi, \psi) = 0\,. \tag{2.1.15}$$

With the scalar product defined by (2.1.12)-(2.1.14) one defines the *norm* $\|\varphi\|$ of a vector φ by

$$\|\varphi\| = +\sqrt{(\varphi, \varphi)}\,. \tag{2.1.16}$$

The norm of a vector is an extension of the notion of length of a vector in $\mathbb{R}^3$. For any vector ψ different from the zero vector one can always define a vector $\hat{\psi} = \psi/\|\psi\|$, which has the property $\|\hat{\psi}\| = 1$ and which is called a *normalized* vector.

Sometimes one needs in a vector space a more general notion than the scalar product, the bilinear Hermitian form.

Definition A complex-valued function $h(\varphi, \psi)$ of two vector arguments is a *Hermitian form* if it satisfies

$$h(\varphi, \psi) = \overline{h(\psi, \varphi)}\,, \tag{2.1.17}$$

$$h(\varphi, \alpha\psi) = \alpha h(\varphi, \psi)\,, \tag{2.1.18}$$

$$h(\varphi_1 + \varphi_2, \psi) = h(\varphi_1, \psi) + h(\varphi_2, \psi)\,. \tag{2.1.19}$$

If in addition h satisfies

$$h(\varphi, \varphi) \geq 0 \tag{2.1.20}$$

for every vector φ, then h is said to be a *positive Hermitian form*. A positive Hermitian form is called *positive definite* if from $h(\varphi, \varphi) = 0$ it follows that $\varphi = 0$. Thus a Hermitian form fulfills (2.1.12) and (2.1.13), but not the condition (2.1.14) for a scalar product. However, a positive definite Hermitian form is a scalar product.

Positive Hermitian forms, which are not necessarily scalar products, satisfy the *Cauchy-Schwartz-Bunyakovski inequality*:

$$|h(\varphi, \psi)|^2 \leq h(\varphi, \varphi) h(\psi, \psi)\,. \tag{2.1.21}$$

If h is positive definite, equality holds iff $\varphi = \alpha\psi$ for some $\alpha \in \mathbb{C}$.

Sometimes we have different realizations of the same algebraic structure. In these cases, the spaces are, from an algebraic point of view, the same.

Definition An *isomorphism* between two algebraic structures $\mathcal{A}$ and $\mathcal{B}$ is a one-to-one correspondence between the sets $\mathcal{A}$ and $\mathcal{B}$ (i.e., to every $a \in \mathcal{A}$ there corresponds exactly one $b \in \mathcal{B}$ and vice versa: $a \leftrightarrow b$), which preserves the algebraic operations.

For example, two linear scalar product spaces $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are isomorphic if there exists a mapping $f : \mathbf{\Phi} \to \mathbf{\Psi}$ which is one-to-one and onto and that fulfills

$$f(\alpha\varphi + \beta\psi) = \alpha f(\varphi) + \beta f(\psi)\,, \quad \forall \alpha\,, \beta \in \mathbb{C}\,,\ \forall \varphi\,, \psi \in \mathbf{\Phi}\,, \tag{2.1.22}$$

$$(\varphi, \psi)_{\mathbf{\Phi}} = (f(\varphi), f(\psi))_{\mathbf{\Psi}}\,, \quad \forall\,, \varphi\,, \psi \in \mathbf{\Phi}\,, \tag{2.1.23}$$

i.e., f preserves the sum, the multiplication and the scalar product. Isomorphic scalar product spaces (and in particular Hilbert spaces) are also called *isometric*. It often happens that two scalar product spaces are isomorphic as vector spaces, i.e., there is a one-to-one correspondence which fulfills (2.1.22), but are not isomorphic as scalar product spaces, i.e., the correspondence does not fulfill (2.1.23).

2.1.3 Linear Operators

Vectors in $\mathbb{R}^3$ can be transformed into each other. One example is the rotation R of a vector $\vec{a}$ into a vector $\vec{b} = R\vec{a}$. In analogy to this, one defines transformations or *linear operators* on a vector space $\mathbf{\Phi}$. A function A, $A : \mathbf{\Phi} \to \mathbf{\Phi}$, that maps each vector φ in a vector space $\mathbf{\Phi}$ into a vector $\psi \in \mathbf{\Phi}$, $A\varphi = \psi$, is called a *linear operator* if for all $\varphi, \psi \in \mathbf{\Phi}$ and $\alpha \in \mathbb{C}$ it fulfills the conditions

$$A(\varphi + \psi) = A\varphi + A\psi\,, \tag{2.1.24}$$

$$A(\alpha\varphi) = \alpha A\varphi\,. \tag{2.1.25}$$

An operator is called *antilinear* if it fulfills

$$A(\alpha\varphi) = \overline{\alpha} A\varphi \tag{2.1.26}$$

instead of (2.1.25), where $\overline{\alpha}$ is the complex conjugate of α.

For two operators defined on the whole space $\mathbf{\Phi}$, the operations of addition $A + B$, multiplication by a complex number αA, and multiplication AB, are defined in the following way:

$$(A + B)\varphi := A\varphi + B\varphi\,, \qquad (\alpha A)\varphi := \alpha(A\varphi)\,, \qquad (AB)\varphi := A(B\varphi)\,, \tag{2.1.27}$$

for all $\varphi \in \mathbf{\Phi}$. It is easily verified that $A + B$, αA and AB are linear operators defined on the whole space $\mathbf{\Phi}$ if A and B are linear operators defined on the whole space $\mathbf{\Phi}$. In finite

dimensional spaces with a topology (linear topological spaces defined in Section 2.3) there is a large class of operators that can be defined on the whole space, the continuous operators. In general this is not the case and the definition of $A+B$ and AB is more complicated and involves questions on the domains and on the ranges of the operators.

For every linear operator A defined on the whole space $\mathbf{\Phi}$, one can define an operator $A^\dagger$ on the elements ψ in $\mathbf{\Phi}$ for which

$$(A^\dagger\psi, \varphi) := (\psi, A\varphi)\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.1.28}$$

The operator $A^\dagger$ is called the *adjoint operator* of A. An operator for which $A^\dagger = A$ is called *self-adjoint* or *Hermitian*.[1]

In the general case, an operator A need not to be defined on the whole space $\mathbf{\Phi}$ but only on certain subset $\mathcal{D}(A)$ of $\mathbf{\Phi}$.

Definition Let $\mathbf{\Phi}, \mathbf{\Psi}$ be two linear spaces and let $\mathcal{D}(A)$ be a subspace of $\mathbf{\Phi}$. A mapping $A : \mathcal{D}(A) \subset \mathbf{\Phi} \to \mathbf{\Psi}$ is called a *linear operator* if

$$A(\alpha\varphi + \beta\psi) = \alpha A\varphi + \beta A\psi\,, \quad \forall\, \alpha, \beta \in \mathbb{C} \text{ and } \forall\, \varphi, \psi \in \mathcal{D}(A)\,, \tag{2.1.29}$$

and is called an *antilinear operator* if

$$A(\alpha\varphi + \beta\psi) = \overline{\alpha} A\varphi + \overline{\beta} A\psi\,, \quad \forall\, \alpha, \beta \in \mathbb{C} \text{ and } \forall\, \varphi, \psi \in \mathcal{D}(A)\,. \tag{2.1.30}$$

$\mathcal{D}(A)$ is the *domain* of A and $\mathcal{R}(A) = \{A\varphi \mid \varphi \in \mathcal{D}(A)\} \subset \mathbf{\Psi}$ is the *range* of A.

Let $A_i : \mathbf{\Phi} \supset \mathcal{D}(A_i) \to \mathbf{\Psi}$ $(i = 1, 2)$ be two linear operators with domains $\mathcal{D}(A_i)$. Then $A_1 + A_2$ is a linear operator with domain $\mathcal{D}(A_1) \cap \mathcal{D}(A_2)$ defined as

$$(A_1 + A_2)(\varphi) := A_1\varphi + A_2\varphi \tag{2.1.31}$$

for every φ in $\mathcal{D}(A_1) \cap \mathcal{D}(A_2)$. In the same way, αA_i is the operator defined on $\mathcal{D}(A_i)$ as

$$(\alpha A_i)(\varphi) := \alpha A_i\varphi \tag{2.1.32}$$

for each $\varphi \in \mathcal{D}(A_i)$. The product of A_1 and A_2 is defined as

$$(A_1A_2)(\varphi) = A_1(A_2\varphi) \tag{2.1.33}$$

for the vectors φ in $\mathbf{\Phi}$ such that φ is in $\mathcal{D}(A_2)$ and $A_2\varphi$ is in $\mathcal{D}(A_1)$. With these operations of addition and multiplication by scalars, the set of all linear operators mapping $\mathbf{\Phi}$ into $\mathbf{\Psi}$ form a vector space.

[1] We will usually use the term Hermitian if we do not want to distinguish between the mathematically precisely defined notions *self-adjoint, essentially self-adjoint*, and *symmetric*. We will present all these concepts in Section 2.5 along with the precise definition of the adjoint operator.

Of special interest are the zero operator, denoted 0, and the unit operator or identity operator, denoted I, which are defined by

$$0\varphi = 0\,, \qquad I\varphi = \varphi\,, \tag{2.1.34}$$

for every $\varphi \in \mathbf{\Phi}$. Note that 0 on the left side of the first equation is the zero operator, while 0 on the right is the zero vector in (2.1.3).

The definition of linear operators was inspired by the properties of transformations on the three-dimensional space. Linear operators on a vector space $\mathbf{\Phi}$ may be thought of as analogous to transformations on the three-dimensional Euclidean space, but they can also have other physical interpretations. In particular, in quantum physics they represent physical observables.

Very important notion for quantum physics is that of an eigenvalue and an eigenvector of an operator in a vector space.

Definition A nonzero vector $\psi \in \mathbf{\Phi}$ is called an eigenvector of the linear operator A if

$$A\psi = \lambda\psi \qquad \text{with} \qquad \lambda \in \mathbb{C}. \tag{2.1.35}$$

λ is called the *eigenvalue* of A corresponding to the eigenvector ψ.

For a given operator A, there may be many (perhaps infinitely many) different eigenvectors with different eigenvalues. There may also be n (finite or infinite) many different eigenvectors with the same eigenvalue λ. In this case, λ is called n-fold degenerate. In a finite dimensional space every linear operator (matrices) has at least one eigenvector. In an infinite dimensional space this is in general not fulfilled. For instance, the operator differentiation $-i\frac{d}{dx}$ defined on the Hilbert space $L^2(\mathbb{R})$ has no eigenvector belonging to $L^2(\mathbb{R})$.

If A is a Hermitian operator defined on a scalar product space, then eigenvectors and eigenvalues have the following properties:

1. All eigenvalues are real.
2. If φ_1 and φ_2 are eigenvectors of A with eigenvalues λ_1 and λ_2, respectively, and if $\lambda_1 \neq \lambda_2$, then φ_1 and φ_2 are orthogonal to each other, i.e., $(\varphi_1, \varphi_2) = 0$.

In quantum physics, an operator represents an observable of a physical system. Its eigenvalues then represent the numbers which are obtained in a measurement of this observable.

In the finite dimensional case (and in some special infinite dimensional cases), the eigenvectors of a Hermitian operator can be used to expand any state (wave function) in terms of them. In the infinite dimensional case, this expansion will need the concept of a *generalized eigenvector* and a *generalized eigenvalue* (see Section 3.5).

Definition An operator B is called the *inverse* of an operator A if $BA = AB = I$. The operator B is denoted by A^{-1}.

A linear operator U is called a *unitary* operator if $U^\dagger U = UU^\dagger = I$.

Because of the definition of the inverse operator, one can define a unitary operator also by the condition $U^\dagger = U^{-1}$. It is worthwhile noting that not every operator has an inverse.

Another important notion is that of the commutator of two operators.

Definition Let A and B be two operators defined on $\mathbf{\Phi}$. The *commutator* of A and B is defined by

$$[A, B] \equiv AB - BA \quad \text{or} \quad [A, B]\varphi = AB\varphi - AB\varphi\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.1.36}$$

A and B are said to *commute* if

$$[A, B] \equiv AB - BA = 0 \quad \text{or} \quad AB\varphi - AB\varphi = 0\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.1.37}$$

The collection of linear operators defined on the whole linear space forms a new algebraic structure, where the algebraic operations of sum of two operators, product of a number with an operator and product of two operators are defined by (2.1.27). This algebraic structure is called an *associative algebra*. An associative algebra can also be defined abstractly without any reference to linear operators by the following definition:

Definition A set $\mathcal{A}$ is an (*associative*) *algebra with unit element* iff

(A1) $\mathcal{A}$ is a vector space.

(A2) For every pair $A, B \in \mathcal{A}$, a product $AB \in \mathcal{A}$ is defined such that

$$(AB)C = A(BC)\,, \tag{2.1.38}$$
$$A(B + C) = AB + AC\,, \tag{2.1.39}$$
$$(A + B)C = AC + BC\,, \tag{2.1.40}$$
$$(\alpha A)B = A(\alpha B) = \alpha AB\,. \tag{2.1.41}$$

(A3) There exists an element $I \in \mathcal{A}$ such that

$$IA = AI = A\,, \quad \forall A \in \mathcal{A}\,. \tag{2.1.42}$$

A subset $\mathcal{A}_1$ of an algebra $\mathcal{A}$ is called a *subalgebra* of $\mathcal{A}$ if $\mathcal{A}_1$ is an algebra with the same definitions of the operations of addition, multiplication by a number, and multiplication as inherited from $\mathcal{A}$. That is, if from $A, B \in \mathcal{A}_1$ and $\alpha \in \mathbb{C}$, it follows that $A + B \in \mathcal{A}_1$, $\alpha A \in \mathcal{A}_1$, and $AB \in \mathcal{A}_1$.

(A4) An algebra $\mathcal{A}$ is called a $*$-*algebra* if we have on the algebra a $\dagger$-*operation* (involution), $A \to A^\dagger$, that has the following defining properties:

$$(\alpha A + \beta B)^\dagger = \overline{\alpha} A^\dagger + \overline{\beta} B^\dagger\,, \tag{2.1.43}$$

$$(AB)^\dagger = B^\dagger A^\dagger \,, \tag{2.1.44}$$
$$(A^\dagger)^\dagger = A \,, \tag{2.1.45}$$
$$I^\dagger = I \,, \tag{2.1.46}$$

where $A, B \in \mathcal{A}$ and $\alpha, \beta \in \mathbb{C}$.

From the definition (2.1.27) of the sum and the product of two operators and the product of an operator with a number, and from the definition (2.1.28) of the adjoint operator, one can see that the set of linear operators fulfills all the axioms (A1)-(A4) of a $*$-algebra. Thus the set of linear operators defined on the whole vector space $\mathbf{\Phi}$ forms a $*$-algebra. A subalgebra of this algebra is called an *operator $*$-algebra*. It can be shown that in a certain sense every $*$-algebra can be realized as an operator $*$-algebra in a scalar-product space (generalization of the Gelfand-Naimark-Segal reconstruction theorem). In Quantum Mechanics, physical systems are assumed to be described by operator algebras.

A set $X_1, X_2, \ldots, X_n$ of elements of $\mathcal{A}$ is called a *set of generators*, and $\mathcal{A}$ is said to be *generated* by the X_i $(i = 1, 2, \ldots, n)$ iff each element of $\mathcal{A}$ can be written as

$$A = cI + \sum_{i=1}^{n} c^i X_i + \sum_{i,j=1}^{n} c^{ij} X_i X_j + \ldots \,, \tag{2.1.47}$$

where $c, c^i, c^{ij}, \ldots \in \mathbb{C}$.

Defining algebraic relations are relations among the generators

$$P(X_i) = 0 \,, \tag{2.1.48}$$

where $P(X_i)$ is a polynomial with complex coefficients of the n variables X_i. An element $B \in \mathcal{A}$,

$$B = bI + \sum b^i X_i + \sum b^{ij} X_i X_j + \ldots \,, \tag{2.1.49}$$

where $b, b^i, \ldots \in \mathbb{C}$, is *equal* to the element A in (2.1.47) iff (2.1.49) can be brought into the form (2.1.47) with the same coefficients $c, c^i, c^{ij}, \ldots$ by the use of the defining relations (2.1.48).

2.1.4 Antilinear Functionals

In the previous section, we have introduced the concept of an eigenvector of an operator in a vector space. In Quantum Mechanics, some of the eigenvectors that we need are antilinear mappings from a space of states into the complex numbers. In this section, we define them and explain some of their basic properties.

Definition Let $\mathbf{\Phi}$ be a complex linear space. A *functional* (or a *function*) on $\mathbf{\Phi}$ is a mapping F from the space $\mathbf{\Phi}$ into the complex numbers $\mathbb{C}, F : \mathbf{\Phi} \to \mathbb{C}$. (If $\mathbf{\Phi}$ is a real space then the mapping is into the real numbers $\mathbb{R}$.)

If F satisfies

$$F(\alpha\varphi + \beta\psi) = \overline{\alpha}F(\varphi) + \overline{\beta}F(\psi)\,, \quad \forall\varphi,\psi \in \mathbf{\Phi}\,,\ \forall\alpha,\beta \in \mathbb{C}\,, \tag{2.1.50}$$

then F is called an *antilinear functional*. If F satisfies

$$F(\alpha\varphi + \beta\psi) = \alpha F(\varphi) + \beta F(\psi)\,, \quad \forall\varphi,\psi \in \mathbf{\Phi}\,,\ \forall\alpha,\beta \in \mathbb{C}\,, \tag{2.1.51}$$

then F is called a *linear functional*. (If $\mathbf{\Phi}$ is a real space there is no distinction between linear and antilinear functionals.) A linear or antilinear functional is thus a special case of a linear or antilinear operator between two linear spaces (see (2.1.29) and (2.1.30)) if the space $\mathbf{\Psi}$ is the space of complex numbers $\mathbb{C}$.

A functional is also the analog of a complex-valued function $F(x)$ of a real variable x varying on $\mathbb{R}$, $F : \mathbb{R} \to \mathbb{C}$, only now the variable is not a real number $x \in \mathbb{R}$ but a vector $\varphi \in \mathbf{\Phi}$. We will consider here antilinear functionals rather than linear functionals (in the mathematical literature one usually considers linear functionals).

An example of an antilinear functional on a scalar product space is given by

$$\begin{aligned} F_\psi : \mathbf{\Phi} &\to \mathbb{C} \\ \varphi &\to F_\psi(\varphi) = (\varphi,\psi)\,, \end{aligned} \tag{2.1.52}$$

where ψ is a *fixed* element in $\mathbf{\Phi}$ and (φ,ψ) is the scalar product of ψ with φ, where φ varies over $\mathbf{\Phi}$. Because of this example and because in the general case we want to consider a functional to be a generalization of the scalar product, one uses for the antilinear functional $F(\varphi)$ the Dirac's bra-ket symbol (see reference [1])

$$F(\varphi) \equiv \langle\varphi|F\rangle\,. \tag{2.1.53}$$

We shall use the two notations concurrently. Dirac kets will be given a mathematical meaning as antilinear functionals (which in addition are continuous, notion that will be defined in Section 2.2).

Any two antilinear functionals F_1 and F_2 on a linear space $\mathbf{\Phi}$ may be added and multiplied by numbers according to

$$(\alpha F_1 + \beta F_2)(\varphi) = \alpha F_1(\varphi) + \beta F_2(\varphi)\,, \quad \alpha,\beta \in \mathbb{C}\,, \tag{2.1.54}$$

or, using the notation (2.1.53),

$$\langle\varphi|\alpha F_1 + \beta F_2\rangle = \alpha\langle\varphi|F_1\rangle + \beta\langle\varphi|F_2\rangle\,. \tag{2.1.55}$$

The functional $\alpha F_1 + \beta F_2$ defined by (2.1.54) is again an antilinear functional over $\mathbf{\Phi}$. Thus, the set of antilinear functionals on a vector space $\mathbf{\Phi}$ is a linear space itself. This space is called the *conjugate space* or *dual space* (more precisely, the *algebraic dual* or *algebraic conjugate space*) of the space $\mathbf{\Phi}$ and is denoted by $\mathbf{\Phi}^\times_{alg}$.

2.2 Topological Spaces

2.2.1 Introduction

When we defined the vector space we took a set $\mathbf{\Phi}$ of elements (which we called $\varphi, \psi, \ldots$) and endowed this set with an algebraic structure by defining two operations, addition of two elements and multiplication of $\varphi \in \mathbf{\Phi}$ by an $\alpha \in \mathbb{C}$. We demanded that these operations fulfilled certain rules (see Section 2.1.2). The resulting structured set was called a linear space. (We thereafter defined another algebraic operation on $\mathbf{\Phi}$, the scalar product—see Section 2.1.2—and called $\mathbf{\Phi}$ a scalar product space). Now we take a set, which we call again $\mathbf{\Phi}$ (but which is not yet a vector space), and endow it with another structure, a topological structure. The resulting structured set will be called a *topological space*.

The topology on a space provides us with a way of phrasing such concepts of nearness, continuity, convergence, completion, etc that we are familiar with for the space of real numbers. We shall start with the concept of "open set," which is a generalization of the notion of open set in $\mathbb{R}$. However, there are several equivalent ways of defining a topology (via open sets, or closed sets, or neighborhoods,...) and for more restricted cases one can define the topology in more specific ways, e.g. by convergence of sequences. We want to start in the most general setting and then to specialize the concepts without much discussions in order to arrive rapidly at the particular spaces that we need in Quantum Mechanics.

2.2.2 Open Sets and Neighborhoods

Definition Let $\mathbf{\Phi}$ be a set and let $\mathcal{P}(\mathbf{\Phi}) = \{S \mid S \subset \mathbf{\Phi}\}$ be the collection of all subsets of $\mathbf{\Phi}$. A subset $\tau_{\mathbf{\Phi}}$ of $\mathcal{P}(\mathbf{\Phi})$ is called a *topology* of $\mathbf{\Phi}$ if the following conditions are fulfilled:

$$\text{(O1)} \quad \emptyset \in \tau_{\mathbf{\Phi}} \text{ and } \mathbf{\Phi} \in \tau_{\mathbf{\Phi}} \ (\emptyset \text{ is the empty set})\,. \tag{2.2.1}$$

$$\text{(O2)} \quad \text{The union of arbitrarily many elements of } \tau_{\mathbf{\Phi}} \text{ is an element of } \tau_{\mathbf{\Phi}}\,. \tag{2.2.2}$$

$$\text{(O3)} \quad \text{The intersection of a finite number of elements of } \tau_{\mathbf{\Phi}} \text{ is in } \tau_{\mathbf{\Phi}}\,. \tag{2.2.3}$$

The pair $(\mathbf{\Phi}, \tau_{\mathbf{\Phi}})$ is called a *topological space* and the elements of $\tau_{\mathbf{\Phi}}$ are called *open sets*.

With the given definition of topology we can define the convergence of sequences of elements (points) $\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots \equiv \{\varphi_n\}_{n=0}^{\infty}$ of the set $\mathbf{\Phi}$, which is a generalization of the notion of convergence for real numbers.

Definition A sequence of points $\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots \in \mathbf{\Phi}$ is said to *converge to* $\varphi \in \mathbf{\Phi}$ if for every open set O with $\varphi \in O$ there exists a positive integer $N = N(O)$ such that $\varphi_n \in O$ for all $n > N(O)$.

This definition means that beginning from a large enough N the elements of the sequence are as close to φ as we desire.

Example Let $\mathbf{\Phi}$ be the set of real numbers $\mathbb{R}$. The meaning of the convergence of the sequence $\{y_n\}$, written as $\lim_{n\to\infty} y_n = x$ (or $y_n \to x$), is the following: the open sets O containing x in the previous definition are given by

$$U_\epsilon(x) \equiv \{y \in \mathbb{R} \mid |x - y| < \epsilon\,,\ \epsilon > 0\}\,. \tag{2.2.4}$$

Then, according to the definition of convergence, for every $U_\epsilon(x)$ there exists an N_ϵ such that for all $n > N_\epsilon$, $y_n \in U_\epsilon(x)$, i.e., $|x - y_n| < \epsilon$. This is the well-known definition of convergence of a sequence of real numbers. The open sets $U_\epsilon(x)$ in (2.2.4) are called *neighborhoods* of x. The generalization of the concept of a neighborhood to a topological space is the following:

Definition If $\mathbf{\Phi}$ is a topological space and $\varphi \in \mathbf{\Phi}$, a *neighborhood* (hereafter abbreviated *nhood*) of φ is a set U which contains an open set O containing φ (that is, $\varphi \in O \subset U$). The collection $\mathcal{U}_\varphi$ of all nhoods of φ is the *nhood system* at φ. Nhoods need not be open but we shall only use systems of open nhoods, i.e., $U \in \mathcal{U}_\varphi$ which also are in $\tau_{\mathbf{\Phi}}$.

One can easily see that a sequence $\{\varphi_n\}_{n=0}^{\infty}$ converges to an element φ iff each nhood of φ contains every point of the sequence whose index is larger than some positive integer depending on the given nhood. Thus, it is a generalization of the notion of convergence for real numbers.

Definition A subset $S \subset \mathbf{\Phi}$ is said to be a *topological subspace* of $\mathbf{\Phi}$ if S is given the topology

$$\tau_S = \{S \cap O \mid O \in \tau_{\mathbf{\Phi}}\}\,. \tag{2.2.5}$$

To describe a given topology, we do not need to know the whole collection of open sets: it is enough to know a proper subcollection.

Definition A base $\mathcal{B}$ of a topology $\tau_{\mathbf{\Phi}}$ on $\mathbf{\Phi}$ is a subcollection of $\tau_{\mathbf{\Phi}}$ such that every open set O is a union of some open sets in $\mathcal{B}$, i.e., each $O \in \tau_{\mathbf{\Phi}}$ can be given as

$$O = \bigcup_\alpha B_\alpha, \quad B_\alpha \in \mathcal{B}. \tag{2.2.6}$$

Thus, given a base $\mathcal{B}$ we generate all the open sets (and therefore we describe the topology completely) taking all possible unions of sets in $\mathcal{B}$. In much the same way that a base describes the whole collection of open sets, a nhood system can be completely described by a nhood base.

Definition A *nhood base* (or a *system of basic nhoods*) at φ in the topological space $\mathbf{\Phi}$ is a subcollection $\mathcal{B}_\varphi$ taken from the nhood system $\mathcal{U}_\varphi$, having the property that each $U \in \mathcal{U}_\varphi$ contains some $V \in \mathcal{B}_\varphi$. Once a nhood base at φ has been chosen (there are many to choose from, all producing the same nhood system at φ) its elements are called *basic nhoods*.

Obviously, the nhood system at φ is itself a nhood base at φ. In the topological space of the real numbers $\mathbb{R}$, the open set (2.2.4) is a nhood of x and $\{U_\epsilon(x),\ \epsilon > 0\}$ is a system of basic nhoods at x. But also

$$\mathcal{B}_x = \{U_{1/m}(x) \mid \quad m = 1, 2, \ldots\} \tag{2.2.7}$$

is a system of basic nhoods at the point $x \in \mathbb{R}$ which consists of a countable number of nhoods. For the real numbers we know that a sequence $\{y_n\}$ is already convergent to a point x, $y_n \to x$, iff for every $m \in \mathbb{N}$, $|x - y_n| < \frac{1}{m}$ for all positive integers n greater than a certain natural number $N = N(m)$ depending on m. Thus, the countable system of nhoods (2.2.7) defines already the convergence in $\mathbb{R}$ and defines the topology completely.

In general, a topological space does not need to have a countable system of (basic) nhoods at each of its points. But there are many spaces which have this property.

Definition A space $\mathbf{\Phi}$ is said to satisfy the *first axiom of countability* if it has a countable system of basic nhoods at each of its points. We also called these spaces *first countable*.

Most of the spaces in which we are interested satisfy the first axiom of countability. The most important feature of this kind of topologies is that we can describe them completely using convergence on sequences (that is, specifying which sequences converge to which points).

Using the above definitions one can prove that in a topological space $\mathbf{\Phi}$ a system of nhoods $\mathcal{U}_\varphi$ at a point φ has the properties:

(N1) If $U \in \mathcal{U}_\varphi$, then $\varphi \in U$, (2.2.8)

(N2) If $U, V \in \mathcal{U}_\varphi$, then $U \cap V \in \mathcal{U}_\varphi$, (2.2.9)

(N3) If $U \in \mathcal{U}_\varphi$, then there is a $V \in \mathcal{U}_\varphi$ such that $U \in \mathcal{U}_\psi$ for each $\psi \in V$, (2.2.10)

(N4) If $U \in \mathcal{U}_\varphi$, and $U \subset V$ then $V \in \mathcal{U}_\varphi$, (2.2.11)

and furthermore,

(N5) $O \subset \mathbf{\Phi}$ is open iff O contains a nhood of each of its points. (2.2.12)

Conversely, if in a set $\mathbf{\Phi}$ a collection $\mathcal{U}_\varphi$ of subsets of $\mathbf{\Phi}$ is assigned to each $\varphi \in \mathbf{\Phi}$ so as to satisfy (2.2.8)-(2.2.11) and if we define "open" using (2.2.12), the result is a topology on $\mathbf{\Phi}$ (i.e., a collection of subsets of $\mathbf{\Phi}$ satisfying (2.2.1)-(2.2.3)) in which $\mathcal{U}_\varphi$ is a nhood system at φ, for each $\varphi \in \mathbf{\Phi}$. Therefore, whenever nhoods have been assigned to each point in a set, satisfying the properties (2.2.8)-(2.2.11), the topology is completely specified. This means that we can equivalently describe a topology (that is, to describe the concepts of nearness, continuity, convergence,...) using as starting point the open sets or the nhood systems at each point. Obviously, one can also describe the topology completely assigning a system of basic nhoods to each point.

A given set $\mathbf{\Phi}$ can be equipped with various topologies. Different topologies on the same set lead to different meanings of nearness, continuity, convergence,... If $\mathbf{\Phi}$ is equipped with two different topologies, say with τ_1 and τ_2, and if $\tau_1 \subset \tau_2$, then τ_1 is called *coarser*

than τ_2 and the convergence with respect to τ_1 *weaker* than the convergence with respect to τ_2. Correspondingly, τ_2 is called *finer* than τ_1 and the convergence with respect to τ_2 is called *stronger* than with respect to τ_1. Since every $U \in \tau_1$ is also in τ_2, it follows from the definition of convergence that every strongly convergent sequence is also weakly convergent.

One can arrive at the same topology in a space (i.e., the same system of open sets) starting from two different systems of nhoods. For example, in defining the natural topology on the real line we can, on the one hand, take as nhoods the open intervals (2.2.4) with real ϵ's and, on the other hand, take the nhoods (2.2.7) with rational ϵ's. As mentioned above, both systems of nhoods describe the same topology. In general, we will call two different systems of nhoods *equivalent*, if they lead to the same topology. The following simple condition is both necessary and sufficient for the equivalence of two given nhood systems $\{U\}$ and $\{V\}$: every nhood U contains a nhood V, and every nhood V contains a nhood U.

A topology can also be described in terms of closed sets. To introduce this notion, we first need the following definition:

Definition Let $(\mathbf{\Phi}, \tau_{\mathbf{\Phi}})$ be a topological space and let $S \subset \mathbf{\Phi}$. $\varphi \in \mathbf{\Phi}$ is called an *adherence point* of S if for every $U \in \mathcal{U}_\varphi$, then $U \cap S \neq \emptyset$.

In particular, every point of the set S is an adherence point. There are two possibilities for the adherence points of a set S:

1. There exists a nhood of φ (the adherence point) which contains only a finite number of points of S. We are not interested in this case.

2. Every nhood of the adherence point φ contains an infinite number of distinct points of S. Then φ is called a *limit point* of S.

A limit point φ of S may or may not belong to S. A set S is said to be *closed* if it contains *all* of its adherence points. If a set S is not closed one obtains the *closure* $\overline{S}$ of S by adjoining to S those of its adherence points which do not already belong to it. Thus the closure $\overline{S}$ of S is the collection of all adherence points of S. The closure of any set S is closed, and S is closed iff $\overline{S} = S$. The concepts of open and closed set are dual to each other. In fact, a set $M \subset \mathbf{\Phi}$ is closed (i.e., $\overline{M} = M$) iff its complement $\mathbf{\Phi} - M$ is open.

Definition A set D in a topological space $\mathbf{\Phi}$ is called *dense* in $\mathbf{\Phi}$ if $\overline{D} = \mathbf{\Phi}$. A topological space $\mathbf{\Phi}$ is *separable* iff $\mathbf{\Phi}$ has a countable dense subset.

The real line is separable, since the rational numbers are dense in $\mathbb{R}$, and most of the spaces used in Quantum Mechanics are separable.

2.2.3 Separation Axioms

The above definition of a topology is still too general. The topologies that are of importance in physics satisfy more requirements. These topologies all fulfill strong conditions for the

meaning of separation of two points φ and ψ in $\mathbf{\Phi}$. These conditions will allow us to "distinguish" between two different points of the space using only the topology.

Definition A topological space $\mathbf{\Phi}$ is a T_0-*space* (or, the topology on $\mathbf{\Phi}$ is T_0) if whenever φ and ψ are distinct points in $\mathbf{\Phi}$, there is an open set containing one and not the other.

A topological space $\mathbf{\Phi}$ is a T_1-*space* if whenever φ and ψ are distinct points in $\mathbf{\Phi}$, there is a nhood of each not containing the other.

$\mathbf{\Phi}$ is said to be a T_2-*space* (also called *Hausdorff*) if whenever φ and ψ are distinct points of $\mathbf{\Phi}$, there are disjoint open sets U and V in $\mathbf{\Phi}$ with $\varphi \in U$ and $\psi \in V$.

Every T_2-space is T_1, and every T_1-space is T_0. In a T_1-space, every finite set is closed. In a T_2-space, every convergent sequence has exactly one (unique) limit point. For this reason, the minimum that we will require of our topologies is that they be Hausdorff spaces. But often we will make even stronger separation demands on our spaces.

Definition A topological space $\mathbf{\Phi}$ is said to be *regular* if whenever S is closed and φ is not in S, then there are disjoint open sets U and V with $\varphi \in U$ and $S \subset V$.

We define a T_3-*space* to be a regular T_1-space.

A topological space $\mathbf{\Phi}$ is *normal* if whenever S and P are disjoint closed sets in $\mathbf{\Phi}$, there are disjoint open sets U and V with $S \subset U$ and $P \subset V$.

A normal T_1-space will be called T_4.

Roughly speaking, in T_3- and T_4-spaces we can "distinguish" (or "separate") points from sets and sets from sets, respectively. Every T_4-space is T_3, and every T_3-space is T_2. Most spaces we shall consider will be T_4. The class of T_4-spaces include all metrizable and therefore all locally convex spaces whose topology is given by a countable number of seminorms. These include countable normed spaces, countable Hilbert spaces, and, in particular, normed and scalar product spaces. The definition of these kinds of spaces will be given is Section 2.4.1. All the spaces that we shall use in Quantum Mechanics for the space $\mathbf{\Phi}$ of a rigged Hilbert space $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ will be countable Hilbert spaces and therefore T_4.

2.2.4 Continuity and Homeomorphic Spaces

An important notion that depends upon the topology is the notion of a continuous mapping. Intuitively, a map f is continuous at a given point φ if the images of the points close to φ are close to $f(\varphi)$. Thus the concept of continuity is derived from that of nearness, and therefore is given by the topology.

Definition Let $(\mathbf{\Phi}, \tau_{\mathbf{\Phi}})$ and $(\mathbf{\Psi}, \tau_{\mathbf{\Psi}})$ be two topological spaces and $f : \mathbf{\Phi} \to \mathbf{\Psi}$. Then f is *continuous* at $\varphi \in \mathbf{\Phi}$ iff for each nhood V of $f(\varphi)$ in $\tau_{\mathbf{\Psi}}$, there is a nhood U of φ in $\tau_{\mathbf{\Phi}}$ such that $f(U) \subset V$. We say f is *continuous on* $\mathbf{\Phi}$ iff f is continuous at each $\varphi \in \mathbf{\Phi}$.

One can use the open sets to describe continuous maps on the whole space. A map

$f : \mathbf{\Phi} \to \mathbf{\Psi}$ is continuous on $\mathbf{\Phi}$ iff the inverse image of every open set of $\mathbf{\Psi}$ is an open set of $\mathbf{\Phi}$, i.e., $O \in \tau_{\mathbf{\Psi}} \Rightarrow f^{-1}(O) \in \tau_{\mathbf{\Phi}}$.

In the case of spaces that satisfy the first axiom of countability, we can use the sequences (that determine completely the topology) to describe the continuity of a function at a given point. A map $f : \mathbf{\Phi} \to \mathbf{\Psi}$, where $\mathbf{\Phi}$ and $\mathbf{\Psi}$ satisfy the first axiom of countability, is continuous at a point φ iff whenever $\varphi_n \to \varphi$ with respect to $\tau_{\mathbf{\Phi}}$, then $f(\varphi_n) \to f(\varphi)$ with respect to $\tau_{\mathbf{\Psi}}$.

A map is called a *topological map* (or *homeomorphism*) if it is one-to-one, onto and continuous and f^{-1} is also continuous. In this case, we say that $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are *homeomorphic*. Homeomorphic spaces are, from a topological point of view, the same. That is, there is no topological property that allows us to distinguish them. Moreover, a *topological property* is anything that is conserved under homeomorphisms.

In order to convey the meaning of the combination of an algebraic structure with a topological structure, as is needed for the definition of a linear topological space in Section 2.3, we have to define the direct product of two topological spaces.

Definition Let $(\mathbf{\Phi}_1, \tau_1)$ and $(\mathbf{\Phi}_2, \tau_2)$ be topological spaces. Then the topology on the direct product space $\mathbf{\Phi}_1 \times \mathbf{\Phi}_2$ is generated by the base

$$\mathcal{B} = \{O_1 \times O_2 \mid O_1 \in \tau_1, O_2 \in \tau_2\}, \tag{2.2.13}$$

i.e., the (topological) product space is $(\mathbf{\Phi}_1 \times \mathbf{\Phi}_2, \tau)$, where τ is the collection of arbitrary unions of the sets that belong to $\mathcal{B}$ in (2.2.13).

2.3 Linear Topological Spaces

2.3.1 Introduction

A *linear topological space* (also called a *topological vector space*) is a combination of a linear structure (see Section 2.1.2) and a topological structure (see Section 2.2), both introduced on one and the same set $\mathbf{\Phi}$. However, these structures are not independent of each other. The linear operations, which are mappings on $\mathbf{\Phi}$, are required to be continuous in order that these two structures match each other. The general procedure to construct topological algebraic structures (topological algebras, topological groups, topological vector spaces) is:

1. One endows a given set $\mathbf{\Phi}$ with an algebraic structure.

2. One endows the same set $\mathbf{\Phi}$ with a topological structure.

3. One demands that the algebraic operations on $\mathbf{\Phi}$ be continuous mappings.

The reason why one constructs these mathematical structures is that there exist realizations of such structures (with some additional properties) that are very useful in mathematics and in physics. For instance, linear topological spaces are realized in mathematics by classes

of functions (e.g., the Schwartz space). In physics, these abstract mathematical entities are used to describe some structures in nature. For example, topological groups (in particular parameter or Lie groups) are the mathematical image of symmetry transformations of the registration apparatuses (detector) relative to the preparation apparatuses (accelerator). Linear topological spaces and their algebras of linear operators provide the mathematical framework to describe the states and the observables of quantum physics, respectively.

For the combination of a topological structure with the algebraic structure, the following definition is an example of the general procedure described above.

Definition A set $\mathbf{\Phi}$ is called a *linear topological space (l.t.s.)* or a *topological vector space (t.v.s.)* if

$$\text{(LT1)} \quad \mathbf{\Phi} \text{ is a linear space}. \tag{2.3.1}$$

$$\text{(LT2)} \quad \mathbf{\Phi} \text{ is a topological space}. \tag{2.3.2}$$

$$\text{(LT3)} \quad \text{The algebraic operations are continuous}. \tag{2.3.3}$$

Assumption (2.3.3) means that the mapping

$$\begin{aligned} : \mathbb{C} \times \mathbf{\Phi} &\to \mathbf{\Phi} \\ (\alpha, \varphi) &\to \alpha\varphi \end{aligned} \tag{2.3.4}$$

and the mapping

$$\begin{aligned} : \mathbf{\Phi} \times \mathbf{\Phi} &\to \mathbf{\Phi} \\ (\varphi, \psi) &\to \varphi + \psi \end{aligned} \tag{2.3.5}$$

are continuous. The continuity of these operations gives a precise meaning to intuitive notions such as an "infinite linear combination" of vectors or the limit of an infinite sequence of vectors. A l.t.s. is often denoted by $(\mathbf{\Phi}, \tau_{\mathbf{\Phi}}, +, \cdot)$ in order to specify the linear and the topological structures. We shall just denote a l.t.s. by $\mathbf{\Phi}$ if no confusion is possible.

From the continuity of the algebraic operations it follows that if $U(0)$ is a nhood of the zero element, then $V = \varphi + U(0)$ (i.e., the set obtained by adding φ to all the elements of $U(0)$, also called the *translate of* $U(0)$ *by* φ) is a nhood of φ. In other words, the nhood system at φ is just the family of translates by φ of members of the nhood system at 0. Therefore, the topology of a l.t.s. can be completely specified by the system of nhoods at the zero element.

If $\mathcal{U}_0$ is a base of nhoods at the zero element in the l.t.s. $\mathbf{\Phi}$, then $\mathbf{\Phi}$ is T_2 if and only if $\bigcap_{U \in \mathcal{U}_0} U = \{0\}$, i.e., iff the intersection of the nhoods of zero is precisely zero. We shall always assume that the topology of a l.t.s. is T_2. Moreover, we shall consider mostly T_4 spaces. In particular, for all the spaces $\mathbf{\Phi}$ in the Rigged Hilbert Space $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ we shall choose exclusively T_4 spaces.

The simplest example of a l.t.s. is the real line $\mathbb{R}$ when endowed with the usual addition and multiplication (which provide the linear algebraic structure) and with the topology of

the absolute value defined in Section 2.2.2. In a similar manner, the complex numbers $\mathbb{C}$ can be also considered as a l.t.s.

A useful concept in $\mathbb{R}$ is that of a bounded set. A set $S \subset \mathbb{R}$ is *bounded* if there exists an $M > 0$ such that $|x| < M$ for all $x \in S$. The generalization of this notion to an arbitrary l.t.s. is:

Definition A subset B of a l.t.s. $\mathbf{\Phi}$ is said to be *bounded* if for every nhood of zero $U(0)$ there exists a $\lambda > 0$ such that $B \subset \lambda U(0)$. $\lambda U(0) = \{\lambda\varphi \mid \varphi \in U(0)\}$, the set obtained by multiplying each element of $U(0)$ by λ, is called a *multiple* of $U(0)$.

Roughly speaking, a set is bounded if every nhood of zero has a multiple that swallows it up. By using the nhoods of $\mathbb{R}$ in Section 2.2.2, one can show that this definition agrees with the above definition of boundedness of $S \subset \mathbb{R}$.

It is easy to see that if τ_1 and τ_2 are two topologies on a l.t.s. $\mathbf{\Phi}$ and if $\tau_1 \subset \tau_2$, then every set B which is bounded with respect to the finer topology τ_2 is also bounded with respect to the coarser topology τ_1.

2.3.2 Cauchy Sequences

In the topological vector space of real numbers $\mathbb{R}$, a sequence $\{y_n\}_{n=0}^{\infty}$ is called *Cauchy* if for every $\epsilon > 0$ there is a positive integer $N = N(\epsilon)$ (depending only on ϵ) such that for all $n, m \geq N$ we have $|y_n - y_m| < \epsilon$. This means that a sequence is Cauchy if beginning from a large enough N the elements of the sequence are more and more close to each other. We can reformulate this definition in terms of nhoods of the zero element in $\mathbb{R}$: a system of nhoods at $x = 0$ is the collection (see Section 2.2.2) $\mathcal{U}_0 = \{U_\epsilon(0) \mid \epsilon > 0\}$ where $U_\epsilon(0) = \{y \in \mathbb{R} \mid |y| < \epsilon\}$. Then a sequence $\{y_n\}_{n=0}^{\infty}$ of real numbers is Cauchy iff for every nhood $U_\epsilon(0)$ of 0, there is a positive integer $N(U_\epsilon)$ such that $y_n - y_m \in U_\epsilon(0)$ for all $n, m > N$. We shall generalize this concept to an arbitrary l.t.s.

Definition A sequence $\{\varphi_n\}_{n=0}^{\infty}$ of elements in a l.t.s. $\mathbf{\Phi}$ is called *Cauchy* if for every nhood U of the zero element there exists a natural number $N = N(U)$, depending only on U, such that $\varphi_n - \varphi_m \in U$ for all $n, m > N$.

Every convergent sequence is Cauchy, but the converse is not always true, i.e., a Cauchy sequence need not converge to a point in the space. In the l.t.s. of the real numbers $\mathbb{R}$, a sequence is Cauchy iff it is convergent to some (unique) real number. In the l.t.s. of rational numbers $\mathbb{Q}$ this is not the case, since there are Cauchy sequences of rational numbers which do not converge to any rational number (for example, any sequence of rational numbers converging to π).

Definition A l.t.s. $\mathbf{\Phi}$ is called *complete* (more precisely, *sequentially complete*) if every Cauchy sequence has a limit in $\mathbf{\Phi}$.

This definition means that in a sequentially complete space we always get to a point in the space whenever we follow a sequence of elements that become more and more close to each other. When the same set is endowed with two different topologies we usually say that the space is τ-complete, if we want to emphasize which topology we are considering.

In general, we seek spaces that are complete. This is why if a l.t.s. is not complete we complete it by adjoining all the limit elements of Cauchy sequences to it. Then, the incomplete space can be viewed as a dense subspace of its completion.

Definition A complete l.t.s. $\mathbf{\Phi}^c$ is said to be the *completion* of an incomplete l.t.s. $\mathbf{\Phi}$ if there is a map $i : \mathbf{\Phi} \to \mathbf{\Phi}^c$ which is one-to-one, linear and continuous with continuous inverse i^{-1} such that $i(\mathbf{\Phi})$ is dense in $\mathbf{\Phi}^c$.

Note that the function i (usually called an *embedding*) is not onto (if so, $\mathbf{\Phi}$ would already be a complete space). The completion of a space $\mathbf{\Phi}$ is unique up to a linear homeomorphism which leaves $\mathbf{\Phi}$ pointwise fixed. As an example, $\mathbb{R}$ is a completion of $\mathbb{Q}$.

Completeness is a very important requirement in mathematics. Without it one cannot prove existence theorems nor define derivatives or integrals. In physics, completeness cannot be established directly from physical observation because completeness involves an infinite number of entities (Cauchy sequences) and all physical observations involve only a finite number of states. Thus, it cannot be "deduced" directly from experiments and only the overall success of a mathematical theory can show which completion—more precisely, completion with respect to which topology—is preferable for quantum physics.

We have given above only the definition of sequential completeness, which is sufficient when the topology is fully described in terms of the convergence of sequences (that is, when the topology satisfies the first axiom of countability). If the space is not first countable, its completion cannot be defined in terms of Cauchy sequences. It has to be defined in terms of *nets*, which we do not want to introduce here. With this more general definition of completion, every l.t.s. can be completed in the sense of the above definition, the completion is unique (up to a linear homeomorphism) and the space can be considered as a dense subspace of its completion. The space $\mathbf{\Phi}$ of the Rigged Hilbert Space $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ will always be chosen to satisfy the first axiom of countability. Therefore, it can be completed using Cauchy sequences. The space $\mathbf{\Phi}^\times$ will in general not be first countable, and its completion must be constructed using the general definition.

Since any metrizable space (a class that includes scalar product spaces, normed spaces and countably normed spaces) is first countable (see Section 2.3.3), we can complete it by using Cauchy sequences. Vaguely speaking, the completion is accomplished in the following way: two Cauchy sequences $(\varphi_1, \varphi_2, \varphi_3, \ldots)$ and $(\psi_1, \psi_2, \psi_3, \ldots)$ in $\mathbf{\Phi}$ are considered equivalent if beginning from a large enough term their elements are more and more close to each other. More precisely, $(\varphi_1, \varphi_2, \varphi_3, \ldots) \sim (\psi_1, \psi_2, \psi_3, \ldots)$ iff for every $U \in \mathcal{U}_0$ there is a positive integer $N(U)$ such that $\varphi_n - \psi_m \in U$ for all $n, m > N$. We denote by $[(\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots)]$ the set of sequences which are equivalent to $(\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots)$. On

this space of equivalence sequences, one defines an algebraic addition

$$[(\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots)] + [(\psi_1, \psi_2, \ldots, \psi_n, \ldots)] := [(\varphi_1 + \psi_1, \varphi_2 + \psi_2, \ldots, \varphi_n + \psi_n, \ldots)] \quad (2.3.6)$$

and a multiplication by scalars

$$\lambda[(\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots)] := [\lambda(\varphi_1, \varphi_2, \ldots, \varphi_n, \ldots)] \,. \quad (2.3.7)$$

We define the metric on this space as

$$d^c([\{\varphi_n\}_{n=0}^{\infty}], [\{\psi_n\}_{n=0}^{\infty}]) := \lim_{n\to\infty} d(\varphi_n, \psi_n) \,, \quad (2.3.8)$$

where d is the metric on the incomplete space and d^c will be the metric on the complete space. Finally, we define the map $i : \mathbf{\Phi} \to \mathbf{\Phi}^c$ as $i(\varphi) = [(\varphi, \varphi, \ldots, \varphi, \ldots)]$, i.e., the elements φ of the incomplete l.t.s. $\mathbf{\Phi}$ are represented in $\mathbf{\Phi}^c$ by the infinite rows $(\varphi, \varphi, \varphi, \ldots)$. In the end, i is a 1:1, linear, continuous mapping and $i(\mathbf{\Phi})$ is dense in $\mathbf{\Phi}^c$. Moreover, we can extend other algebraic operations on $\mathbf{\Phi}$ to $\mathbf{\Phi}^c$ in the same way we extended the sum and the products by scalars. For example, we can extend a scalar product on $\mathbf{\Phi}$ to $\mathbf{\Phi}^c$ via the definition

$$([\{\varphi_n\}_{n=0}^{\infty}], [\{\psi_n\}_{n=0}^{\infty}])_c := \lim_{n\to\infty} (\varphi_n, \psi_n) \quad (2.3.9)$$

where $(\,\cdot\,,\,\cdot\,)_c$ is the scalar product on $\mathbf{\Phi}^c$ and $(\,\cdot\,,\,\cdot\,)$ is the scalar product on $\mathbf{\Phi}$.

2.3.3 Normed, Scalar Product and Metric Spaces

In a linear space $\mathbf{\Phi}$, we can introduce algebraic operations that have in principle nothing to do with a topology, but that can be used to define one. For instance, in Section 2.1.2 we introduced a scalar product on a vector space. The resulting structure, called scalar product space, has significance even without any topological considerations. However, this scalar product can be used to define several topologies on the scalar product space (a Hilbert space topology, a nuclear topology,...). Another example of an algebraic operation that can give rise to a topology is the norm.

Definition Let $\mathbf{\Phi}$ be a linear space. A *norm* $\|\cdot\|$ on $\mathbf{\Phi}$ is a function which associates to each $\varphi \in \mathbf{\Phi}$ a finite real number $\|\varphi\|$ fulfilling

$$\text{(N1)} \quad \|\varphi + \psi\| \le \|\varphi\| + \|\psi\| \,, \quad \forall\, \varphi, \psi \in \mathbf{\Phi} \,. \quad (2.3.10)$$

$$\text{(N2)} \quad \|\alpha\varphi\| = |\alpha|\, \|\varphi\| \,, \quad \forall\, \varphi \in \mathbf{\Phi}, \forall \alpha \in \mathbb{C} \,. \quad (2.3.11)$$

$$\text{(N3)} \quad \|\varphi\| \ge 0 \,, \text{ and } \|\varphi\| = 0 \text{ only if } \varphi = 0 \,. \quad (2.3.12)$$

A linear space $\mathbf{\Phi}$ equipped with a norm $\|\cdot\|$ is usually denoted by $(\mathbf{\Phi}, \|\cdot\|)$, and it is called a *normed space*. From (2.3.10) and (2.3.11), it follows that $\|0\| = 0$.

With the use of the norm we can specify a system of nhoods at 0 to define a topology, called the *norm topology*. We define the nhoods of the zero element by

$$U_\epsilon(0) = \{\varphi \mid \|\varphi\| < \epsilon\}\,, \quad \epsilon > 0\,. \tag{2.3.13}$$

Then the nhoods of any ψ are defined by

$$U_\epsilon(\psi) = \psi + U_\epsilon(0) = \{\varphi \mid \|\varphi - \psi\| < \epsilon\}\,. \tag{2.3.14}$$

The system of nhoods at zero

$$\mathcal{U}_0 = \{U_\epsilon(0) \mid \epsilon > 0\} \tag{2.3.15}$$

provides a topology for the normed space $(\mathbf{\Phi}, \|\cdot\|)$. Equipped with this topology, $(\mathbf{\Phi}, \|\cdot\|)$ is a l.t.s. In place of (2.3.15), one can choose a countable system of nhoods at zero

$$\mathcal{W}_0 = \{U_{1/m}(0) \mid m = 1, 2, ...\}\,. \tag{2.3.16}$$

One can show that the systems of nhoods (2.3.15) and (2.3.16) are equivalent, i.e., they yield the same topology. In particular, this means that every normed space satisfies the first axiom of countability.

In the l.t.s. $(\mathbf{\Phi}, \|\cdot\|)$, we can give a meaning to the topological notions we have discussed above (convergence of sequences, completeness,...). For example, according to the general definition given in Section 2.3.2, a sequence $\{\varphi_n\}_{n=0}^\infty$ is Cauchy if for every $U_\epsilon(0)$ in (2.3.13) there exists an $N = N(U_\epsilon)$ such that for all $n, m > N$, $\varphi_n - \varphi_m \in U_\epsilon(0)$. This means that for every $\epsilon > 0$ there exists a natural number $N = N(\epsilon)$ such that for all $n, m > N$, $\|\varphi_n - \varphi_m\| < \epsilon$. This is the definition of Cauchy sequences that one usually finds in tracts on normed spaces. As in the general case, a normed space $\mathbf{\Phi}$ is called *complete* if every Cauchy sequence converges to an element in $\mathbf{\Phi}$. If a normed space $(\mathbf{\Phi}, \|\cdot\|)$ is not complete then it can be completed. A complete normed space is called a *Banach* space.

Now, given a scalar product $(\,\cdot\,,\,\cdot\,)$ on a linear space $\mathbf{\Phi}$ we can define the *norm provided by the scalar product* as

$$\|\varphi\| := +\sqrt{(\varphi, \varphi)}\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.3.17}$$

It is easy to see that (2.3.17) is a well defined norm that satisfies the requirements (2.3.10)-(2.3.12) if the scalar product satisfies (2.1.12)-(2.1.14). Therefore, we can make a scalar product space $\mathbf{\Phi}$ a l.t.s. by using the system of nhoods at zero (2.3.15) or (2.3.16) with $\|\cdot\|$ defined by (2.3.17). Although a scalar product always describes a norm (through (2.3.17)), the converse is not always true. Therefore a scalar product space is always a normed space but the converse does not necessarily hold.

Definition A scalar product space is called a *Hilbert space* if it is complete with respect to the topology generated by the norm given by the scalar product as in (2.3.17). We shall usually denote a Hilbert space by $\mathcal{H}$.

Thus a Hilbert space is the completion of the scalar product space of Section 2.1.2 with respect to the topology given by the system of nhoods (2.3.15) or (2.3.16) . Since the Hilbert

space has been so important in mathematics and physics, a scalar product space (in which one does not introduce any topology) is often called a *pre-Hilbert space*. Every pre-Hilbert space becomes a Hilbert space when we complete it with respect to the topology given by (2.3.15) with (2.3.17). It is worthwhile noting that the Hilbert space topology is not the only topology for which one can complete a scalar product space $\mathbf{\Phi}$. In Section 2.4 we will discuss other different topologies that can be introduced on $\mathbf{\Phi}$.

Definition A real-valued function d, defined for each pair of elements φ, ψ of a set $\mathbf{\Phi}$, is called a *metric* if it satisfies

$$\text{(M1)} \quad d(\varphi+\psi) \le d(\varphi,\phi)+d(\phi,\psi)\,, \quad \forall\,\varphi,\phi,\psi\in\mathbf{\Phi}\,. \tag{2.3.18}$$

$$\text{(M2)} \quad d(\varphi,\psi)=d(\psi,\varphi)\,, \quad \forall\,\varphi,\psi\in\mathbf{\Phi}\,. \tag{2.3.19}$$

$$\text{(M3)} \quad d(\varphi,\psi)\ge 0\,,\ d(\varphi,\varphi)=0\,,\ \text{and } d(\varphi,\psi)>0 \text{ if } \varphi\ne\psi\,. \tag{2.3.20}$$

A set $\mathbf{\Phi}$ provided with a metric is called a *metric space* and $d(\varphi,\psi)$ is called the *distance* between φ and ψ.

Let $V(\varphi,\epsilon)$ be the set of all elements $\psi\in\mathbf{\Phi}$ such that $d(\varphi,\psi)<\epsilon$. Then, the collection

$$\mathcal{U}_\varphi=\{V(\varphi,\epsilon)\mid \epsilon>0\} \tag{2.3.21}$$

is a system of basic nhoods at φ that generate a topology on $\mathbf{\Phi}$. Endowed with this topology, a metric space is a l.t.s. A topological space is called *metrizable* if its topology can be defined by a metric d. Every metrizable space is first countable, since the system of nhoods

$$\{V(\varphi,1/n)\mid n=1,2,\ldots\} \tag{2.3.22}$$

is equivalent to (2.3.21). A metrizable space is also T_4.

The real numbers and the complex numbers are both metrizable spaces, the metric being given by

$$d(x,y):=|x-y|\,,\quad x,y\in\mathbb{R}\,(\in\mathbb{C})\,. \tag{2.3.23}$$

If we are given a norm $\|\cdot\|$ defined on a linear space, we can define a metric associated to it by $d(\varphi,\psi)=\|\varphi-\psi\|$. Therefore, normed and scalar product spaces are metrizable, and their topology as metrizable spaces coincides with the topology defined by the norm or by the scalar product.

2.3.4 Continuous Linear Operators and Continuous Antilinear Functionals

Linear operators and antilinear functionals were defined in Sections 2.1.3 and 2.1.4. In quantum physics, the operators (representing quantum mechanical observables and quantum mechanical states) are linear and the functionals (representing *kets* or *generalized states*) are antilinear. Therefore, we shall use here linear operators and antilinear functionals; corresponding mathematical statements hold for antilinear operators and linear functionals.

Definition Let $\mathbf{\Phi}$ and $\mathbf{\Psi}$ be two l.t.s. A map $A : \mathcal{D}(A) \subset \mathbf{\Phi} \to \mathbf{\Psi}$ is called a *continuous linear mapping* or just a *continuous operator* iff

1. A is linear (cf. Section 2.1.3),
2. A is continuous (cf. Section 2.2.4).

The notion of continuity of an operator on a l.t.s. can be localized at zero, in the same way that the topology can be localized at zero. More precisely, a linear mapping A from a l.t.s. $\mathbf{\Phi}$ into another l.t.s. $\mathbf{\Psi}$ is continuous on the whole space $\mathbf{\Phi}$ iff it is continuous at the zero element. Therefore, a linear mapping $A : \mathbf{\Phi} \to \mathbf{\Psi}$ is continuous iff for every nhood U of $0 \in \mathbf{\Psi}$ there exists a nhood V of $0 \in \mathbf{\Phi}$ such that $A(V) \subset U$. When the l.t.s. $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are first countable (that is, the topology can be described in terms of convergence of sequences), then the sequential criterion for continuity (see Section 2.2.4) can also be localized at zero: an operator $A : \mathbf{\Phi} \to \mathbf{\Psi}$ is continuous iff whenever $\varphi_n \to 0$ in $\mathbf{\Phi}$, then $A(\varphi_n) \to 0$ in $\mathbf{\Psi}$.

The notion of boundedness is related to the continuity of an operator:

Definition A linear operator $A : \mathbf{\Phi} \to \mathbf{\Psi}$ is called *bounded* iff it transforms every $\tau_{\mathbf{\Phi}}$-bounded set $B \subset \mathbf{\Phi}$ into a $\tau_{\mathbf{\Psi}}$-bounded set $A(B) \subset \mathbf{\Psi}$ (cf. Section 2.3.1 for the definition of a bounded set).

One can show that every continuous operator defined on a l.t.s. is bounded. Moreover, if the l.t.s. $\mathbf{\Phi}$ and $\mathbf{\Psi}$ satisfy the first axiom of countability, an operator $A : \mathbf{\Phi} \to \mathbf{\Psi}$ is continuous if and only if it is bounded. Therefore, in all normed, countably normed and metrizable spaces (which are first countable) one can use the words continuous operator and bounded operators interchangeably.

Continuous operators as compared to non-continuous operators have nicer properties and are easier to handle because they can always be defined on the whole space $\mathbf{\Phi}$. Even if initially they are only defined on a dense subspace $\mathcal{D}(A)$, their definition can be extended to the whole space in a continuous manner. As an example of this extension, consider two first countable l.t.s. $\mathbf{\Phi}$ and $\mathbf{\Psi}$ such that $\mathbf{\Psi}$ is complete. Let $A : \mathcal{D}(A) \subset \mathbf{\Phi} \to \mathbf{\Psi}$ be a densely defined continuous operator. Then A can be uniquely extended to the whole space $\mathbf{\Phi}$ in a continuous way as follows: if $\varphi \in \mathbf{\Phi}$ but φ is not in $\mathcal{D}(A)$ we can always find a sequence $\{\varphi_n\}$ in $\mathcal{D}(A)$ such that $\varphi_n \to \varphi$ with respect to $\tau_{\mathbf{\Phi}}$. Since $\{\varphi_n\}$ is $\tau_{\mathbf{\Phi}}$-Cauchy, $\{A\varphi_n\}$ is $\tau_{\mathbf{\Psi}}$-Cauchy, and $\{A\varphi_n\}$ has a well defined limit ψ in $\mathbf{\Psi}$. We can define the action of A on φ to be this limit ψ

$$A\varphi := \lim_{n\to\infty} A\varphi_n\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.3.24}$$

The operator defined in (2.3.24) is well defined on the whole space $\mathbf{\Phi}$, extends the action of A on $\mathcal{D}(A)$ and is continuous. For the spaces $\mathbf{\Phi}$ of the RHS $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ and for the operators defined on them this extension will always be possible. In fact, we shall always assume that every continuous linear (as well as antilinear) operator has already been extended to the whole space $\mathbf{\Phi}$.

If $A : \mathbf{\Phi} \to \mathbf{\Psi}$ is a continuous linear operator then (αA), $\alpha \in \mathbb{C}$, is also a continuous linear operator. If A, B are continuous linear operators then $A + B$ and $A \cdot B$ are also continuous linear operators. Thus if the generators X_i of an algebra $\mathcal{A}$ are given by continuous operators then the whole algebra is an algebra of continuous operators and every $A \in \mathcal{A}$ given by (2.1.47) with a finite numbers of terms are defined on the whole space $\mathbf{\Phi}$. (The question of the convergence of infinite sums of the form (2.1.47) can only be addressed after a topology has been introduced on $\mathcal{A}$). If one wants to do calculations it is of great importance to have an algebra of continuous operators which are defined on the whole space, because then one does not have to worry about domain questions, i.e., one does not have to answer the question whether $B\varphi$ is in the domain $\mathcal{D}(A)$ of an operator A to calculate $AB\varphi$. Also one will not have to deal with the absurd situation that the expectation value $(\varphi, A\varphi)$, representing average value of a quantum mechanical observable A measured in quantum mechanical state φ, is "infinite" when φ is not in $\mathcal{D}(A)$. It would, therefore, be desirable that all quantum mechanical observables were given by continuous operators on a suitable l.t.s. This means that the mathematical image of all quantum mechanical observables should be a set (perhaps an algebra) of continuous operators on some l.t.s. Only vectors φ of such l.t.s. can represent physical states. The non-continuous operators should be forbidden because they may lead to nonphysical infinite predictions.

Much of the trouble of the Hilbert Space formalism comes from domain questions. Already the simplest operators of Quantum Mechanics, the operators momentum P and position Q, which fulfill the algebraic relation $PQ - QP = -i1$ (Heisenberg commutation relation), cannot be represented by continuous operators in the Hilbert space $\mathcal{H}$. Thus the Hilbert space contains some "non-physical states" in which these operators are not defined. This is one of the reasons why we have to introduce a countably norm topology $\tau_{\mathbf{\Phi}}$ in addition to the algebraic structure of a scalar product space. The completion with respect to this topology generates a space $\mathbf{\Phi}$. This space, which is as subspace of $\mathcal{H}$, allows for a representation by $\tau_{\mathbf{\Phi}}$-continuous operators that satisfy the Heisenberg commutation relation or similar algebraic relations (e.g., the commutation relations of non-compact groups of importance in physics). Our task is thus to find a topology $\tau_{\mathbf{\Phi}}$ such that the phenomenological commutation relations of Quantum Mechanics are represented by continuous operators on some space $\mathbf{\Phi}$. For the Heisenberg commutation relations and many other algebraic relations (including the commutation relations of all Lie groups) a countably Hilbert space (cf. Section 2.4) will do the job.

The concept and properties of a continuous antilinear functional $F : \mathbf{\Phi} \to \mathbb{C}$ follows from the case of a continuous linear mapping just changing linearity for antilinearity and considering the space $\mathbb{C}$ as a l.t.s.

Definition A map $F : \mathbf{\Phi} \to \mathbb{C}$ is called a *continuous antilinear functional* if

1. F is antilinear (cf. Section 2.1.3),

2. F is continuous (cf. Section 2.2.4).

Dirac kets, Lippmann-Schwinger kets and Gamow vectors will be represented by continuous antilinear functionals.

The collection $\mathbf{\Phi}^\times$ of continuous antilinear functionals on a l.t.s. $\mathbf{\Phi}$, i.e., the set

$$\mathbf{\Phi}^\times = \{F : \mathbf{\Phi} \to \mathbb{C} \,|\, F \text{ is antilinear and } \tau_{\mathbf{\Phi}}\text{−continuous}\}\,, \tag{2.3.25}$$

is called the *conjugate* of $\mathbf{\Phi}$, the *topological dual* of $\mathbf{\Phi}$, or the *adjoint* of $\mathbf{\Phi}$. The conjugate space depends, as all topological notions do, on the particular topology that has been chosen. The conjugate space is a linear space under the usual sum of two functionals and multiplication of a functional by a complex number. Since the elements of $\mathbf{\Phi}^\times$ must be continuous, the topological dual is always a subspace of the algebraic dual defined in Section 2.1.4. A topology can also be assigned to $\mathbf{\Phi}^\times$ to make it a l.t.s.

Example If $(\mathbf{\Phi}, \|\cdot\|)$ is a Banach space, an antilinear functional F on $\mathbf{\Phi}$ is continuous iff the quantity

$$\|F\|_{\mathbf{\Phi}^\times} := \sup_{\varphi\in\mathbf{\Phi},\,\varphi\neq 0} \frac{|F(\varphi)|}{\|\varphi\|} \tag{2.3.26}$$

is a finite real number. $\|F\|_{\mathbf{\Phi}^\times}$ is called the *norm* of the antilinear functional F. One can prove that (2.3.26) is indeed a well defined norm that satisfies (2.3.10)-(2.3.12). Moreover, the adjoint space $\mathbf{\Phi}^\times$ of a Banach space $\mathbf{\Phi}$ is a Banach space itself when we define the norm of a functional by (2.3.26). An antilinear functional F over a Banach space is bounded iff there exists a positive constant K such that

$$|F(\varphi)| \leq K\|\varphi\|\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.3.27}$$

Since a Banach space is first countable, F is continuous iff F is bounded. In fact, $\|F\|_{\mathbf{\Phi}^\times}$ in (2.3.26) is the minimum of the real numbers K that satisfy (2.3.27).

The adjoint $\mathcal{H}^\times$ of a Hilbert space $\mathcal{H}$, that in particular is a Banach space, can be constructed in a similar fashion and can be endowed with the norm topology generated by (2.3.26). Once this is done, the following important theorem holds:

Theorem (Riesz-Frechet) For every $\tau_{\mathcal{H}}$-continuous antilinear functional F on a Hilbert space $\mathcal{H}$ there exists a unique vector $f_F \in \mathcal{H}$ such that

$$F(g) = (g, f_F)\,, \quad \forall\, g \in \mathcal{H}\,, \tag{2.3.28}$$

and such that $\|f_F\|_{\mathcal{H}} = \|F\|_{\mathcal{H}^\times}$.

The Riesz-Frechet theorem provides a one-to-one continuous linear mapping of $\mathcal{H}^\times$ onto $\mathcal{H}$,

$$\begin{aligned} : \mathcal{H}^\times &\to \mathcal{H} \\ F &\to f_F\,, \end{aligned} \tag{2.3.29}$$

that preserves the norms of the spaces. Therefore, a Hilbert space and its adjoint are isometric spaces (cf. Section 2.1.2). This is usually abbreviated as

$$\mathcal{H} \simeq \mathcal{H}^{\times} . \tag{2.3.30}$$

In general, two l.t.s. $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are called *isomorphic* if there exists a one-to-one mapping h of $\mathbf{\Phi}$ onto $\mathbf{\Psi}$ which is linear and continuous and such that its inverse is continuous. The mapping h is called an *isomorphism*.[2] Thus an isomorphism is a mapping that preserves the linear topological structure of the spaces. Two isomorphic spaces are, from a linear topological point of view, the same, and are usually identified,

$$\mathbf{\Phi} \simeq \mathbf{\Psi} . \tag{2.3.31}$$

When $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are normed spaces, a linear mapping h of $\mathbf{\Phi}$ onto $\mathbf{\Psi}$ is an isomorphism iff there are positive constants K_1 and K_2 with

$$K_1\|\varphi\| \leq \|h(\varphi)\| \leq K_2\|\varphi\| . \tag{2.3.32}$$

Two isomorphic metric spaces are usually called isometric.

A continuous linear operator A defined on the whole of a l.t.s. $\mathbf{\Phi}$,

$$A : \mathbf{\Phi} \to \mathbf{\Phi} , \tag{2.3.33}$$

can be extended into $\mathbf{\Phi}^{\times}$ by

$$\langle \varphi | A^{\times} F \rangle := \langle A\varphi | F \rangle , \quad \varphi \in \mathbf{\Phi} , \ F \in \mathbf{\Phi}^{\times} . \tag{2.3.34}$$

The dual extension $A^{\times}$ defined by (2.3.34) is a well defined linear operator on $\mathbf{\Phi}^{\times}$

$$A^{\times} : \mathbf{\Phi}^{\times} \to \mathbf{\Phi}^{\times} . \tag{2.3.35}$$

2.4 Countably Hilbert Spaces

2.4.1 Introduction

In Section 2.3 we studied how to combine a linear and a topological structure. The resulting l.t.s. structure is still too general for the purposes of Quantum Mechanics. We now distinguish a class of l.t.s. that is of service in Quantum Mechanics: *countably Hilbert spaces*. A countably Hilbert space is a linear space on which a countable number of scalar products is defined, i.e., for every $\varphi, \psi \in \mathbf{\Phi}$ there exist

$$(\varphi, \psi)_1, \ (\varphi, \psi)_2, \ldots, (\varphi, \psi)_p, \ldots , \tag{2.4.1}$$

[2] Since algebraic isomorphisms were also designated as isomorphisms in Section 2.1.2, the terms *topological isomorphism* and *topologically isomorphic* may be used to avoid misunderstanding.

which fulfill the defining conditions (2.1.12)-(2.1.14) of the scalar product. From these scalar products one can define the norms

$$\|\varphi\|_p := \sqrt{(\varphi,\varphi)_p}\,, \quad p = 1, 2, \ldots \tag{2.4.2}$$

One can also define a countably set of arbitrary norms $\|\varphi\|_p$ not necessarily given by scalar products. In this case, the space is called *countably normed*. The scalar products (norms) in a countably Hilbert (normed) space must be related to each other. This relation makes these norms match each other in the sense given by the following definitions:

Definition Let $\|\cdot\|_1$ and $\|\cdot\|_2$ be two norms defined on the same linear space $\mathbf{\Phi}$. These two norms are called *comparable* if for every $\varphi \in \mathbf{\Phi}$ there exists a constant $C > 0$ such that

$$\|\varphi\|_1 \leq C\|\varphi\|_2\,, \quad \forall\, \varphi \in \mathbf{\Phi}\,. \tag{2.4.3}$$

The norm $\|\cdot\|_1$ is called *weaker* than the norm $\|\cdot\|_2$ and $\|\cdot\|_2$ is called *stronger* than $\|\cdot\|_1$. Two norms are *equivalent* if there exist two constants C and D such that

$$\|\varphi\|_1 \leq C\|\varphi\|_2\,, \quad \|\varphi\|_2 \leq D\|\varphi\|_1\,, \tag{2.4.4}$$

for every $\varphi \in \mathbf{\Phi}$.

Every sequence that is Cauchy with respect to the stronger norm is also Cauchy with respect to the weaker norm. If two norms are equivalent, a sequence is Cauchy with respect to one of the norms iff it is Cauchy with respect to the other norm.

Definition Two norms are called *compatible* iff every sequence $\{\varphi_n\}_{n=1}^{\infty} \subset \mathbf{\Phi}$ which is Cauchy with respect to both norms and which converges to 0 with respect to one of them, also converges to 0 with respect to the other norm.

Let $\|\cdot\|_1$ and $\|\cdot\|_2$ be two comparable and compatible norms on a linear space $\mathbf{\Phi}$ such that $\|\cdot\|_1$ is weaker than $\|\cdot\|_2$. We can complete $\mathbf{\Phi}$ with respect to the norm $\|\cdot\|_1$ to obtain a complete normed space $\mathbf{\Phi}_1$. Similarly, we can complete $\mathbf{\Phi}$ with respect to the norm $\|\cdot\|_2$ to obtain $\mathbf{\Phi}_2$. We then have

$$\mathbf{\Phi}_1 \supset \mathbf{\Phi}_2 \supset \mathbf{\Phi}\,. \tag{2.4.5}$$

If $\|\cdot\|_1$ and $\|\cdot\|_2$ are equivalent, then both completions yield the same space,

$$\mathbf{\Phi}_1 = \mathbf{\Phi}_2 \supset \mathbf{\Phi}\,. \tag{2.4.6}$$

Definition A space $\mathbf{\Phi}$ is a *countably Hilbert space* (or a *countably scalar product space*) if an increasing denumerable number of scalar products

$$(\varphi,\varphi)_1 \leq (\varphi,\varphi)_2 \leq \cdots \leq (\varphi,\varphi)_p \leq \cdots \tag{2.4.7}$$

are defined on $\mathbf{\Phi}$ such that the norms

$$\|\varphi\|_p := \sqrt{(\varphi,\varphi)_p}\,, \quad p = 0, 1, 2, \ldots \tag{2.4.8}$$

are comparable and compatible. The nhoods of zero that generate the topology are given by

$$U_{p,\epsilon}(0) = \{\varphi \mid \|\varphi\|_p < \epsilon\}\,, \quad \epsilon > 0,\, p = 1, 2, \ldots \tag{2.4.9}$$

The topology generated by (2.4.9) make $\mathbf{\Phi}$ a linear topological space, i.e., the algebraic operations are continuous.

Instead of (2.4.9), one can also choose the countable number of nhoods

$$U_{p,m}(0) = \{\varphi \mid \|\varphi\|_p < \frac{1}{m}\}\,, \quad p, m = 1, 2, \ldots \tag{2.4.10}$$

It is not hard to see that the systems of nhoods (2.4.9) and (2.4.10) are equivalent. Therefore, in a countably scalar product space the first axiom of countability holds, and its topology $\tau_{\mathbf{\Phi}}$ is completely specified by the definition of convergence of sequences. As it is easily seen, a sequence $\{\varphi_n\}_{n=1}^{\infty}$ of elements in a countably Hilbert space $\mathbf{\Phi}$ converges to zero with respect to this topology iff it converges to zero with respect to every norm $\|\cdot\|_p$, $p = 0, 1, 2, \ldots$ In symbols,

$$\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} 0 \quad \text{iff} \quad \|\varphi_n\|_p \xrightarrow[n\to\infty]{\tau_{\mathbb{C}}} 0\,, \qquad \text{for every } p = 1, 2, 3, \ldots \tag{2.4.11}$$

and

$$\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \quad \text{iff} \quad \|\varphi_n - \varphi\|_p \xrightarrow[n\to\infty]{\tau_{\mathbb{C}}} 0\,, \qquad \text{for every } p = 1, 2, 3, \ldots \tag{2.4.12}$$

Since a countably Hilbert space is first countable, the continuity of the linear combinations $\alpha\varphi + \beta\psi$ can be equivalently stated in terms of sequences as:

1. if $\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \varphi$ then also $\alpha\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \alpha\varphi$ for every $\alpha \in \mathbb{C}$,
2. if $\alpha_n \xrightarrow[n\to\infty]{\tau_{\mathbb{C}}} \alpha$ then also $\alpha_n\varphi \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \alpha\varphi$ for every $\varphi \in \mathbf{\Phi}$,
3. if $\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \varphi$ and $\psi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \psi$ then $\varphi_n + \psi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \varphi + \psi$.

If a given system of countable scalar products $(\,\cdot\,,\,\cdot\,)_p$ does not fulfill the inequalities (2.4.7), it can be replaced by a new equivalent system of scalar products that has this property. We just need to define a new increasing sequence of scalar products as

$$(\varphi,\varphi)'_p := \sum_{i=1}^{p} (\varphi,\varphi)_i\,, \quad p = 1, 2, 3, \ldots \tag{2.4.13}$$

The systems of scalar products $(\,\cdot\,,\,\cdot\,)'_p$ and $(\,\cdot\,,\,\cdot\,)_p$ yield the same topology. Therefore, the condition (2.4.7) does not restrict the class of spaces considered.

When the sequence of norms in (2.4.8) cannot be defined in terms of scalar products, we call the space *countably normed*. A countably Hilbert space is always countably normed,

but not vice versa. At first glance, it may appear that the class of countably Hilbert spaces constitutes a narrow class of countably normed spaces, because the norms $\|\varphi\|_p = \sqrt{(\varphi,\varphi)_p}$ are only special cases of general countable collections of norms. However, due to the fact that we are considering denumerable collections of norms, the difference is much less pronounced than for the case of one norm (Banach space) and one scalar product (Hilbert space). Under very mild assumptions any initial system of norms $\|\varphi\|'_p$ on a given countably normed space can be replaced by another system of norms $\|\varphi\|_p = \sqrt{(\varphi,\varphi)_p}$ defined by some scalar products without altering the topology on the space. We will always consider that this is the case.

Example An important example of countably Hilbert space is the *Schwartz space*—also called the space of *test functions*. We consider the set $\mathcal{S}(\mathbb{R})$ of functions $\varphi(\cdot) : \mathbb{R} \to \mathbb{C}$ which are infinitely differentiable and the derivatives $\partial^k\varphi(x)/\partial x^k$ of which tend to 0 as $x \to \infty$ faster than any power of $1/|x|$, for $k = 0, 1, 2, \ldots$ The norms that define the topology are

$$\|\varphi\|_p = \sup_{k,q\le p} \left| x^k \frac{\partial^q \varphi(x)}{\partial x^q} \right| , \quad p = 0, 1, 2, \ldots \tag{2.4.14}$$

As mentioned before, we usually can find a sequence of scalar products that generate the same topology as the sequence of norms do. In the case of $\mathcal{S}(\mathbb{R})$, these scalar products are defined by

$$(\varphi,\psi)_p = \int_{-\infty}^{\infty} (1+x^2)^{2p} \sum_{0\le q\le p} \frac{\partial^q \overline{\varphi(x)}}{\partial x^q} \frac{\partial^q \psi(x)}{\partial x^q}\, dx\,, \quad p = 1, 2, \ldots . \tag{2.4.15}$$

The norms (2.4.14) and the scalar products (2.4.15) lead to equivalent topologies on $\mathcal{S}(\mathbb{R})$. Therefore, $\mathcal{S}(\mathbb{R})$ is a countably Hilbert space.

Example The linear space $K(a)$ of all infinitely differentiable functions $\varphi(x)$ that vanish whenever $|x| > a$ can be made a countably normed space by defining the norms

$$\|\varphi\|_p := \sup_{k=0,1,\ldots,p} \left| \frac{d^k\varphi(x)}{dx^k} \right| , \quad p = 0, 1, 2, \ldots \tag{2.4.16}$$

A countably Hilbert space is always metrizable, i.e., we can define a metric on it that yields the original topology. In terms of the norms (2.4.8), this metric is given by

$$d(\varphi,\psi) = \sum_{n=1}^{\infty} \frac{1}{2^n} \frac{\|\varphi-\psi\|_n}{1+\|\varphi-\psi\|_n} . \tag{2.4.17}$$

The function defined in (2.4.17) meets the conditions (2.3.18)-(2.3.20) for a metric. Thus one can apply all the results for the well studied metric spaces to the countably Hilbert spaces.

A countably Hilbert (normed) space is called *Frechet* or an *F-space* if it is complete with respect to the topology generated by the sequence of scalar products (norms). To find a necessary and sufficient condition for a countably Hilbert space $\mathbf{\Phi}$ to be complete, we denote by $\mathbf{\Phi}_n$ the completion of $\mathbf{\Phi}$ relative to the norm $\|\varphi\|_n = \sqrt{(\varphi,\varphi)_n}$. Then $\mathbf{\Phi}_n$ is a Hilbert space. Since

$$\|\varphi\|_1 \leq \|\varphi\|_2 \leq \cdots \leq \|\varphi\|_n \leq \cdots, \tag{2.4.18}$$

we have (cf. Eq. (2.4.5))

$$\mathbf{\Phi}_1 \supset \mathbf{\Phi}_2 \supset \ldots \supset \mathbf{\Phi}_n \supset \ldots \mathbf{\Phi}\,. \tag{2.4.19}$$

One can prove that $\mathbf{\Phi}$ is complete with respect to the topology given by the nhoods (2.4.9) iff

$$\mathbf{\Phi} = \bigcap_{n=1}^{\infty} \mathbf{\Phi}_n\,. \tag{2.4.20}$$

We shall always assume that our countably Hilbert space is Frechet, i.e., it fulfills (2.4.20).

In Section 2.2.2 we saw that different systems of nhoods in a topological space can lead to equivalent topologies. The question arises whether the topology in a countably normed space is really not equivalent to the topology given by one single norm. On the one hand, every normed space $(\mathbf{\Phi}, \|\cdot\|)$ is a countably normed space: one has just to choose a countable system of norms $\|\cdot\|_p$, $p = 1, 2, \ldots$, such that $\|\cdot\|_p$ is equivalent to $\|\cdot\|$ for every p. On the other hand, given a countably normed space $\mathbf{\Phi}$, whose topology is given by the infinite sequence of norms

$$\|\cdot\|_1 \leq \|\cdot\|_2 \leq \cdots \leq \|\cdot\|_p \leq \cdots, \tag{2.4.21}$$

its topology is equivalent to the topology given by a single norm $\|\cdot\|$ iff there is only a finite number of non-equivalent norms in the sequence (2.4.21). Therefore, the essential difference between a normed space and a countably normed space is that in the latter the topology is given by an infinite number of non-equivalent norms.

2.4.2 Dual Space of a Countably Hilbert Space

The dual space $\mathbf{\Phi}^\times$ (cf. Section 2.3.4) of a countably Hilbert space $\mathbf{\Phi}$ is the collection of antilinear functionals on $\mathbf{\Phi}$ that are continuous with respect to the topology generated by the norms (2.4.8). If we denote the adjoint of the Hilbert spaces $\mathbf{\Phi}_n$ in (2.4.19) by $\mathbf{\Phi}_n^\times$, then these spaces form an increasing chain

$$\mathbf{\Phi}_1^\times \subset \mathbf{\Phi}_2^\times \subset \ldots \subset \mathbf{\Phi}_n^\times \subset \ldots \subset \mathbf{\Phi}^\times\,, \tag{2.4.22}$$

as opposed to the decreasing chain (2.4.19). Since a countably Hilbert space is first countable, a linear functional F on $\mathbf{\Phi}$ is continuous iff it is bounded (see Section 2.3.4). One can also see that F is bounded iff there exist a positive constant K and a norm $\|\cdot\|_q$ in the sequence (2.4.8) such that

$$F(\varphi) \leq K\|\varphi\|_q \tag{2.4.23}$$

holds for every $\varphi \in \mathbf{\Phi}$. This means that an antilinear functional is continuous (bounded) with respect to the sequence of norms (2.4.8) iff it is continuous (bounded) with respect to one norm in this sequence. Therefore, the dual space of a countably Hilbert space can be written as (compare to Eq. (2.4.20))

$$\mathbf{\Phi}^\times = \bigcup_{n=1}^{\infty} \mathbf{\Phi}_n^\times \,. \tag{2.4.24}$$

One can introduce a topology in the linear space $\mathbf{\Phi}^\times$ in various ways. For instance, one can take as the nhoods of zero in $\mathbf{\Phi}^\times$ the sets

$$U_W(\varphi_1, \varphi_2, \ldots, \varphi_n; \epsilon) = \{F \in \mathbf{\Phi}^\times \mid |F(\varphi_k)| \leq \epsilon \,, \quad 1 \leq k \leq n\} \,. \tag{2.4.25}$$

Here $\varphi_1, \varphi_2, \ldots, \varphi_n$ are elements of $\mathbf{\Phi}$, and ϵ is an arbitrary positive number. The topology generated by these nhoods is called the *weak topology* on the space $\mathbf{\Phi}^\times$ and is denoted by τ_W. Along with the weak topology one can construct the *strong topology*, whose nhoods of zero are defined by

$$U_S(B; \epsilon) = \left\{ F \in \mathbf{\Phi}^\times \mid \sup_{\varphi \in B} |F(\varphi)| < \epsilon \right\} \,, \tag{2.4.26}$$

where B is any bounded set in $\mathbf{\Phi}$ (cf. Section 2.3.1), and $\epsilon > 0$. We denote the strong topology by τ_S. As the names indicate, the strong topology is actually stronger than the weak topology, i.e., $\tau_W \subset \tau_S$.

We consider, finally, the adjoint space $\mathbf{\Phi}^{\times\times}$ of $\mathbf{\Phi}^\times$. In this space also, one can define different topologies. We shall only consider a topology built from the strongly bounded sets in $\mathbf{\Phi}^\times$ (that is, bounded with respect to τ_S). With each τ_S-bounded set B and each number $\epsilon > 0$ we associate the set

$$U(B, \epsilon) = \left\{ \widetilde{\varphi} \in \mathbf{\Phi}^{\times\times} \mid \sup_{F \in B} |\widetilde{\varphi}(F)| < \epsilon \right\} \,. \tag{2.4.27}$$

We take the collection of all sets $U(B; \epsilon)$ for a system of nhoods at zero in $\mathbf{\Phi}^{\times\times}$. With this topology the second adjoint $\mathbf{\Phi}^{\times\times}$ is isomorphic to the original countably normed space $\mathbf{\Phi}$, i.e., $\mathbf{\Phi} \simeq \mathbf{\Phi}^{\times\times}$. A l.t.s. $\mathbf{\Phi}$ for which $\mathbf{\Phi} \simeq \mathbf{\Phi}^{\times\times}$ is called *reflexive*. Thus any countably Hilbert space is reflexive. In particular, every Hilbert space is also reflexive (cf. Eq. (2.3.30)).

2.4.3 Countably Hilbert Spaces in Quantum Mechanics

The primary structure that physicists work with is a linear space Ψ with a (primary) scalar product (φ, ψ) defined on it and an algebra of linear operators $\mathcal{A}$. The (primary) scalar product constitutes one of the most fundamental entities: $|(\varphi, \psi)|^2$ represents the probability to find the property ψ in the state φ, which are the quantities that are to be compared with the experimental data. The linear operators $A \in \mathcal{A}$ represent the observables measured in the quantum system upon consideration. This algebraic structure has, in principle, no topology attached to it. But in Quantum Mechanics we need a topological structure so

that the elements of the algebra of observables are continuous operators and all algebraic operations are allowed. This is the reason why we need a sequence of scalar products.

Therefore, we consider the case of a linear space Ψ in which, in addition to a sequence of scalar products (2.4.7), there is also another scalar product

$$\begin{aligned} (\,\cdot\,,\,\cdot\,) : \Psi \times \Psi &\longmapsto \mathbb{C} \\ \psi \times \varphi &\longmapsto (\psi, \varphi) \end{aligned} \tag{2.4.28}$$

defined on it. In principle the scalar product (2.4.28) is unrelated to the other scalar products (2.4.7) that generate a countably Hilbert space topology $\tau_{\mathbf{\Phi}}$. To make the scalar product (2.4.28) and the sequence (2.4.7) match each other, we assume that (2.4.28) is a $\tau_{\mathbf{\Phi}}$-continuous mapping. Thus, in addition to (2.1.12)-(2.1.14), we demand that

$$\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \quad \text{implies} \quad (\varphi_n, \psi) \xrightarrow[n\to\infty]{\tau_{\mathbb{C}}} (\varphi, \psi)\,, \quad \forall\, \psi \in \Psi\,. \tag{2.4.29}$$

We are now going to show that whenever a primary scalar product (2.4.28) is continuous with respect to the topology generated by a denumerable sequence of scalar products, we can include this scalar product as the first element of that sequence without altering the topology:

From (2.4.29) we can see that the linear functional

$$\begin{aligned} F_\psi : \Psi &\longmapsto \mathbb{C} \\ \varphi &\longmapsto F_\psi(\varphi) = (\psi, \varphi) \end{aligned} \tag{2.4.30}$$

and the antilinear functional

$$\begin{aligned} \overline{F}_\psi : \Psi &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \overline{F}_\psi(\varphi) = (\varphi, \psi) \end{aligned} \tag{2.4.31}$$

are $\tau_{\mathbf{\Phi}}$-continuous. Since any continuous functional on a countably Hilbert space is bounded, there is a norm $\|\cdot\|_q$ and a constant $C > 0$ such that

$$|F_\psi(\varphi)| \le C\|\varphi\|_q\,, \quad |\overline{F}_\psi(\varphi)| \le C\|\varphi\|_q\,, \quad |(\psi, \varphi)| \le C\|\psi\|_q\,\|\varphi\|_q\,. \tag{2.4.32}$$

We now define the sequence of scalar products

$$(\varphi, \psi)'_0 := (\varphi, \psi)\,, \tag{2.4.33}$$

$$(\varphi, \psi)'_p := C(\varphi, \psi)_{p+q-1}\,, \quad p = 1, 2, \ldots \tag{2.4.34}$$

The new sequence of scalar products contains the original scalar product as the zeroth element, satisfies

$$(\varphi, \varphi) \equiv (\varphi, \varphi)'_0 \le (\varphi, \varphi)'_1 \le \cdots \le (\varphi, \varphi)'_p \le \cdots, \tag{2.4.35}$$

and generates the same topology as the original scalar products $(\varphi, \varphi)_p$ do.

Therefore, we can always assume that the scalar product (2.4.28) is already the zeroth scalar product of the sequence

$$(\varphi,\varphi)_0 \leq (\varphi,\varphi)_1 \leq \cdots \leq (\varphi,\varphi)_p \leq \cdots \tag{2.4.36}$$

of scalar products that will define the topologies on Ψ. We are mostly interested in two topologies induced by the scalar products (2.4.36) on Ψ. The first topology is generated by the nhoods of zero given by

$$U_m(0) = \{\varphi \mid \|\varphi\|_0 < \frac{1}{m}\}\,, \quad m = 1, 2, \ldots \tag{2.4.37}$$

This is the Hilbert space topology (cf. Section 2.3.3) and is denoted by $\tau_{\mathcal{H}}$. The second topology is the countably Hilbert space topology $\tau_{\mathbf{\Phi}}$, whose nhoods of zero are given by

$$U_{p,m}(0) = \{\varphi \mid \|\varphi\|_p < \frac{1}{m}\}\,, \quad p = 0, 1, 2, \ldots,\ m = 1, 2, \ldots \tag{2.4.38}$$

If we complete the linear space Ψ with respect to these two topologies, we obtain the chain of spaces

$$\Psi \subset \mathbf{\Phi} \subset \mathcal{H}\,. \tag{2.4.39}$$

$\mathcal{H}$ is obtained by adjoining to Ψ the limit elements of $\tau_{\mathcal{H}}$-Cauchy sequences whereas $\mathbf{\Phi}$ is obtained by adjoining to Ψ the limit elements of $\tau_{\mathbf{\Phi}}$-Cauchy sequences. The algebraic space Ψ is $\tau_{\mathbf{\Phi}}$-dense in $\mathbf{\Phi}$ and $\tau_{\mathcal{H}}$-dense in $\mathcal{H}$, and the complete countably Hilbert space $\mathbf{\Phi}$ is $\tau_{\mathcal{H}}$-dense in $\mathcal{H}$. The second inclusion in (2.4.39) comes from the fact that every $\tau_{\mathbf{\Phi}}$-Cauchy sequence is also $\tau_{\mathcal{H}}$-Cauchy because $\{U_m(0)\} \subset \{U_{p,m}(0)\}$ (and then $\tau_{\mathcal{H}} \supset \tau_{\mathbf{\Phi}}$), but not vice versa.

In applications to physics, the scalar products (2.4.36) are introduced in order to obtain a topology so that all the elements of the algebra of observables are continuous. They are defined in terms of the (primary) scalar product and the algebra of observables. For example, the countable number of scalar products can be defined as

$$(\varphi,\psi)_p \equiv (\varphi, A^p\psi)\,, \quad p = 0, 1, 2, \ldots,\ A \in \mathcal{A}\,, \tag{2.4.40}$$

where $(\,\cdot\,,\,\cdot\,)$ is the (primary) scalar product that describes the probabilities. The quantities $|(\varphi,\psi)_p| = |(\varphi, A^p\psi)| = |(\varphi,\chi)|$ have also an interpretation, namely the probability to find the property represented by φ in the transformed state $\chi = A^p\psi$. Therefore, the scalar products $(\varphi,\psi)_p$, and therewith the topology $\tau_{\mathbf{\Phi}}$ and the space $\mathbf{\Phi}$, depend upon the particular system under study.

2.5 Linear Operators on Hilbert Spaces

2.5.1 Introduction

In Quantum Mechanics, the observables are represented by a linear operators defined on some linear scalar product space $(\Psi, (\,\cdot\,,\,\cdot\,))$. The completion of this space with respect to

the Hilbert space topology leads to the Hilbert space $\mathcal{H}$ (see Section 2.4.3). Therefore, any observable can be viewed as an operator defined on the domain Ψ of the Hilbert space $\mathcal{H}$. This will allow us to apply the Hilbert space methods to these operators. Some of these methods will be very useful in the Rigged Hilbert Space theory.

2.5.2 Bounded Operators on a Hilbert Space

Certain classes of bounded operators play an essential role in Quantum Mechanics: nuclear operators are needed in the construction of the nuclear Rigged Hilbert Space (see Section 2.6) and operators with finite trace (which are defined below) are to represent mixed states. Before introducing the concept of bounded operator, we need some preliminary definitions.

Definition Let $\mathcal{H}$ be a Hilbert space and $\mathcal{M}$ be a closed subspace of $\mathcal{H}$. The *orthogonal complement* $\mathcal{M}^\perp$ of $\mathcal{M}$ is the set of elements in $\mathcal{H}$ which are orthogonal to every element of $\mathcal{M}$,

$$\mathcal{M}^\perp := \{f \in \mathcal{H} \mid (f, g) = 0\,,\ \forall g \in \mathcal{M}\}\,. \tag{2.5.1}$$

If $\mathcal{M}$ is a closed subspace of a Hilbert space $\mathcal{H}$, then every $f \in \mathcal{H}$ can be uniquely written as $f = g + g_\perp$, where $g \in \mathcal{M}$ and $g_\perp \in \mathcal{M}^\perp$. We usually say that $\mathcal{H}$ is the *direct sum* of the spaces $\mathcal{M}$ and $\mathcal{M}^\perp$, and denote

$$\mathcal{H} = \mathcal{M} \oplus \mathcal{M}^\perp\,. \tag{2.5.2}$$

Definition A set $\{e_n\}_{n=1}^\infty \subset \mathcal{H}$ is an *orthonormal basis* for $\mathcal{H}$ if:

1. The elements of the basis are orthonormal to each other,

$$(e_n, e_m) = \delta_{nm}\,, \quad n, m = 1, 2, \ldots, \tag{2.5.3}$$

   where δ_{nm} is the Kronecker delta.

2. Every $f \in \mathcal{H}$ can be expanded in terms of this basis as a series of the form

$$f = \sum_{n=1}^\infty (e_n, f) e_n\,, \tag{2.5.4}$$

   which converges in the sense of the norm of $\mathcal{H}$.

In a general Hilbert space, an orthonormal basis need not be countable. It can be proven though, that a Hilbert space is separable iff it has a countable orthonormal basis. We shall only consider separable Hilbert spaces.

Example Define l_2 to be the set of sequences $\{x_n\}_{n=1}^\infty$ of complex numbers which satisfy $\sum_{n=1}^\infty |x_n|^2 < \infty$ with the scalar product

$$(\{x_n\}_{n=1}^\infty, \{y_n\}_{n=1}^\infty) := \sum_{n=1}^\infty \overline{x}_n\, y_n\,. \tag{2.5.5}$$

l_2 is a separable Hilbert space and the set

$$\{(1,0,0,\ldots,0,\ldots),(0,1,0,\ldots,0,\ldots),(0,0,1,\ldots,0,\ldots),\ldots,(0,0,0,\ldots,1,\ldots),\ldots\} \tag{2.5.6}$$

is an orthonormal basis for l_2.

Example The space $L^2(\mathbb{R},dx)$ is the set of complex-valued functions on $\mathbb{R}$ which satisfy $\int_{-\infty}^{\infty}|f(x)|^2dx<\infty$. $L^2(\mathbb{R},dx)$ is a Hilbert space under the scalar product

$$(f,g)=\int_{-\infty}^{\infty}\overline{f(x)}\,g(x)\,dx\,. \tag{2.5.7}$$

The Hermite polynomials form an orthonormal basis for $L^2(\mathbb{R},dx)$.

We now list some definitions and results concerning bounded linear operators defined on a Hilbert space $\mathcal{H}$. Corresponding statements hold for operators of a Hilbert space $\mathcal{H}_1$ into another Hilbert space $\mathcal{H}_2$.

Definition A linear operator A defined on a Hilbert space $\mathcal{H}$ is called *bounded* if there exists a positive number K such that

$$\|Af\|\leq K\|f\| \tag{2.5.8}$$

holds for every $f\in\mathcal{H}$. This definition of bounded operator is equivalent to the definition given in Section 2.3.4.

The collection of all bounded operators on $\mathcal{H}$ is denoted by $\mathcal{L}(\mathcal{H})$. The space $\mathcal{L}(\mathcal{H})$ is a linear space under the usual sum of two operators and multiplication of an operator by a number. The *norm* of a bounded operator is defined by

$$\|A\|:=\sup_{f\in\mathcal{H},f\neq 0}\frac{\|Af\|}{\|f\|}\,. \tag{2.5.9}$$

One can prove that (2.5.9) is a well defined norm that satisfies the conditions (2.3.10)-(2.3.12). The space $\mathcal{L}(\mathcal{H})$ becomes a Banach space when the norm of its elements is defined by (2.5.9).

In Section 2.1.2 we gave a preliminary definition of the adjoint of an operator. Now we give a more thorough definition.

Definition Let A be a bounded operator on a Hilbert space $\mathcal{H}$. The adjoint operator $A^\dagger$ of A is defined on the elements g for which there exists a $z\in\mathcal{H}$ fulfilling

$$(Af,g)=(f,z) \tag{2.5.10}$$

for every $f\in\mathcal{H}$. The adjoint is then defined by $A^\dagger g=z$. Thus (2.5.10) can be restated as

$$(Af,g)=(f,A^\dagger g)\,,\quad \forall f\in\mathcal{H}\,,\ \forall g\in\mathcal{D}(A^\dagger)\,. \tag{2.5.11}$$

A bounded operator A is called *Hermitian* or *self-adjoint* if $A = A^\dagger$, i.e., if

$$(Af, g) = (f, Ag)\,, \quad \forall f, g \in \mathcal{H}\,. \tag{2.5.12}$$

An important class of operators on Hilbert spaces is that of projections.

Definition If $P \in \mathcal{L}(\mathcal{H})$ and $P^2 = P$, then P is called a *projection*. If in addition $P = P^\dagger$, then P is called an *orthogonal projection*.

The range $\mathcal{R}(P)$ of a projection P is always a closed subspace on which P acts like the identity. If in addition P is orthogonal, then P acts like the zero operator on $(\mathcal{R}\,(P))^\perp$. Conversely, given a closed subspace $\mathcal{M}$ of $\mathcal{H}$, we can define a projection operator $P_\mathcal{M}$ onto $\mathcal{M}$ as follows: since $\mathcal{M}$ induces on $\mathcal{H}$ a decomposition of the form (2.5.2), any $f \in \mathcal{H}$ can be written as $f = g + g_\perp$, where $g \in \mathcal{M}$ and $g_\perp \in \mathcal{M}^\perp$. We define $P_\mathcal{M} f = P_\mathcal{M}(g + g_\perp) := g$. The operator $P_\mathcal{M}$ is a well defined orthogonal projection. Therefore, there is a one to one correspondence between orthogonal projections and closed subspaces.

Definition An operator U on $\mathcal{H}$ is called *unitary* if $\|Uf\| = \|f\|$ for every $f \in \mathcal{H}$. A unitary operator satisfies the relations

$$U^\dagger U = UU^\dagger = I\,. \tag{2.5.13}$$

Given a closed subspace $\mathcal{M} \subset \mathcal{H}$, an operator $U \in \mathcal{L}(\mathcal{H})$ is called a *partial isometry on* $\mathcal{M}$ if U is unitary when restricted to $\mathcal{M}$, i.e., if

$$U^\dagger U = P_\mathcal{M}\,, \tag{2.5.14}$$

where $P_\mathcal{M}$ is the projection onto $\mathcal{M}$.

Evidently, any unitary operator is a partial isometry on the whole of $\mathcal{H}$. A unitary operator U is always bounded and $\|U\| = 1$.

If A is a matrix on $\mathbb{C}^n$, then the *eigenvalues* of A are the complex numbers λ such that the determinant of $\lambda I - A$ is equal to zero. The set of such λ is called the *spectrum* of A. It can consist of at most n points since $\det(\lambda I - A)$ is a polynomial of degree n. If λ is not an eigenvalue, then $(\lambda I - A)$ has an inverse since $\det(\lambda I - A) \neq 0$. In this case, λ is in the *resolvent* set of A. These notions can be extended to the case of a linear transformation on a Hilbert space.

Definition Let $A \in \mathcal{L}(\mathcal{H})$. A complex number λ is said to be in the *resolvent* set, $\mathrm{Re}(A)$, of A if $\lambda I - A$ is a bijection with a bounded inverse. If $\lambda \notin \mathrm{Re}(A)$, then λ is said to be in the *spectrum*, $\mathrm{Sp}(A)$, of A. We distinguish two subsets of the spectrum:

1. An $f \in \mathcal{H}$ which satisfies $Af = \lambda f$ for some $\lambda \in \mathbb{C}$ is called an *eigenvector* of A; λ is called the corresponding *eigenvalue*. If λ is an eigenvalue, then λ is in the spectrum of A. The set of all eigenvalues is called the *discrete spectrum* of A.

2. If λ is not an eigenvalue and if λ is not in $\mathrm{Re}(A)$, then λ is said to be in the *continuous spectrum* of A.

A very important class of bounded operators is that of compact operators.

Definition An operator $A \in \mathcal{L}(\mathcal{H})$ is called *compact* (or *completely continuous*) if for every bounded sequence $\{f_n\} \subset \mathcal{H}$, $\{Af_n\}$ has a subsequence convergent in $\mathcal{H}$.

Example The simplest example of compact operator is an operator A of the form

$$Af := \lambda(e, f)h\,, \tag{2.5.15}$$

where e and h are fixed vectors of unit length, and λ is a fixed number. This operator maps all of $\mathcal{H}$ onto the one-dimensional subspace spanned by h, and is called a *one-rank operator*. We can also define a linear operator A as

$$Af := \sum_{i=1}^{N} \lambda_i(e_i, f)\, h_i \tag{2.5.16}$$

for some fixed collections of vectors $\{e_i\}_{i=1}^N$ and $\{h_i\}_{i=1}^N$ in $\mathcal{H}$. The range of this operator is the finite dimensional subspace spanned by the vectors $\{h_i\}_{i=1}^N$. The operator A in (2.5.16) is called a *finite rank* operator. Every finite rank operator is compact.

The spectrum $\mathrm{Sp}(A)$ of a compact operator A is a discrete set having no limit points excepts perhaps $\lambda = 0$. Further, any nonzero $\lambda \in \mathrm{Sp}(A)$ is an eigenvalue of finite multiplicity (i.e., the corresponding space of eigenvectors is finite dimensional).

A self adjoint compact operator, i.e., a compact operator A such that $(Af, g) = (f, Ag)$ for every $f, g \in \mathcal{H}$, has a particularly simple structure. If A is a compact self adjoint operator, then one can choose an orthonormal basis $e_1, e_2, \ldots$ in $\mathcal{H}$ which consists of eigenvectors of A, $Ae_n = \lambda_n e_n$. The eigenvalues $\lambda_1, \lambda_2, \ldots$ corresponding to the eigenvectors $e_1, e_2, \ldots$ are real and converge to zero as $n \to \infty$, i.e., $\lim_{n\to\infty} \lambda_n = 0$. Conversely, every operator A which is defined in terms of some orthonormal basis $e_1, e_2, \ldots,$ by $Ae_n = \lambda_n e_n$, where the λ_n are real numbers and $\lim_{n\to\infty} \lambda_n = 0$, is self adjoint and compact.

An operator A is *positive-definite* if $(Af, f) \geq 0$ for every vector $f \in \mathcal{H}$. The eigenvalues of a positive-definite operator are either positive or equal to zero. A compact operator differs from a positive-definite operator only by an isometric factor, i.e., the following theorem holds:

Theorem Let A be a compact operator on a Hilbert space $\mathcal{H}$. Then A has the form

$$A = U|A|\,, \tag{2.5.17}$$

where $|A|$ is a positive-definite compact operator, and U is a partial isometry on the range of $|A|$.

Any compact operator can be approximated by a sum of one-rank operators (2.5.15). Specifically, a compact operator A can be represented as the sum of a series

$$Af = \sum_{n=1}^{\infty} \lambda_n \, (e_n, f) \, h_n \, . \tag{2.5.18}$$

The e_n are the eigenvectors of the operator $|A|$ in the decomposition (2.5.17) corresponding to the eigenvalues λ_n, i.e., $|A|e_n = \lambda_n e_n$. The h_n are given by $h_n = Ue_n$. (In particular, the e_n and the h_n are the elements of two orthonormal basis in $\mathcal{H}$, and $\lambda_1, \lambda_2, \ldots$ are positive numbers that tend to zero as $n \to \infty$). Conversely, every series of the form (2.5.18), in which e_n, h_n, λ_n have the aforementioned properties, defines a compact operator.

The requirement that the eigenvalues λ_n (of the operator $|A|$ appearing in the decomposition $A = U|A|$ of a compact operator A) tend to zero is too weak. We now consider operators that satisfy more stringent conditions.

Definition A compact operator $A = U|A|$ is called *Hilbert-Schmidt* if $\sum_{n=1}^{\infty} \lambda_n^2 < \infty$, where the λ_n are the eigenvalues of the operator $|A|$.

Therefore, an operator is of Hilbert-Schmidt type iff admits a decomposition of the form (2.5.18) such that the series $\sum_{n=1}^{\infty} \lambda_n^2$ converges. One can also see that in order an operator A be of Hilbert-Schmidt type, it is necessary and sufficient that the series $\sum_{n=1}^{\infty} \|Ae_n\|^2$ converge for at least one orthonormal basis $e_1, e_2, \ldots$ in $\mathcal{H}$.

An even more restrictive requirement that the operator A be Hilbert-Schmidt is that it be a nuclear operator.

Definition A compact operator is called *nuclear* (or *trace class*) if $\sum_{n=1}^{\infty} \lambda_n < \infty$, where the λ_n are the eigenvalues of the operator $|A|$ appearing in the decomposition $A = U|A|$. Since the convergence of the series $\sum_{n=1}^{\infty} \lambda_n^2$ follows from the convergence of $\sum_{n=1}^{\infty} \lambda_n$, every nuclear operator is of Hilbert-Schmidt type.

It is clear that an operator A is nuclear iff it admits a decomposition of the form (2.5.18) such that the series $\sum_{n=1}^{\infty} \lambda_n$ converges. The nuclear operators will serve in the definition of nuclear spaces (cf. Section 2.6), which are the most important class of l.t.s. used in Quantum Mechanics.

The trace of an operator is a generalization of the usual notion of the sum of the diagonal elements of a matrix. For any positive operator $A \in \mathcal{L}(\mathcal{H})$ we define

$$\mathrm{Tr}(A) := \sum_{n=1}^{\infty} (e_n, Ae_n) \, , \tag{2.5.19}$$

where $\{e_n\}$ is an orthonormal basis of $\mathcal{H}$. The number $\mathrm{Tr}(A)$ is called the *trace of* A and is independent of the orthonormal basis chosen. When $\mathrm{Tr}(A)$ is finite, then A is called an *operator with finite trace*. If A is a positive-definite compact operator, then A is nuclear iff

A has a finite trace. In this case,

$$\mathrm{Tr}(A) = \sum_{n=1}^{\infty} (e_n, Ae_n) = \sum_{n=1}^{\infty} \lambda_n \,. \tag{2.5.20}$$

In Quantum Mechanics, a general (mixed) state is assumed to be described by a positive operator W with finite trace. W is usually chosen such that $\mathrm{Tr}(W) = 1$ (if $\mathrm{Tr}(W) \neq 1$, we just define the equivalent normalized state $W' \equiv W/\mathrm{Tr}(W)$). If A is a linear operator representing a physical observable, then the quantity $\mathrm{Tr}(AW)$ is to represent the probability to observe A in the state W.

2.5.3 Unbounded Operators on a Hilbert Space

Most important observables that occur in Quantum Mechanics are represented by linear operators that are unbounded with respect to the Hilbert space topology. In this section we will introduce some of the basic definitions and theorems necessary for dealing with this type of operators.

An operator A is *unbounded* if the quantity (2.5.9) is not finite. Unbounded operators are usually defined on some subdomain of the Hilbert space. We will always suppose that this domain is dense.

In order to compare operators that are not defined on the whole of $\mathcal{H}$, we introduce the following definition:

Definition Let A and B be two operators defined on $\mathcal{H}$. Let $\mathcal{D}(A)$ be the domain of A and $\mathcal{D}(B)$ the domain of B. A is said to be an *extension* of B if $\mathcal{D}(B) \subset \mathcal{D}(A)$ and $Af = Bf$ for every $f \in \mathcal{D}(B)$. In this case we shall write $B \subset A$. One may also call B the *restriction* of A to $\mathcal{D}(B)$.

For some operators A there is a natural way of defining an extension $\overline{A}$. One takes a Cauchy sequence $\{f_n\}$ in $\mathcal{D}(A)$. If the sequence $\{Af_n\}$ is also Cauchy, and if one denotes by f and g the limits of $\{f_n\}$ and $\{Af_n\}$ respectively, it is natural to define $\overline{A}f = g$. Since f is not necessarily in $\mathcal{D}(A)$, one may define an extension $\overline{A}$ of A by applying the above procedure to all Cauchy sequences $\{f_n\}$ in $\mathcal{D}(A)$ which are such that $\{Af_n\}$ is also Cauchy. However, this construction makes sense only if the element g is independent of the choice of a particular Cauchy sequence $\{f_n\}$ converging to f, i.e., if whenever $\{f_n\}$ and $\{f'_n\}$ are two Cauchy sequences in $\mathcal{D}(A)$ converging to the same limit f and $\{Af_n\}$ and $\{Af'_n\}$ are also Cauchy, then $\lim_{n\to\infty} Af_n = \lim_{n\to\infty} Af'_n$. An operator A verifying this condition is said to be *closable*, and the extension $\overline{A}$ is called the *closure* of A. An operator A is said to be *closed* if $A = \overline{A}$.

Closedness is a weaker condition than continuity since, if an operator A on $\mathcal{H}$ is continuous, then

$$\lim_{n\to\infty} f_n = f \,, \quad f_n \in \mathcal{D}(A) \,, \tag{2.5.21}$$

implies that the sequence $\{Af_n\}$ converges, while if it is only closed, then the convergence of the sequence $\{f_n\} \subset \mathcal{D}(A)$ does not imply the convergence of the sequence $\{Af_n\}$.

The spectral notions for a bounded operator can be generalized to the unbounded case when the operator is closed.

Definition Let A be a closed operator on a Hilbert space $\mathcal{H}$. A complex number λ is in the *resolvent set*, $\mathrm{Re}(A)$, of A if $\lambda I - A$ is a bijection from $\mathcal{D}(A)$ onto $\mathcal{H}$ with a bounded inverse. The definitions of *spectrum, discrete spectrum* and *continuous spectrum* are the same for unbounded operators as they are for bounded operators. We will sometimes refer to the spectrum of nonclosed, but closable operators. In this case we always mean the spectrum of the closure.

The adjoint of an unbounded operator A can be defined in a similar way to the bounded case whenever the domain of A is dense in $\mathcal{H}$.

Definition Let $A : \mathcal{H} \to \mathcal{H}$ be a linear operator (not necessarily bounded) on a Hilbert space $\mathcal{H}$ whose domain $\mathcal{D}(A)$ is a dense linear subspace of $\mathcal{H}$. The domain $\mathcal{D}(A^\dagger)$ of the adjoint operator $A^\dagger$ is the set of all vectors $f \in \mathcal{H}$ for which there exists a $z \in \mathcal{H}$ fulfilling

$$(f, Ag) = (z, g) \tag{2.5.22}$$

for every $g \in \mathcal{D}(A)$. Then, by definition, $A^\dagger f = z$. Since $\mathcal{D}(A)$ is dense, the vector z is uniquely determined and $A^\dagger$ is well defined. We then write (2.5.22) as

$$(A^\dagger f, g) = (f, Ag)\,, \quad \forall g \in \mathcal{D}(A)\,, \forall f \in \mathcal{D}(A^\dagger)\,. \tag{2.5.23}$$

The adjoint operator is always closed. The relation between an unbounded operator A and its adjoint $A^\dagger$ can be more complicated than for the bounded case:

Definition An operator A on $\mathcal{H}$ is called *symmetric* if $\mathcal{D}(A)$ is dense in $\mathcal{H}$ and $(Af, g) = (f, Ag)$ for every f, $g \in \mathcal{D}(A)$. This means that a densely defined operator is symmetric iff $A \subset A^\dagger$. A is called *self-adjoint* if $\mathcal{D}(A)$ is dense in $\mathcal{H}$ and $A = A^\dagger$. A is called *essentially self adjoint* (*e.s.a.*) if $\overline{A}$ is self adjoint.

If A is a symmetric operator, then A is closable and $\overline{A} = A^{\dagger\dagger}$. An e.s.a. operator has a unique self adjoint extension that coincides with its adjoint. Physical observables are assumed to be represented by e.s.a. operators.

Evidently, any self adjoint operator is e.s.a., and any e.s.a. operator is symmetric. In fact, an operator A (not necessarily bounded) is

$$\text{symmetric} \quad \text{iff} \quad A \subset \overline{A} = A^{\dagger\dagger} \subset A^\dagger\,, \tag{2.5.24}$$

$$\text{e.s.a.} \quad \text{iff} \quad A \subset \overline{A} = A^{\dagger\dagger} = A^\dagger\,, \tag{2.5.25}$$

$$\text{self adjoint} \quad \text{iff} \quad A = \overline{A} = A^{\dagger\dagger} = A^\dagger\,. \tag{2.5.26}$$

The spectrum of a self-adjoint operator is always a closed subset of the real axis.

In Quantum Mechanics, the elements A of the algebra of observables $\mathcal{A}$ are defined on some linear scalar product space $(\Psi, (\,\cdot\,,\,\cdot\,))$, and are required to fulfill $(A\varphi, \psi) = (\varphi, A\psi)$ for every φ, $\psi \in \Psi$ (i.e., they are required to be symmetric). These operators are usually unbounded. When this is the case, they cannot be extended to the whole Hilbert space $\mathcal{H}$ (which is the completion of Ψ with respect to the Hilbert space topology) due to the following theorem:

Theorem (Hellinger-Toeplitz) Let A be an everywhere defined linear operator on a Hilbert space $\mathcal{H}$ with $(f, Ag) = (Af, g)$ for all f and g in $\mathcal{H}$. Then A is bounded.

The Hellinger-Toeplitz theorem tells us that symmetric unbounded operators cannot be defined on the whole of $\mathcal{H}$. Thus such operators can be only extended at most into certain dense subspaces of $\mathcal{H}$. Given two unbounded densely defined operators A and B in $\mathcal{A}$, the definition of $A+B$ or AB may be difficult: $A+B$ is a priori only defined on $\mathcal{D}(A) \cap \mathcal{D}(B)$, and AB is only defined on the elements $\varphi \in \mathcal{D}(B)$ such that $B\varphi \in \mathcal{D}(A)$. However, if there exists a common invariant subdomain $\mathbf{\Phi}$ for the algebra of operators $\mathcal{A}$, i.e., a subspace $\mathbf{\Phi}$ such that $\mathbf{\Phi} \subset \mathcal{D}(A)$ and $A : \mathbf{\Phi} \to \mathbf{\Phi}$ for every $A \in \mathcal{A}$, then all algebraic operations are allowed and domain questions do not arise. The need for this domain, that is not provided by the Hilbert space theory, is one of the reasons why we need to go beyond the Hilbert space to the Rigged Hilbert Space.

As an example, let $L^2(\mathbb{R}, dx)$ be the Hilbert space of square integrable functions on the real line. Then the multiplication (position) operator

$$Q : f(x) \to x f(x) \tag{2.5.27}$$

and the differentiation (momentum) operator

$$P : f(x) \to \frac{1}{i} \frac{df(x)}{dx} \tag{2.5.28}$$

are not bounded on $L^2(\mathbb{R}, dx)$. Therefore, the commutation relation

$$[Q, P] = QP - PQ = iI \tag{2.5.29}$$

is not defined for every element in the Hilbert space. However, the actions of P and Q can be restricted to the Schwartz space $\mathcal{S}(\mathbb{R})$, that is included in the domains of P and Q. On this subdomain both P and Q are bounded (continuous) with respect to the topology generated by the scalar products (2.4.15). On $\mathcal{S}(\mathbb{R})$, the commutation relation (2.5.29) is well defined and all algebraic operations are allowed. This will serve as a motivation for a physicist to consider using countably Hilbert spaces such as $\mathcal{S}(\mathbb{R})$ rather than just the Hilbert space $L^2(\mathbb{R}, dx)$.

2.6 Nuclear Rigged Hilbert Spaces

2.6.1 Introduction

The class of countably Hilbert spaces that is of service in Quantum Mechanics is that of nuclear spaces. Nuclear spaces will appear in connection with the spectral analysis of self adjoint operators. This spectral analysis will be provided by the Gelfand-Maurin theorem (see Section 3.5).

In order to introduce the concept of nuclearity, we consider a countably Hilbert space $\mathbf{\Phi}$ on which an increasing sequence of scalar products

$$(\varphi,\varphi)_1 \leq (\varphi,\varphi)_2 \leq \cdots \leq (\varphi,\varphi)_n \leq \cdots \tag{2.6.1}$$

is defined. We consider the Hilbert spaces $\mathbf{\Phi}_n$ which are obtained by completing the space $\mathbf{\Phi}$ with respect to the norms $\|\varphi\|_n = \sqrt{(\varphi,\varphi)_n}$. These completions lead to the chain of spaces

$$\mathbf{\Phi}_1 \supset \mathbf{\Phi}_2 \supset \cdots \supset \mathbf{\Phi}_n \supset \cdots \supset \mathbf{\Phi}\,. \tag{2.6.2}$$

By construction, $\mathbf{\Phi}$ is dense in each space $\mathbf{\Phi}_n$. We denote by $\varphi^{[n]}$ and $\varphi^{[m]}$ the same element $\varphi \in \mathbf{\Phi}$, considered as an element of $\mathbf{\Phi}_n$ and $\mathbf{\Phi}_m$, respectively. If $m \leq n$, then it follows from (2.6.1) that the identity mapping

$$\begin{array}{rcl} : \mathbf{\Phi} \subset \mathbf{\Phi}_n & \to & \mathbf{\Phi} \subset \mathbf{\Phi}_m \\ \varphi^{[n]} & \to & \varphi^{[m]} \end{array} \tag{2.6.3}$$

is a continuous mapping from a dense set in $\mathbf{\Phi}_n$ onto a dense set in $\mathbf{\Phi}_m$. We can extend this mapping to a continuous linear transformation $T^n{}_m$ which maps the space $\mathbf{\Phi}_n$ onto a dense subset of $\mathbf{\Phi}_m$ (cf. Section 2.3.4).

A countably Hilbert space $\mathbf{\Phi}$ is called *nuclear* if for any m there is an n such that the mapping $T^n{}_m$ of the space $\mathbf{\Phi}_n$ into the space $\mathbf{\Phi}_m$ is nuclear, i.e., it has the form

$$T^n{}_m\varphi = \sum_{k=1}^{\infty} \lambda_k\,(e_k,\varphi)_n\,h_k\,, \tag{2.6.4}$$

where $\varphi \in \mathbf{\Phi}_n$, $\{e_k\}$ and $\{h_k\}$ are orthonormal systems in $\mathbf{\Phi}_n$ and $\mathbf{\Phi}_m$, respectively, $\lambda_k > 0$ and $\sum_{k=1}^{\infty} \lambda_k < \infty$.

We can extend the concept of nuclearity to a countably normed space. However, this generalization does not lead to an extension of the class of spaces considered: in any nuclear countably normed space it is possible to define a sequence of scalar products in such a way that the space becomes a nuclear countably Hilbert space without altering its topology.

Nuclear spaces posses certain properties that make them suitable for the purposes of Quantum Mechanics. Here we list the most relevant:

1. Any closed subspace of a nuclear space is nuclear.

2. If $\mathbf{\Phi}$ is a nuclear countably Hilbert space, then the strong and the weak topology[3] on $\mathbf{\Phi}$ agree.

3. If $\mathbf{\Phi}$ is nuclear, then the strong and weak topologies on $\mathbf{\Phi}^\times$ (which were defined in Section 2.4.2) coincide.

4. A nuclear space is separable (i.e., it contains a dense countable subset).

5. A nuclear space is complete with respect to the weak convergence.

6. A Hilbert (or a Banach) space is nuclear only if it is finite dimensional.

There is a number of countably Hilbert spaces that are nuclear. For example, the Schwartz space $\mathcal{S}(\mathbb{R})$ (see Section 2.4.1) is nuclear with respect to the topology generated by the scalar products (2.4.15). The space $K(a)$ of Section 2.4.1 is also nuclear.

2.6.2 Nuclear Rigged Hilbert Spaces

By the use of the concepts discussed so far, it is now easy to introduce the basic notion of (nuclear) Rigged Hilbert Space.

Let $\mathbf{\Phi}$ be a nuclear countably Hilbert space. We introduce a scalar product $(\,\cdot\,,\,\cdot\,)$ into $\mathbf{\Phi}$ satisfying (2.1.12)-(2.1.14). This scalar product is also required to be continuous with respect to the countably Hilbert space topology on $\mathbf{\Phi}$. The completion of $\mathbf{\Phi}$ with respect to the norm $\|\varphi\| = \sqrt{(\varphi,\varphi)}$ yields the Hilbert space $\mathcal{H}$. Therefore, the mapping T that brings any element of $\mathbf{\Phi}$ into the completion $\mathcal{H}$ is continuous. Usually, we identify the space $\mathbf{\Phi}$ with the space $T(\mathbf{\Phi})$ and write

$$\mathbf{\Phi} \subset \mathcal{H}\,. \tag{2.6.5}$$

By construction, the topology of $\mathbf{\Phi}$ is stronger (finer) than the topology induced by $\mathcal{H}$ on $\mathbf{\Phi}$. Along with the spaces $\mathbf{\Phi}$ and $\mathcal{H}$ we consider the adjoint space $\mathbf{\Phi}^\times$ of $\mathbf{\Phi}$ and the adjoint space $\mathcal{H}^\times$ of $\mathcal{H}$. The adjoint $T^\times$ of T is an operator mapping $\mathcal{H}^\times$ into $\mathbf{\Phi}^\times$. $T^\times$ is defined by the equation

$$\langle \varphi | T^\times h' \rangle = \langle T\varphi | h' \rangle \tag{2.6.6}$$

for every $h' \in \mathcal{H}^\times$ and $\varphi \in \mathbf{\Phi}$. Since every antilinear functional h' on the Hilbert space $\mathcal{H}$ can be written in the form (see Frechet-Riesz Theorem in Section 2.3.4)

$$h'(f) = (f, h_1)\,, \tag{2.6.7}$$

where h_1 is some element of $\mathcal{H}$, then $T^\times$ can be considered as a mapping of $\mathcal{H}$ into $\mathbf{\Phi}^\times$.

[3] A sequence $\{\varphi_k\}$ of elements in a countably Hilbert space $\mathbf{\Phi}$ is said to be *weakly* convergent to φ if $\lim_{n\to\infty} F(\varphi_k) = F(\varphi)$ for every functional F on $\mathbf{\Phi}$. By strong convergence we mean the convergence with respect to the countably Hilbert topology generated by the scalar products (2.6.1).

A *Rigged Hilbert Space*[4] (abbreviated *RHS*) or a *Gelfand triplet* is a triplet of spaces $\mathbf{\Phi}$, $\mathcal{H}$, $\mathbf{\Phi}^\times$, having the properties stated above: $\mathbf{\Phi}$ is a nuclear countably Hilbert space on which a scalar product is defined, $\mathcal{H}$ is the completion of $\mathbf{\Phi}$ with respect to this scalar product, and $\mathbf{\Phi}^\times$ is the adjoint space of $\mathbf{\Phi}$. For any RHS there exists a continuous linear operator T which maps $\mathbf{\Phi}$ one-to-one onto a dense subset of $\mathcal{H}$, and its adjoint $T^\times$ maps $\mathcal{H}$ one-to-one onto a dense subset in $\mathbf{\Phi}^\times$. Therefore, we will denote a RHS by

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times . \tag{2.6.8}$$

Since T is continuous, then there exists a norm $\|\varphi\|_m$ and an $M > 0$ such that

$$\|T\varphi\| = \sqrt{(\varphi, \varphi)} \leq M\|\varphi\|_m . \tag{2.6.9}$$

Thus T can be extended onto the entire space $\mathbf{\Phi}_n$, $n \geq m$. We denote the corresponding operator by T_n. It can be proven that there is a value of n for which T_n, mapping the Hilbert space $\mathbf{\Phi}_n$ into $\mathcal{H}$, is a nuclear operator. The operator $T_n^\times$, mapping $\mathcal{H}$ into $\mathbf{\Phi}_n^\times$, is also nuclear.

The nuclearity of T_n will allow us to write T in a simple form. Since T_n is nuclear, there exist orthonormal basis $\{h_k\}$ and $\{e_k\}$ in $\mathcal{H}$ and $\mathbf{\Phi}_n$ such that for every element $\varphi \in \mathbf{\Phi}_n$ one has

$$T_n\varphi = \sum_{k=1}^{\infty} \lambda_k (e_k, \varphi) h_k , \tag{2.6.10}$$

where $\lambda_k \geq 0$ and the series $\sum_{k=1}^{\infty} \lambda_k$ converges. Since $T_n\varphi = T\varphi$ if φ belongs to $\mathbf{\Phi}$, then for elements $\varphi \in \mathbf{\Phi}$ formula (2.6.10) takes the form

$$T\varphi = \sum_{k=1}^{\infty} \lambda_k (e_k, \varphi) h_k . \tag{2.6.11}$$

One can associate with a RHS a two-sided infinite decreasing chain of spaces

$$\mathbf{\Phi}^\times \supset \cdots \supset \mathbf{\Phi}_{-n} \supset \cdots \supset \mathbf{\Phi}_0 \supset \cdots \supset \mathbf{\Phi}_n \supset \cdots \supset \mathbf{\Phi} , \tag{2.6.12}$$

such that for any integer n there exists a nuclear mapping T_n^{n+1} of the space $\mathbf{\Phi}_{n+1}$ onto a dense subset of $\mathbf{\Phi}_n$, and such that

$$\mathbf{\Phi} = \bigcap_{n=1}^{\infty} \mathbf{\Phi}_n , \quad \mathbf{\Phi}^\times = \bigcup_{n=1}^{\infty} \mathbf{\Phi}_{-n} . \tag{2.6.13}$$

In order to construct the chain (2.6.12), we take into account the fact that a nuclear space $\mathbf{\Phi}$ is the intersection of a decreasing chain of Hilbert spaces (see Section 2.4.1)

$$\mathbf{\Phi} = \bigcap_{n=1}^{\infty} \mathbf{\Phi}_n , \quad \mathbf{\Phi}_1 \supset \mathbf{\Phi}_2 \supset \cdots \supset \mathbf{\Phi}_n \supset \cdots \supset \mathbf{\Phi} , \tag{2.6.14}$$

[4]The word "rigged" in Rigged Hilbert Space has a nautical connotation, such as the phrase "fully rigged ship"; it has nothing to do with any unsavory practice such as "fixing" or predetermining a result. The phrase "rigged Hilbert space" is a direct translation of the phrase "osnashchyonnoe Hilbertovo prostranstvo" from the original Russian.

and for every n the mapping T_n^{n+1} is nuclear. Now the space $\mathbf{\Phi}^\times$ is the union of an increasing chain of Hilbert spaces (see Section 2.4.2)

$$\mathbf{\Phi}^\times = \bigcup_{n=1}^{\infty} \mathbf{\Phi}_{-n}\,, \quad \mathbf{\Phi}_{-1} \subset \mathbf{\Phi}_{-2} \subset \cdots \subset \mathbf{\Phi}_{-n} \subset \cdots \subset \mathbf{\Phi}^\times\,, \tag{2.6.15}$$

where $\mathbf{\Phi}_{-n} \equiv \mathbf{\Phi}_n^\times$. We denote by T_n^{n+1}, for $n < -1$, the operator adjoint to T_{-n-1}^{-n}. This operator is also nuclear. In order to connect the chains (2.6.14) and (2.6.15), we note that there is a value n for which the operator T_n , mapping $\mathbf{\Phi}_n$ into $\mathcal{H}$, is nuclear. Then the mapping T_{-n} of $\mathcal{H}$ into $\mathbf{\Phi}_{-n}$ is also nuclear. Without loss of generality we may suppose that $n = 1$. We now denote $\mathcal{H}$ by $\mathbf{\Phi}_0$, and the mappings T_1 and T_{-1} by $T^1_{\ 0}$ and $T^0_{\ -1}$, respectively. We thereby obtain the sequence of spaces (2.6.12).

Example We define the scalar product on $\mathcal{S}(\mathbb{R})$ by

$$(\varphi, \psi) = \int_{-\infty}^{+\infty} \overline{\varphi(x)}\psi(x)dx\,. \tag{2.6.16}$$

Completion of $\mathcal{S}(\mathbb{R})$ with respect to this scalar product yields the Hilbert space $L^2(\mathbb{R}, dx)$. Since $\mathcal{S}(\mathbb{R})$ is nuclear and the scalar product (2.6.16) is continuous with respect to the topology on $\mathcal{S}(\mathbb{R})$, then the triplet

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dx) \subset \mathcal{S}(\mathbb{R})^\times \tag{2.6.17}$$

is a (nuclear) Rigged Hilbert Space. The space $\mathcal{S}(\mathbb{R})^\times$ is called the *space of tempered distributions*. The "plane waves" $e^{i\lambda x}$ may be considered as elements of $\mathcal{S}(\mathbb{R})^\times$. The functional associated to each plane wave $e^{i\lambda x}$ is defined by

$$\langle\varphi|F_\lambda\rangle \equiv \langle\varphi|e^{i\lambda x}\rangle := \int_{-\infty}^{\infty} \overline{\varphi(x)}\, e^{i\lambda x}dx\,. \tag{2.6.18}$$

It is easy to see that $|F_\lambda\rangle$ is a well defined continuous antilinear functional on $\mathcal{S}(\mathbb{R})$.

Chapter 3

The Rigged Hilbert Space of the Harmonic Oscillator

In this chapter, we construct the RHS of the harmonic oscillator. This system is studied from a different point of view to that taken in Quantum Mechanics textbooks. Instead of assuming that the position and momentum operators are given by the multiplication and derivative operators, we shall make three simple algebraic assumptions: the Heisenberg commutation relation, the expression of the Hamiltonian in terms of the position and momentum operators, and the existence of an eigenvector of the Hamiltonian. From these algebraic assumptions, we shall construct the RHS of the harmonic oscillator and the Schrödinger representation of the algebra of the harmonic oscillator.

> As I sat there, brooding on the old unknown world, I thought of Gatsby's wonder when he first picked out the green light at the end of Daisy's dock. He had come a long way to this blue lawn and his dream must have seemed so close that he could hardly fail to grasp it. He did not know that it was already behind him, somewhere back in the vast obscurity beyond the city, where the dark fields of the republic rolled on under the night.
>
> Gatsby believed in the green light, the orgiastic future that year by year recedes before us. It eluded us then, but that's no matter—tomorrow we will run faster, stretch out our arms farther.... And one fine morning——
>
> So we beat on, boats against the current, borne back ceaselessly into the past.
>
> F. Scott Fitzgerald, *The Great Gatsby*

3.1 Introduction

We shall treat in detail one of the simplest physical models, the one-dimensional harmonic oscillator, using the framework of the preceding sections. Our formulation will easily generalize to more complicated physical models, and we will list the algebras for which these generalizations are already known.

The standard approach to the harmonic oscillator is to start out with the (position) Schrödinger realization of the algebra of operators, i.e., one takes for granted the well known differential expressions for the operators position Q, momentum P and energy H of the harmonic oscillator. From these expressions one derives, for instance, the Heisenberg commutation relation. These operators are implicitly assumed to be defined on the same domain, which is assumed to remain stable under their action, and so all algebraic operations such as the multiplication of two operators are allowed. The operators Q and P are assumed to have eigenkets $|x\rangle$ and $|p\rangle$ satisfying $Q|x\rangle = x|x\rangle$ and $P|p\rangle = p|p\rangle$ for every real x and p, although a satisfactory mathematical meaning within a Hilbert space formulation is not possible. Dirac basis expansion is also used, although the Hilbert space spectral decomposition does not correspond to it.

Here we shall obtain this realization but starting from a different point. We shall just assume some algebraic relations to be fulfilled by the operators P, Q and H, namely the Heisenberg commutation relation and the expression of H in terms of P and Q. We shall make an additional essential assumption: the existence of an eigenvector of the energy operator. The operators will be defined on a common linear space that remains stable under their actions.

From this algebraic starting point, we shall derive first that H possesses a countable number of eigenvalues $\hbar w(n + 1/2)$, $n = 0, 1, 2, \ldots$, corresponding to some eigenvectors ϕ_n, as it appears in the literature. The linear space spanned by the ϕ_n will be called Ψ. In Section 3.3 this linear space is equipped with two different topologies: the usual Hilbert space topology, which generates the Hilbert space $\mathcal{H}$ from Ψ, and a stronger nuclear topology, which generates the space $\mathbf{\Phi}$ from Ψ. This nuclear topology will make the elements of the algebra continuous operators.

In Section 3.4, the space of antilinear functionals is defined, and the Rigged Hilbert Space

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times} \tag{3.1.1}$$

for the harmonic oscillator is constructed. Section 3.5 gives the definition of generalized eigenvectors. This definition will provide the proper mathematical setting for the eigenket equations $Q|x\rangle = x|x\rangle$ and $P|p\rangle = p|p\rangle$. The eigenkets $|p\rangle$ and $|x\rangle$ will be continuous antilinear functionals over $\mathbf{\Phi}$, i.e., they will be elements of $\mathbf{\Phi}^{\times}$. A statement of the Gelfand-Maurin Theorem will be given, which will guarantee the existence of a complete set of generalized eigenvectors of the position and momentum operators, as it is usually assumed. It will be shown that this theorem is the mathematical statement that justifies the heuristic Dirac basis vector expansion. In Section 3.6, we derive the Schrödinger representation of the harmonic oscillator. In this representation the standard expressions for P, Q and H in

terms of differential operators will be obtained. The realization of the RHS (3.1.1) by spaces of functions and distributions is also described in Section 3.6. The space $\mathbf{\Phi}$ will be realized by the Schwartz space $\mathcal{S}(\mathbb{R})$, and $\mathbf{\Phi}^\times$ by the space of tempered distributions $\mathcal{S}(\mathbb{R})^\times$. Thus the RHS (3.1.1) will be realized in the position representation by

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dx) \subset \mathcal{S}(\mathbb{R})^\times \,. \tag{3.1.2}$$

Therefore, we shall provide a proper mathematical framework for the operations that are needed in physics, and we will throw light onto the problem of how the Schrödinger realization of the algebra of operators can be singled out. The important point is that this realization, which is introduced *ad hoc* in the literature, can be derived from proper algebraic assumptions within the RHS formalism.

3.2 Algebraic Operations

The algebra (cf. Section 2.1.3) $\mathcal{A}$ of observables for the one dimensional harmonic oscillator is generated by the operators H (representing the observable energy), P (representing the observable momentum) and Q (representing the observable position). The defining algebraic relations are:

$$H = \frac{1}{2\mu}P^2 + \frac{\mu\omega^2}{2}Q^2 \,, \qquad [P, Q] = -i\hbar I \,, \tag{3.2.1}$$

where $\hbar$ is a universal constant (Planck's constant), μ, ω are characteristic constants of the system (mass and frequency, respectively) and $[P, Q] \equiv PQ - QP$ is the commutator of P and Q. The elements of $\mathcal{A}$ are assumed to be linear operators defined on a linear space Ψ. There is a scalar product $(\,\cdot\,,\,\cdot\,)$ defined on Ψ that provides the probability amplitudes (but Ψ is not a Hilbert space). Further, P, Q and H are supposed to be symmetric operators of Ψ into Ψ. That is,

$$A : \Psi \to \Psi \,, \tag{3.2.2}$$

and

$$(A\varphi, \psi) = (\varphi, A\psi), \quad \forall \varphi, \psi \in \Psi \,, \tag{3.2.3}$$

where the operator A can be P, Q or H. The assumptions about the algebra of observables stated so far do not specify the mathematical structure completely. There are many realizations of the vector space Ψ on which $\mathcal{A}$ is an algebra of operators. We have to make one further assumption in order to fully specify the realization of $\mathcal{A}$, i.e., the realization of (3.2.1). This additional requirement can be formulated in the following way:

$$\begin{aligned} &\textit{there exists at least one non-degenerate eigenvalue of} \\ &H \textit{ whose corresponding eigenvector is an element of } \Psi \,. \end{aligned} \tag{3.2.4}$$

In short, our starting point is to assume that the physics of the harmonic oscillator is described by an algebra of observables that satisfy the (algebraic) assumptions (3.2.1)-(3.2.4).

In order to construct the space Ψ, we make the elements of $\mathcal{A}$ act on the eigenvector of (3.2.4). The representation of $\mathcal{A}$ by linear operators on Ψ obtained in this way is called the ladder representation. The procedure to find the ladder representation is well known and will be sketched only very briefly. One defines

$$a := \frac{1}{\sqrt{2}}\left(\sqrt{\frac{\mu\omega}{\hbar}}Q + \frac{i}{\sqrt{\mu\omega\hbar}}P\right), \tag{3.2.5}$$

$$a^\dagger := \frac{1}{\sqrt{2}}\left(\sqrt{\frac{\mu\omega}{\hbar}}Q - \frac{i}{\sqrt{\mu\omega\hbar}}P\right), \tag{3.2.6}$$

$$N := a^\dagger a = \frac{1}{\omega\hbar}H - \frac{1}{2}I\,. \tag{3.2.7}$$

These operators clearly fulfill, as a consequence of (3.2.3),

$$(\varphi, a\psi) = (a^\dagger\varphi, \psi)\,, \quad \forall\,\varphi,\psi \in \Psi\,, \tag{3.2.8}$$

$$(\varphi, N\psi) = (N\varphi, \psi)\,, \quad \forall\,\varphi,\psi \in \Psi\,. \tag{3.2.9}$$

Eq. (3.2.1) implies that a and $a^\dagger$ fulfill

$$[a, a^\dagger] = a\,a^\dagger - a^\dagger a = I\,. \tag{3.2.10}$$

Assumption (3.2.4) implies that there exists a $\varphi_\lambda \neq 0$ in Ψ, such that

$$N\varphi_\lambda = \lambda\varphi_\lambda\,. \tag{3.2.11}$$

From (3.2.9) and (3.2.11) it follows that

$$\lambda(\varphi_\lambda, \varphi_\lambda) = (\varphi_\lambda, N\varphi_\lambda) = (N\varphi_\lambda, \varphi_\lambda) = \overline{\lambda}(\varphi_\lambda, \varphi_\lambda)\,. \tag{3.2.12}$$

Therefore, $\lambda = \overline{\lambda}$, i.e., λ is real. From the commutation relation (3.2.10), it then follows that

$$\begin{aligned} N(a\varphi_\lambda) &= a^\dagger a\,a\varphi_\lambda = (a\,a^\dagger - I)a\varphi_\lambda = a(a^\dagger a - I)\varphi_\lambda \\ &= a(N - I)\varphi_\lambda = a(\lambda - 1)\varphi_\lambda = (\lambda - 1)a\varphi_\lambda\,. \end{aligned} \tag{3.2.13}$$

This implies that either $a\varphi_\lambda$ is an eigenvector of N with eigenvalue $(\lambda - 1)$ or $a\varphi_\lambda = 0$. Further, from (3.2.8) and from the commutation relation (3.2.10) it follows that

$$\|a^\dagger\varphi_\lambda\|^2 = (\varphi_\lambda, a^\dagger a\varphi_\lambda) + (\varphi_\lambda, I\varphi_\lambda) = \|a\varphi_\lambda\|^2 + \|\varphi_\lambda\|^2 \neq 0\,, \tag{3.2.14}$$

since φ_λ is different from the zero vector. This means that $a^\dagger\varphi_\lambda \neq 0$. In addition, equation (3.2.10) implies that

$$N(a^\dagger\varphi_\lambda) = (\lambda + 1)a^\dagger\varphi_\lambda\,, \tag{3.2.15}$$

i.e., $a^\dagger\varphi_\lambda$ is an eigenvector of N with eigenvalue $(\lambda + 1)$.

We now start with the eigenvector φ_λ, which was *assumed* to exist, and successively define the vectors

$$\varphi_{\lambda-m} = a^m \varphi_\lambda \qquad m = 0, 1, 2, 3, \ldots \tag{3.2.16}$$

Since according to (3.2.13) each application of a lowers the eigenvalue by 1, we have

$$N\varphi_{\lambda-m} = (\lambda - m)\varphi_{\lambda-m}\,, \quad m = 0, 1, 2, \ldots \tag{3.2.17}$$

This means that $\varphi_{\lambda-m} = a^m\varphi_\lambda$, $m = 0, 1, 2, \ldots$, are eigenvectors of N with eigenvalue $(\lambda - m)$ unless $\varphi_{\lambda-m}$ is the zero vector. We shall now show that after a finite number of steps m_0, the vector $\varphi_{\lambda-m_0}$ is the zero vector

$$\varphi_{\lambda-m_0} = a^{m_0}\varphi_\lambda = 0\,. \tag{3.2.18}$$

To prove this statement, we calculate the scalar product of (3.2.16) and (3.2.17)

$$(\varphi_{\lambda-m}, N\varphi_{\lambda-m}) = (\lambda - m)\,(\varphi_{\lambda-m}, \varphi_{\lambda-m}) = (\varphi_{\lambda-m}, a^\dagger a\varphi_{\lambda-m}) = \|a\varphi_{\lambda-m}\|^2\,. \tag{3.2.19}$$

If $\varphi_{\lambda-m} \neq 0$, then (3.2.19) leads to

$$(\lambda - m) = \frac{\|a\varphi_{\lambda-m}\|^2}{\|\varphi_{\lambda-m}\|^2}\,. \tag{3.2.20}$$

Since the norm of a non-zero vector is always positive, equation (3.2.20) implies that $(\lambda - m) \geq 0$ whenever $\varphi_{\lambda-m} \neq 0$. Now, if $\varphi_{\lambda-m}$ were different from zero for every $m = 1, 2, \ldots$, then $\lambda - m \geq 0$ could not be fulfilled, since λ is a fixed real number. Therefore, there must exist an $m_0 \in \mathbb{N}$ such that

$$\varphi_{\lambda-m} \neq 0 \quad \text{for}\, m < m_0\,, \tag{3.2.21}$$

and

$$\varphi_{\lambda-m_0} = a\varphi_{\lambda-(m_0-1)} = 0\,. \tag{3.2.22}$$

This proves (3.2.18).

After normalization, we denote the last non-zero vector by

$$\phi_0 \equiv \frac{\varphi_{\lambda-(m_0-1)}}{\|\varphi_{\lambda-(m_0-1)}\|}\,. \tag{3.2.23}$$

From ϕ_0 (for which $a\phi_0 = 0$) one defines the sequence of vectors

$$\begin{array}{lcl} \phi_0 & & \\ \phi_1 & = & \dfrac{1}{\sqrt{1!}}a^\dagger\phi_0 \\ \phi_2 & = & \dfrac{1}{\sqrt{2!}}(a^\dagger)^2\phi_0 \\ \ldots. & .. & \ldots.. \\ \phi_n & = & \dfrac{1}{\sqrt{n!}}(a^\dagger)^n\phi_0 \\ \ldots. & .. & \ldots.. \end{array} \tag{3.2.24}$$

These vectors have the following properties:

1. They are eigenvectors of the number operator N and of the Hamiltonian H

$$N\phi_n = n\phi_n\,, \quad n = 0, 1, 2, \ldots \tag{3.2.25}$$

$$H\phi_n = \hbar\omega(n + 1/2)\phi_n \quad n = 0, 1, 2, \ldots \tag{3.2.26}$$

2. For every ϕ_n, there exists a ϕ_{n+1} that is different from the zero vector.

3. The actions of $a^\dagger$ and a on the sequence (3.2.24) are given by

$$a^\dagger\phi_n = \sqrt{n+1}\phi_{n+1}\,, \quad a\phi_n = \sqrt{n}\phi_{n-1}\,. \tag{3.2.27}$$

Equation (3.2.26) is usually interpreted by saying that the energy of the harmonic oscillator is quantized and cannot take any arbitrary value. Equation (3.2.27) means that if we start with an eigenstate ϕ_n of H corresponding to the eigenvalue $E_n = \hbar\omega(n+1/2)$, application of the operator $a^\dagger$ yields an eigenvector associated with the eigenvalue $E_{n+1} = \hbar\omega(n+1/2)+\hbar\omega$, and application of a yields, in the same way, the energy $E_{n-1} = \hbar\omega(n + 1/2) - \hbar\omega$. For this reason, $a^\dagger$ is said to be a creation operator and a an annihilation operator: their action on an eigenvector of H makes an energy quantum $\hbar\omega$ appear or disappear.

The space Ψ of the ladder representation of $\mathcal{A}$ is the linear space spanned by the eigenvectors $\phi_0, \phi_1, \ldots, \phi_n, \ldots$ of (3.2.24), i.e., Ψ is the set of all (finite) linear combinations

$$\psi = \sum_{n=0}^{M} \alpha_n\phi_n\,, \tag{3.2.28}$$

where $\alpha_n \in \mathbb{C}$ and M is a natural number which is arbitrarily large but finite. In Ψ we have the scalar product $(\,\cdot\,,\,\cdot\,)$ for which (3.2.3), (3.2.8) and (3.2.9) holds. With respect to this scalar product, the vectors ϕ_n are orthogonal and normalized,

$$(\phi_n, \phi_m) = \delta_{nm}\,. \tag{3.2.29}$$

We call the set of vectors $\{\phi_n\}$ an algebraic orthonormal basis for the space Ψ.

The set Ψ can be also viewed as the linear space of all sequences of the form

$$\psi \equiv (\alpha_0, \alpha_1, \ldots, \alpha_M, 0, 0, \ldots) \equiv \sum_{n=0}^{M} \alpha_n\phi_n\,, \tag{3.2.30}$$

where $\alpha_n \in \mathbb{C}$. The algebraic operations of this linear space are defined componentwise: let

$$\psi = (\alpha_0, \alpha_1, \ldots, \alpha_{M_1}, 0, 0, \ldots) \equiv \sum_{n=0}^{M_1} \alpha_n\phi_n \tag{3.2.31}$$

and

$$\varphi = (\beta_0, \beta_1, \ldots, \beta_{M_2}, 0, 0, \ldots) \equiv \sum_{n=0}^{M_2} \beta_n\phi_n \tag{3.2.32}$$

be two elements of Ψ ($M_2 > M_1$). Then

$$\begin{aligned} \psi + \varphi &:= (\alpha_0 + \beta_0, \alpha_1 + \beta_1, \ldots, \alpha_{M_1} + \beta_{M_1}, \ldots, \beta_{M_2}, 0, 0, \ldots) \\ &= \sum_{n=0}^{M_2} (\alpha_n + \beta_n)\phi_n \,, \end{aligned} \tag{3.2.33}$$

and

$$\alpha\psi := (\alpha\alpha_0, \alpha\alpha_1, \ldots, \alpha\alpha_{M_1}, 0, 0, \ldots) = \sum_{n=0}^{M_1} (\alpha\alpha_n)\phi_n \,. \tag{3.2.34}$$

The scalar product of ψ and φ is

$$(\psi, \varphi) = \sum_{n=0}^{M_2} (\alpha_n\phi_n, \beta_n\phi_n) = \sum_{n=0}^{M_2} \overline{\alpha}_n \, \beta_n \,. \tag{3.2.35}$$

Then the norm of ψ is given by

$$\|\psi\|^2 = \sum_{n=0}^{M_1} (\alpha_n\phi_n, \alpha_n\phi_n) = \sum_{n=1}^{M_1} |\alpha_n|^2 \,. \tag{3.2.36}$$

Since the sums (3.2.30)-(3.2.36) only go up to a finite number, the question of the convergence of these sums does not arise. The algebraic operations (3.2.33), (3.2.34) and (3.2.35) show Ψ is a linear scalar product space (cf. Section 2.1.2).

We now introduce the space spanned by each ϕ_n. This is the subspace

$$R_n = \{\alpha\phi_n \mid \alpha \in \mathbb{C}\} \,. \tag{3.2.37}$$

R_n is a one dimensional subspace called the energy eigenspace associated to the n-th eigenvalue of H, because all of its elements are eigenvectors of the operator H with eigenvalue $E_n = \hbar\omega(n + 1/2)$. Although we can just as well work with the vectors ϕ_n, by using the spaces R_n we obtain a formulation which immediately generalizes to the case where R_n is not one dimensional. The space Ψ, that is given by

$$\Psi = \{\psi = (\alpha_0, \alpha_1, \ldots, \alpha_M, 0, 0, \ldots) \equiv \sum_{n=0}^{M} \alpha_n\phi_n \,; \quad \alpha_n \in \mathbb{C} \,, \; M \in \mathbb{N}\} \,, \tag{3.2.38}$$

is usually rewritten as the algebraic direct sum of the spaces R_n:

$$\Psi = \sum_{\text{algebraic}} \oplus R_n \,. \tag{3.2.39}$$

The right hand side of the equation (3.2.39) means that every $\psi \in \Psi$ can be uniquely written as a finite linear combination

$$\psi \equiv r_0 + r_1 + \cdots + r_M \tag{3.2.40}$$

of elements $r_n = \alpha_n\phi_n \in R_n$ that are orthogonal to each other (i.e., $(r_n, r_m) = 0$ if $n \neq m$).

3.3 Construction of the Topologies

3.3.1 Introduction

The space Ψ has so far an algebraic structure, namely it is a linear space provided with a scalar product. In order to be able to use certain tools (such as the Gelfand-Maurin theorem of Section 3.5) we need to equip Ψ with a topological structure, i.e., we need to construct a linear topological space (cf. Section 2.3).

We will define a topology in terms of the notion of sequence convergence. All the rest of the topological notions such as continuity, denseness, boundedness, closure, completeness, etc. will be derived from the notion of sequence convergence. When this notion fully describes the topology, the topological space is said to be first countable (cf. Section 2.2.2). The topologies introduced in this section are all first countable. Only Section 3.4 will deal with topologies that are not first countable.

Intuitively, a sequence $\{\varphi_n\}$ converges to a point φ if whenever we follow the terms of that sequence we get closer and closer to the limit point φ with respect to a certain sense of closeness. This definition of convergence must be such that the linear and the topological structures can be pieced together. This is accomplished by requiring that the algebraic operations be continuous with respect to the topology under consideration. Therefore, a linear topological space has

1. A linear structure.

2. A topology τ that provides a notion of convergence of sequences. If a sequence $\{\varphi_n\}$ converges to a point φ, then we denote

$$\varphi_n \xrightarrow[n\to\infty]{\tau} \varphi\,. \tag{3.3.1}$$

3. The algebraic operations are continuous. That is,
   (3a) If $\varphi_n \xrightarrow{\tau} \varphi$, then $\alpha\varphi_n \xrightarrow{\tau} \alpha\varphi$ for every $\alpha \in \mathbb{C}$.
   (3b) If $\mathbb{C} \ni \alpha_n \longrightarrow \alpha \in \mathbb{C}$, then $\alpha_n\varphi \xrightarrow{\tau} \alpha\varphi$ for every φ.
   (3c) If $\varphi_n \xrightarrow{\tau} \varphi$ and $\psi_n \xrightarrow{\tau} \psi$, then $\varphi_n + \psi_n \xrightarrow{\tau} \varphi + \psi$.

This is not the most general definition of a linear topological space (cf. Section 2.3) but it is sufficient when the topology is first countable.

A sequence $\{\varphi_n\}$ will be said to be Cauchy if the terms of the sequence get more and more close to each other as $n \to \infty$. We then write

$$\varphi_n - \varphi_m \xrightarrow[n,m\to\infty]{\tau} 0\,. \tag{3.3.2}$$

One may expect that whenever we follow the elements of a Cauchy sequence, we always end up in an element of the space. However, this is the case only in certain kind of spaces, that are called complete. Therefore, a space is complete with respect to a given topology if every Cauchy sequence has a limit that belongs to the space. When a space is not complete, it

can be completed by adding to it all the limit points of Cauchy sequences. In this case, the incomplete space can be viewed as a dense set of the complete space (cf. Section 2.3.2).

We shall introduce two different topologies on Ψ, the Hilbert space topology and a nuclear topology. Completion with respect to each topology will lead to the space $\mathcal{H}$ and $\mathbf{\Phi}$, respectively. These two topologies will be fully described by the definition of convergence of sequences (i.e., they are first countable).

3.3.2 Hilbert Space Topology

First, we introduce into Ψ the well known Hilbert space topology, which we shall denote by $\tau_{\mathcal{H}}$. For each $\psi \in \Psi$, we define the norm of ψ by

$$\|\psi\| := \sqrt{(\psi, \psi)}\,, \tag{3.3.3}$$

where (ψ, ψ) is the scalar product of Ψ. The norm (3.3.3) can be used to introduce a meaning of convergence, i.e., to specify in which sense the terms of a sequence get closer and closer to a limit point. We will say that a sequence $\{\psi_n\}$ in Ψ converges to $\psi \in \Psi$ with respect to the Hilbert space topology $\tau_{\mathcal{H}}$ if

$$\|\psi_n - \psi\| \to 0 \quad \text{as } n \to \infty\,. \tag{3.3.4}$$

This means that $\{\psi_n\}$ tends to ψ if for every $\epsilon > 0$ there is a positive integer $N(\epsilon)$ such that $\|\psi_n - \psi\| < \epsilon$ for every $n > N$. Symbolically, this condition is written as

$$\psi_n \xrightarrow[n\to\infty]{\tau_{\mathcal{H}}} \psi \quad \text{iff} \quad \|\psi_n - \psi\| \xrightarrow[n\to\infty]{} 0\,. \tag{3.3.5}$$

The concept of Cauchy sequence can be stated as: a sequence $\{\psi_n\}$ in Ψ is Cauchy with respect to $\tau_{\mathcal{H}}$ if for every $\epsilon > 0$ there exists a positive integer N such that $\|\psi_n - \psi_m\| < \epsilon$ for every $m, n > N$. In other words, the sequence $\{\psi_n\}$ is Cauchy if

$$\|\psi_n - \psi_m\| \to 0 \quad \text{as } n, m \to \infty\,. \tag{3.3.6}$$

The space Ψ is not complete with respect to the Hilbert space topology. That is to say, there exist Cauchy sequences of elements ψ_n in Ψ (i.e., sequences fulfilling (3.3.6)) that do not have a $\tau_{\mathcal{H}}$-limit element in Ψ (i.e., there is no $\psi \in \Psi$ such that (3.3.4) holds). As an example, let us consider the following infinite sequence:

$$\begin{aligned}
\psi_0 &= (\frac{\phi_0}{1}, 0, 0, \ldots) \equiv \frac{\phi_0}{1} \\
\psi_1 &= (\frac{\phi_0}{1}, \frac{\phi_1}{2}, 0, \ldots) \equiv \frac{\phi_0}{1} + \frac{\phi_1}{2} \\
\ldots. &\ \ldots \ \ldots\ldots\ldots \\
\psi_n &= (\frac{\phi_0}{1}, \frac{\phi_1}{2}, \ldots, \frac{\phi_n}{n+1}, 0, \ldots) \equiv \sum_{i=0}^{n} \frac{\phi_i}{i+1} \\
\ldots. &\ \ldots \ \ldots\ldots\ldots\,,
\end{aligned} \tag{3.3.7}$$

where the ϕ_n are the eigenvectors (3.2.24) of N. The sequence (3.3.7) is $\tau_{\mathcal{H}}$-Cauchy, because for any positive integers n, m ($m > n$ without loss of generality)

$$\|\psi_n - \psi_m\|^2 = \sum_{i=n+1}^{m} \frac{\|\phi_i\|^2}{(i+1)^2} = \sum_{i=n+1}^{m} \frac{1}{(i+1)^2} \xrightarrow[n,m\to\infty]{} 0\,. \tag{3.3.8}$$

But (3.3.7) tends, with respect to $\tau_{\mathcal{H}}$, to

$$z = (\frac{\phi_0}{1}, \frac{\phi_1}{2}, \ldots, \frac{\phi_n}{n+1}, \frac{\phi_{n+1}}{n+2}, \ldots) \equiv \sum_{i=0}^{\infty} \frac{\phi_i}{i+1}\,. \tag{3.3.9}$$

which is an infinite sequence and therefore is not in Ψ. This shows that Ψ is not complete.

The space Ψ can be completed with respect to the topology $\tau_{\mathcal{H}}$ by adding to Ψ all the limit points of $\tau_{\mathcal{H}}$-Cauchy sequences of elements of Ψ. The resulting space, denoted by $\mathcal{H}$, is the Hilbert space. Ψ, that is a scalar product space which is not complete with respect to $\tau_{\mathcal{H}}$, is usually called a pre-Hilbert space. The space $\mathcal{H}$ is the set of infinite sequences

$$h = (r_0, r_1, \ldots, r_n, \ldots) \equiv \sum_{n=0}^{\infty} r_n\,, \tag{3.3.10}$$

where $r_n = \alpha_n \phi_n \in R_n$ and $\alpha_n \in \mathbb{C}$, such that

$$\sum_{n=0}^{\infty} \|r_n\|^2 = \sum_{n=0}^{\infty} |\alpha_n|^2 < \infty\,, \tag{3.3.11}$$

or in a more compact notation

$$\mathcal{H} = \{h \equiv (r_0, r_1, \ldots, r_n, \ldots) \mid \sum_{n=0}^{\infty} \|r_n\|^2 < \infty\,,\ r_n \in R_n\}\,. \tag{3.3.12}$$

Its topology is given by the prescription (3.3.5) for sequence convergence:

$$h_n \xrightarrow[n\to\infty]{\tau_{\mathcal{H}}} h \Leftrightarrow \|h_n - h\| \xrightarrow[n\to\infty]{\tau_{\mathbb{C}}} 0\,. \tag{3.3.13}$$

It can be proven that the space $\mathcal{H}$ defined by (3.3.12) is complete with respect to the topology defined by (3.3.13).

A vector $h \in \mathcal{H}$ given by (3.3.10) is uniquely determined by the sequence of complex numbers

$$h \equiv (\alpha_0, \alpha_1, \ldots, \alpha_n, \ldots)\,, \tag{3.3.14}$$

where $r_n = \alpha_n \phi_n$. This sequence is not arbitrary, but it must fulfill (3.3.11). In fact, it can be shown that the norm (3.3.3) of any $h \in \mathcal{H}$ is given by

$$\|h\|^2 = \sum_{n=0}^{\infty} |\alpha_n|^2\,. \tag{3.3.15}$$

An infinite sequence $(\alpha_0, \alpha_1, \ldots, \alpha_n, \ldots)$ that satisfies (3.3.11) is said to be square summable. The set of square summable sequences is denoted by $l_2(\mathbb{C})$. It is clear that $h \in \mathcal{H}$ iff its corresponding sequence (3.3.14) is square summable. Therefore, (3.3.14) and (3.3.15) set up a one-to-one correspondence of the Hilbert space $\mathcal{H}$ onto the space $l_2(\mathbb{C})$. The spaces $\mathcal{H}$ and $l_2(\mathbb{C})$ are, from a linear topological point of view, the same. We then say that $l_2(\mathbb{C})$ is the realization of $\mathcal{H}$ by the space of square summable sequences. In terms of these sequences, the space $\mathcal{H}$ is given by

$$\mathcal{H} = \{h = \sum_{n=0}^{\infty} \alpha_n \phi_n \mid \alpha_n \in \mathbb{C}\,,\ \sum_{n=0}^{\infty} |\alpha_n|^2 < \infty\}\,. \tag{3.3.16}$$

The α_n of (3.3.14) can be obtained as the scalar product of h with ϕ_n

$$\alpha_n = (\phi_n, h)\,, \qquad n = 0, 1, 2, \ldots \tag{3.3.17}$$

Thus we can write any element $h \in \mathcal{H}$ as

$$h \equiv \sum_{n=0}^{\infty} \phi_n (\phi_n, g) \equiv \sum_{n=0}^{\infty} |\phi_n)(\phi_n, g)\,, \tag{3.3.18}$$

in analogy to the three-dimensional case

$$\vec{x} = \sum_{i=1}^{3} \vec{e}_i (\vec{e}_i \cdot \vec{x}) = \sum_{i=1}^{3} \vec{e}_i\, x_i\,. \tag{3.3.19}$$

Equation (3.3.18) is usually interpreted by saying that the $\{\phi_n\}$ form an orthonormal basis for $\mathcal{H}$ and that the α_n are the components along the basis vectors ϕ_n.

We are now going to show that $\mathcal{H}$ is actually a $\tau_{\mathcal{H}}$-completion of Ψ. First, the algebraic operations on Ψ can be readily extended to the Hilbert space $\mathcal{H}$. The sum of two elements

$$h \equiv (\alpha_0, \alpha_1, \ldots, \alpha_n, \ldots) \equiv \sum_{n=0}^{\infty} \alpha_n \phi_n \tag{3.3.20}$$

and

$$g \equiv (\beta_0, \beta_1, \ldots, \beta_n, \ldots) \equiv \sum_{n=0}^{\infty} \beta_n \phi_n \tag{3.3.21}$$

of $\mathcal{H}$ is defined componentwise as

$$h + g := (\alpha_0 + \beta_0, \alpha_1 + \beta_1, \ldots, \alpha_n + \beta_n, \ldots) \equiv \sum_{n=0}^{\infty} (\alpha_n + \beta_n) \phi_n\,. \tag{3.3.22}$$

It can be proven that if h and g are elements of $\mathcal{H}$, i.e., the sequences (3.3.20) and (3.3.21) satisfy (3.3.11), then $h + g$ is also an element of $\mathcal{H}$, i.e., it obeys

$$\sum_{n=0}^{\infty} |\alpha_n + \beta_n|^2 < \infty\,. \tag{3.3.23}$$

The multiplication of an element h of $\mathcal{H}$ by a complex number α is defined by

$$\alpha h := (\alpha\alpha_0, \alpha\alpha_1, \ldots, \alpha\alpha_n, \ldots) \equiv \sum_{n=0}^{\infty} (\alpha\alpha_n)\phi_n \,. \tag{3.3.24}$$

The scalar product on $\mathcal{H}$ is defined by

$$(h, g) = \sum_{n=0}^{\infty} (\alpha_n\phi_n, \beta_n\phi_n) = \sum_{n=0}^{\infty} \overline{\alpha}_n \, \beta_n \,. \tag{3.3.25}$$

If h and g are in $\mathcal{H}$, then it can be shown that the series (3.3.25) converges and that this scalar product is well defined. Therefore, $\mathcal{H}$ is a linear scalar product space that is complete with respect to the topology $\tau_{\mathcal{H}}$ generated by this scalar product, i.e., $\mathcal{H}$ is a Hilbert space. Since every element $\psi \in \Psi$ is given by a finite sequence of the form

$$\psi = (r_0, r_1, \ldots, r_M, 0, 0, \ldots) \tag{3.3.26}$$

that obviously satisfies (3.3.11), the space Ψ is a subset of $\mathcal{H}$. The algebraic operations (3.3.22), (3.3.24) and (3.3.25) on $\mathcal{H}$ clearly extend the operations (3.2.33), (3.2.34) and (3.2.35) on Ψ. We can see that Ψ is dense in $\mathcal{H}$ with respect to this topology. In fact, every element

$$h \equiv (\alpha_0, \alpha_1, \ldots, \alpha_n, \ldots) \equiv \sum_{n=0}^{\infty} \alpha_n\phi_n \tag{3.3.27}$$

of $\mathcal{H}$ is the $\tau_{\mathcal{H}}$-limit of a sequence of elements of Ψ with the form

$$\psi_n \equiv (\alpha_0, \alpha_1, \ldots, \alpha_n, 0, 0, \ldots) \equiv \sum_{i=0}^{n} \alpha_i\phi_i \,. \tag{3.3.28}$$

In other words, $\mathcal{H}$ is the $\tau_{\mathcal{H}}$-completion of Ψ with respect to the topology defined by the norm $\|\psi\| = \sqrt{(\psi, \psi)}$.

In terms of the spaces R_n, the space $\mathcal{H}$ is usually written as

$$\mathcal{H} = \sum_{\text{Hilbert}} \oplus \, R_n \,. \tag{3.3.29}$$

The right hand side of (3.3.29) is usually called the Hilbertian direct sum or orthogonal direct sum of the R_n because the spaces R_n are orthogonal to each other, since $(r_n, r_m) = 0$ for $n \neq m$, where $r_n \in R_n$ and $r_m \in R_m$.

An example of an element of $\mathcal{H}$ is the sequence

$$z \equiv (1, \frac{1}{2}, \frac{1}{3}, \ldots, \frac{1}{n}, \ldots) \equiv \sum_{n=0}^{\infty} \frac{\phi_n}{n+1} \tag{3.3.30}$$

of (3.3.9). For this sequence, it holds that

$$\|z\|^2 = \sum_{n=0}^{\infty} \frac{\|\phi_n\|^2}{(n+1)^2} = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}\,. \tag{3.3.31}$$

z is the $\tau_{\mathcal{H}}$-limit element of the Cauchy sequence (3.3.7), because for every ψ_n in (3.3.7)

$$\|\psi_n - z\|^2 = \sum_{i=n+1}^{\infty} \frac{\|\phi_i\|^2}{(i+1)^2} = \sum_{i=n+1}^{\infty} \frac{1}{(i+1)^2} \xrightarrow[n\to\infty]{} 0\,. \tag{3.3.32}$$

Summarizing, we started with the linear scalar product space Ψ of finite linear combinations of the eigenvectors ϕ_n. In this space, we introduced the topology $\tau_{\mathcal{H}}$ through the meaning of sequence convergence (3.3.5). The space Ψ was not complete with respect to $\tau_{\mathcal{H}}$, i.e., there were Cauchy sequences of elements of Ψ that did not have a $\tau_{\mathcal{H}}$-limit element in Ψ. Ψ was completed to a space $\mathcal{H}$ by adjoining to it all limit elements of $\tau_{\mathcal{H}}$-Cauchy sequences. Thus, the Hilbertian direct sum was obtained by completing the algebraic direct sum with respect to $\tau_{\mathcal{H}}$:

$$\Psi = \sum_{\text{algebraic}} \oplus R_n \longmapsto \tau_{\mathcal{H}}\text{−completion} \longmapsto \mathcal{H} = \sum_{\text{Hilbert}} \oplus R_n\,. \tag{3.3.33}$$

The operators of the algebra of observables $\mathcal{A}$ can be considered now as linear operators defined on a subdomain of the Hilbert space. These operators can be extended to larger subdomains of $\mathcal{H}$ (see Section 3.3.5). But these extensions are not continuous with respect to $\tau_{\mathcal{H}}$. Moreover, their domains do not remain stable under the actions of the operators. Therefore, algebraic operations such as the sum or multiplication of two operators are not always allowed. Since in physics these kind of operations are always assumed to be well defined, it is reasonable to search for a space $\mathbf{\Phi}$ that

1. remains stable under the action of the elements of the algebra $\mathcal{A}$,

$$A : \mathbf{\Phi} \to \mathbf{\Phi}\,, \tag{3.3.34}$$

   where A is any element of $\mathcal{A}$.

2. Every $A \in \mathcal{A}$ is continuous with respect to certain topology on $\mathbf{\Phi}$. This continuity will allow us to extend the operators from Ψ to their extension on $\mathbf{\Phi}$ in a unique way.

The domain $\mathbf{\Phi}$ is characteristic of the particular physical system (i.e., of the particular algebra of observables) upon consideration. The construction of this domain for the harmonic oscillator is the subject of the next section.

3.3.3 Nuclear Topology

We now construct the space $\mathbf{\Phi}$, which will be the completion of Ψ with respect to a nuclear topology $\tau_{\mathbf{\Phi}}$. We take the original scalar product $(\,\cdot\,,\,\cdot\,)$ and define the quantities

$$(\varphi,\psi)_p := (\varphi,(N+I)^p\psi)\,, \quad \forall\varphi,\psi\in\Psi\,,\ p=0,1,2,\ldots \tag{3.3.35}$$

and

$$\|\psi\|_p := \sqrt{(\psi,\psi)_p}\,, \quad \forall\psi\in\Psi\,. \tag{3.3.36}$$

From the properties of the linear operator N, it is easy to see that $(\varphi,\psi)_p$ of (3.3.35) fulfills the conditions (2.1.12)-(2.1.14) of a scalar product and that the quantities of (3.3.36) form an increasing sequence of norms

$$\|\psi\|_0 \le \|\psi\|_1 \le \|\psi\|_2 \le \cdots \tag{3.3.37}$$

Further, these norms are compatible, i.e., if a sequence converges to zero with respect to one norm and is a Cauchy sequence with respect to another, then it also converges to zero with respect to this other norm (cf. Section 2.4.1).

We now define the notion of convergence that will determine the nuclear topology $\tau_{\mathbf{\Phi}}$. A sequence $\{\psi_n\}$ of elements in Ψ converges to an element ψ with respect to the topology $\tau_{\mathbf{\Phi}}$ if $\{\psi_n\}$ converges to ψ with respect to every norm in (3.3.36):

$$\psi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \psi \Leftrightarrow \|\psi_n-\psi\|_p \to 0\,, \quad \text{for every } p=0,1,2,\ldots \tag{3.3.38}$$

The reason why we introduce the scalar products (3.3.35) and the topology (3.3.38) is that the operator N will be continuous with respect to $\tau_{\mathbf{\Phi}}$ (cf. Section 3.3.5). Moreover, due to the special structure of the algebra of the harmonic oscillator, the continuity of N will imply the continuity of the rest of the observables of this algebra (cf. Section 3.3.5).

From $\psi_n \xrightarrow{\tau_{\mathbf{\Phi}}} \psi$ it follows that $\psi_n \xrightarrow{\tau_{\mathcal{H}}} \psi$, but not vice versa. Therefore $\tau_{\mathbf{\Phi}}$ is stronger (finer) than $\tau_{\mathcal{H}}$, and $\tau_{\mathcal{H}}$ is weaker (coarser) than $\tau_{\mathbf{\Phi}}$.

A sequence $\{\psi_n\}$ in Ψ is $\tau_{\mathbf{\Phi}}$-Cauchy if for every p and for every $\epsilon>0$ there exists a positive integer $N=N(\epsilon,p)$ such that

$$\|\psi_n-\psi_m\|_p < \epsilon \quad \text{for every } n,m>N\,, \tag{3.3.39}$$

i.e., $\{\psi_n\}$ is $\tau_{\mathbf{\Phi}}$-Cauchy if it is Cauchy with respect to every norm of (3.3.36).

We now complete Ψ with respect to $\tau_{\mathbf{\Phi}}$ by adding to Ψ the limit points of all $\tau_{\mathbf{\Phi}}$-Cauchy sequences. The complete linear topological space obtained in this way is denoted by $\mathbf{\Phi}$. $\mathbf{\Phi}$ is called a countably Hilbert space (cf. Section 2.4). Since there are more $\tau_{\mathcal{H}}$-Cauchy sequences than $\tau_{\mathbf{\Phi}}$-Cauchy sequences (because a $\tau_{\mathcal{H}}$-Cauchy sequence must fulfill (3.3.39) only for $p=0$), this implies

$$\Psi \subset \mathbf{\Phi} \subset \mathcal{H}\,. \tag{3.3.40}$$

Thus, Ψ is $\tau_{\mathbf{\Phi}}$-dense in $\mathbf{\Phi}$, and since Ψ is $\tau_{\mathcal{H}}$-dense in $\mathcal{H}$, $\mathbf{\Phi}$ is $\tau_{\mathcal{H}}$-dense in $\mathcal{H}$.

In order to construct $\mathbf{\Phi}$ explicitly, let us see which of the infinite sequences that are elements of $\mathcal{H}$, i.e., that fulfill (3.3.11), are also elements of $\mathbf{\Phi}$. A sequence

$$\varphi = (r_0, r_1, \ldots, r_n, \ldots)\,, \quad r_n \in R_n\,, \tag{3.3.41}$$

is an element of $\mathbf{\Phi}$ iff it is the limit point of the sequence

$$\psi_n = (r_0, r_1, \ldots, r_n, 0, 0, \ldots) \tag{3.3.42}$$

of elements of Ψ with respect to $\tau_{\mathbf{\Phi}}$, i.e., iff

$$\|\psi_n - \varphi\|_p \to 0\,, \quad \text{for every } p = 0, 1, 2, \ldots \tag{3.3.43}$$

Equation (3.3.43) is equivalent to

$$((\psi_n - \varphi), (N+I)^p(\psi_n - \varphi)) \to 0\,, \quad \text{for every } p = 0, 1, 2, \ldots\,, \tag{3.3.44}$$

which is equivalent to

$$\sum_{i=n+1}^{\infty} (r_i, (N+I)^p r_i) = \sum_{i=n+1}^{\infty} (i+1)^p \|r_i\|^2 \xrightarrow[n\to\infty]{} 0\,, \quad \text{for every } p = 0, 1, 2, \ldots \tag{3.3.45}$$

Therefore, φ is the $\tau_{\mathbf{\Phi}}$-limit point of a $\tau_{\mathbf{\Phi}}$-Cauchy sequence of elements of Ψ iff it fulfills (3.3.45). Then the space $\mathbf{\Phi}$ is given by

$$\mathbf{\Phi} = \{\varphi = \sum_{n=0}^{\infty} \alpha_n \phi_n \mid \alpha_n \in \mathbb{C}\,,\ \sum_{n=0}^{\infty} (n+1)^p |\alpha_n|^2 < \infty \quad \text{for every } p = 0, 1, 2, \ldots\}\,. \tag{3.3.46}$$

Obviously, $\mathbf{\Phi}$ is a linear space under the algebraic operations inherited from $\mathcal{H}$.

If we denote the completion of Ψ with respect to each norm $\|\psi\|_p$ of (3.3.36) by $\mathbf{\Phi}_p$, for every $p = 0, 1, 2, \ldots$, then it can be shown that

$$\mathbf{\Phi} = \bigcap_{p=0}^{\infty} \mathbf{\Phi}_p\,. \tag{3.3.47}$$

$\mathbf{\Phi}$ is also called the $\tau_{\mathbf{\Phi}}$-direct sum of the spaces R_n, that is denoted by

$$\mathbf{\Phi} = \sum_{\text{nuclear}} \oplus R_n\,. \tag{3.3.48}$$

This $\tau_{\mathbf{\Phi}}$-direct sum has been constructed by completing the algebraic direct sum with respect to the $\tau_{\mathbf{\Phi}}$ topology

$$\Psi = \sum_{\text{algebraic}} \oplus R_n \longmapsto \tau_{\mathbf{\Phi}}\text{−completion} \longmapsto \sum_{\text{nuclear}} \oplus R_n\,. \tag{3.3.49}$$

The operators in the algebra of observables can be extended to $\mathbf{\Phi}$ (cf. Section 3.3.5). These extensions will be proven to be continuous with respect to $\tau_{\mathbf{\Phi}}$ and the space $\mathbf{\Phi}$ will be proven to remain stable under the action of the operators of the algebra. Therefore, all algebraic operations will be allowed. This is, in fact, the very reason why we have introduced the space $\mathbf{\Phi}$.

3.3.4 Physical Interpretation of Ψ, $\mathbf{\Phi}$ and $\mathcal{H}$

To see what these various spaces might mean for physics, we recall that R_n is the energy eigenspace corresponding to the energy eigenvalue

$$E_n = \hbar\omega\Big(n + \frac{1}{2}\Big)\,. \tag{3.3.50}$$

If $h = (\alpha_0, \alpha_1, \ldots, \alpha_n, \ldots) = \sum_{n=0}^{\infty} \alpha_n \phi_n$, where $\alpha_n = (\phi_n, h)$, then

$$h \in \mathcal{H} \quad \Leftrightarrow \quad \sum_{n=0}^{\infty} |\alpha_n|^2 < \infty\,, \tag{3.3.51}$$

$$h \in \mathbf{\Phi} \quad \Leftrightarrow \quad \sum_{n=0}^{\infty} (n+1)^p |\alpha_n|^2 < \infty \quad \text{for } p = 0, 1, 2, \ldots\,, \tag{3.3.52}$$

$$h \in \Psi \quad \Leftrightarrow \quad \text{all } \alpha_n \text{ but a finite number are equal to } 0\,. \tag{3.3.53}$$

Clearly, direct experimental data can only tell us something about Ψ. In fact for most real physical systems whose idealization is the harmonic oscillator, e.g. diatomic molecules, only the very lowest energy levels are relevant; for higher energy the diatomic molecule is no longer a harmonic oscillator and finally not even an oscillator. $\mathbf{\Phi}$ and $\mathcal{H}$ are both idealizations, though $\mathbf{\Phi}$ appears "closer" to reality.

The reason why we prefer the mathematical idealization provided by $\mathbf{\Phi}$ over the one provided by $\mathcal{H}$ can be vaguely summarized by saying that $\mathbf{\Phi}$ admits Dirac's bra-ket formalism. Two aspects of this formalism are:

1. All algebraic operations involving the observables are allowed and no questions regarding the domain of definition arise.

2. For every observable there exists a complete system of eigenvectors such that every wave function can be expanded in terms of these eigenvectors.

The first aspect follows from the fact that all the elements of the algebra $\mathcal{A}$ leave invariant $\mathbf{\Phi}$, are continuous operators with respect to $\tau_{\mathbf{\Phi}}$ and therefore uniquely defined on the whole space $\mathbf{\Phi}$. This will be discussed in the next section. The second aspect will need the concepts of dual space and generalized eigenfunction, and will be discussed in Section 3.5.

3.3.5 Extension of the Algebra of Operators

The operators of the algebra of observables were assumed to be defined on the space Ψ. Since $\Psi \subset \mathcal{H}$, these observables can be considered as linear operators defined on the subdomain Ψ of the Hilbert space $\mathcal{H}$. They can be extended to larger subdomains of $\mathcal{H}$ by using the notion of closure (see Section 2.5.3). If $\psi_n \in \Psi$ and $\psi_n \xrightarrow{\tau_{\mathcal{H}}} f$, but $f \notin \Psi$, then $A\psi_n \in \Psi$ for every n but A is not defined on f. If $A\psi_n \xrightarrow{\tau_{\mathcal{H}}} g$, then we define the closure $\overline{A}$ of A by $\overline{A}f = g$. We can do this only for those $f \in \mathcal{H}$ which are $\tau_{\mathcal{H}}$-limit points of some sequences

$\psi_n \in \Psi$ and for which $A\psi_n$ $\tau_{\mathcal{H}}$-converges. The domain $\mathcal{D}(\overline{A})$ of $\overline{A}$ is the set of elements for which the above procedure can be applied. Evidently, the closure of an operator extends the operator itself. Thus, in correspondence to the relation

$$\Psi \subset \mathcal{H} \tag{3.3.54}$$

between the spaces, we have the relation

$$A \subset \overline{A} \tag{3.3.55}$$

between the operators. However, in general, $\mathcal{D}(\overline{A}) \neq \mathcal{H}$. This means that there are elements h in $\mathcal{H}$ on which $\overline{A}$ is not defined, i.e., $\|\overline{A}h\| = \infty$.

As an example, we consider the operator N. This operator can be extended from Ψ to larger subdomains of $\mathcal{H}$. But N cannot be extended to the whole of $\mathcal{H}$. For instance, the action of N cannot be extended to the Hilbert space element

$$z \equiv (1, \frac{1}{2}, \ldots, \frac{1}{n+1}, \ldots) \tag{3.3.56}$$

because

$$\psi_n \equiv (1, \frac{1}{2}, \ldots, \frac{1}{n+1}, 0, \ldots) \xrightarrow[n\to\infty]{\tau_{\mathcal{H}}} z\,, \tag{3.3.57}$$

but

$$N\psi_n \equiv (0, 1, \frac{1}{2}, \frac{2}{3}, \ldots, \frac{n}{n+1}, 0, \ldots) \xrightarrow[n\to\infty]{\tau_{\mathcal{H}}} (0, 1, \frac{1}{2}, \frac{2}{3}, \ldots, \frac{n}{n+1}, \ldots)\,, \tag{3.3.58}$$

which is not an element of $\mathcal{H}$. In fact, the largest subdomain of $\mathcal{H}$ to which N can be extended is given by

$$\{h = \sum_{n=0}^{\infty} \alpha_n \phi_n \mid \sum_{n=0}^{\infty} n^2 |\alpha_n|^2 < \infty\}\,. \tag{3.3.59}$$

The extension of any other operator A of the algebra $\mathcal{A}$ can be constructed in a similar way. If $h = \sum_{n=0}^{\infty} \alpha_n \phi_n$ is an element of $\mathcal{H}$, then the action of the extension of A (that is also denoted by A) on h is given by

$$Ah = A\left(\sum_{n=0}^{\infty} \alpha_n \phi_n\right) := \sum_{n=0}^{\infty} \alpha_n (A\phi_n)\,. \tag{3.3.60}$$

This extension, however, is not defined for every element of the Hilbert space, but only for those $h \in \mathcal{H}$ for which $\|Ah\| < \infty$. Therefore, the operators of $\mathcal{A}$ cannot be extended to the whole of $\mathcal{H}$ and their extensions are not $\tau_{\mathcal{H}}$-continuous. The domains of the extensions of the operators of $\mathcal{A}$ are, in general, different for different operators, and do not remain stable under the action of the extensions. In order to avoid domain questions, we need the space $\mathbf{\Phi}$. This space is the largest subspace of $\mathcal{H}$ on which all the extensions of the operators are well defined and that remains stable under the action of these extensions. From now on, we

will always consider the domain of the operators to be $\mathbf{\Phi}$. We will denote the (Hilbert space) extension of P, Q, $H\ldots$ to $\mathbf{\Phi}$ also by P, Q, $H\ldots$ These extensions are also symmetric,

$$(A\varphi, \psi) = (\varphi, A\psi)\,, \qquad \forall \varphi, \psi \in \mathbf{\Phi}\,, \tag{3.3.61}$$

where A can be P, Q or H.

It can be shown that the operator H is not only symmetric but also essentially self-adjoint (e.s.a.) (cf. Section 2.5.3), i.e., it can be shown that

$$\overline{H} = H^\dagger\,. \tag{3.3.62}$$

In fact, it can be proven (see reference [65]) that the requirement that H has at least one eigenvector (see (3.2.4)) is equivalent to the requirement that H is e.s.a.:

$$\text{There exists a } \varphi_E \text{ such that } H\varphi_E = E\varphi_E \quad \text{iff} \quad \overline{H} = H^\dagger\,. \tag{3.3.63}$$

We remark that either of these requirements leads to a representation of $\mathcal{A}$ which integrates to a representation of the group generated by P, Q and I (Weyl group): the requirement that H is e.s.a. because of the Nelson theorem (see [65]) and the requirement that H has one eigenvector because it leads to the ladder representation, and ladder representations are always integrable.

Since $N = 1/(\hbar\omega)H - 1/2I$, N is also e.s.a. That is,

$$N^\dagger = \overline{N}\,. \tag{3.3.64}$$

As a consequence of the fact that P and Q are elements of the Lie algebra of the Weyl group, it follows that P and Q are also e.s.a. by a theorem of Nelson and Stinespring (see [66]). That is,

$$P^\dagger = \overline{P}\,, \qquad Q^\dagger = \overline{Q}\,. \tag{3.3.65}$$

$H + I$ is, except for some constant factors, the Nelson operator, and is also e.s.a.

> In our example, one can easily see that N is e.s.a. without invoking the Nelson theorem. It can be easily proved by using one of the criteria of essentially self-adjointness:
>
> Lemma: An operator A is e.s.a. if $(A+I)^{-1}$ is continuous and has a dense domain in $\mathcal{H}$.
>
> The spectrum (cf. Section 2.5) of $(N+1)^{-1}$ is $1/(n+1)$, $n = 0, 1, 2, \ldots$ Consequently, it is a continuous operator. Its domain is dense in $\mathcal{H}$. Therefore, N is e.s.a. As a consequence, $N + I$ is e.s.a. Further, $(N+I)^p$ is e.s.a.[1] for every $p = 1, 2, \ldots$

The extension of any operator A of $\mathcal{A}$ from Ψ to $\mathbf{\Phi}$ is constructed as follows: given any element $\varphi = \sum_{n=0}^{\infty} \alpha_n \phi_n$ of $\mathbf{\Phi}$, the sequence $\psi_n = \sum_{i=0}^{n} \alpha_i \phi_i$ of elements of Ψ converge

[1] That $(N+I)^p$ is e.s.a. can be proved in many ways. It also follows from the fact that $(N+I)^p$ is an elliptic element in the enveloping algebra of a group representation (see reference [66]).

to φ with respect to $\tau_{\mathbf{\Phi}}$, i.e., $\psi_n \xrightarrow{\tau_{\mathbf{\Phi}}} \varphi$. The action of A on φ is defined by $A\varphi := \tau_{\mathbf{\Phi}} - \lim_{n\to\infty} A\psi_n$, or

$$A\varphi := \sum_{n=0}^{\infty} \alpha_n A\phi_n \,. \tag{3.3.66}$$

These extensions are unique if the operators are $\tau_{\mathbf{\Phi}}$-continuous on Ψ (cf. Section 2.3.4). Since the product and the sum of two continuous operators are continuous operators, the elements of our algebra $\mathcal{A}$ are continuous if a and $a^\dagger$ are continuous operators. In particular, P, Q and H are continuous if a and $a^\dagger$ are continuous. In a space on which the topology can be defined by the convergence of sequences, i.e., a space in which the first axiom of countability holds, a linear operator A is continuous iff for all sequences $\{\varphi_n\}$ with $\varphi_n \xrightarrow{\tau_{\mathbf{\Phi}}} 0$ it follows that $A\varphi_n \xrightarrow{\tau_{\mathbf{\Phi}}} 0$ (cf. Section 2.3.4). Since our topology $\tau_{\mathbf{\Phi}}$ satisfies the first axiom of countability, the operator $a^\dagger$ is continuous if from $\varphi_n \xrightarrow{\tau_{\mathbf{\Phi}}} 0$ it follows that $a^\dagger\varphi_n \xrightarrow{\tau_{\mathbf{\Phi}}} 0$:

To prove that $a^\dagger$ is $\tau_{\mathbf{\Phi}}$-continuous we use a lemma (see Appendix 3.7.4) that states that for every norm $\|\psi\|_p$ of (3.3.36) there is a real constant $\kappa < \infty$ such that

$$(\psi, a(N+I)^p a^\dagger \psi) \le \kappa(\psi, (N+I)^{p+1}\psi)\,, \quad \forall \psi \in \Psi\,. \tag{3.3.67}$$

Let $\psi_n \xrightarrow{\tau_{\mathbf{\Phi}}} 0$ as $n \to \infty$. Then $\|\psi_n\|_p \to 0$ for every $p = 0, 1, 2, \ldots$,

$$(\psi_n, (N+I)^p \psi_n) \to 0 \quad \text{for every } p = 0, 1, 2, \ldots \tag{3.3.68}$$

To show that $a^\dagger\psi_n \xrightarrow{\tau_{\mathbf{\Phi}}} 0$, we have to show that

$$\|a^\dagger \psi_n\|_q \to 0 \tag{3.3.69}$$

for every $q = 0, 1, 2, \ldots$, i.e., that

$$(a^\dagger\psi_n, (N+I)^q a^\dagger \psi_n) = (\psi_n, a(N+I)^q a^\dagger \psi_n) \to 0 \tag{3.3.70}$$

for every $q = 0, 1, 2, \ldots$ By (3.3.67)

$$(\psi_n, a(N+I)^q a^\dagger \psi_n) \le \kappa(\psi_n, (N+I)^{q+1}\psi_n)\,. \tag{3.3.71}$$

By (3.3.68) the right hand side of (3.3.71) tends to zero for every $q = 0, 1, 2, \ldots$, and consequently also the left hand side, which proves (3.3.70). Then $a^\dagger$ is continuous. The proof of the $\tau_{\mathbf{\Phi}}$-continuity of a is analogous.

We remark that the convergence of $\|a^\dagger\varphi_n\|_q \to 0$ as $n \to \infty$ for a fixed q follows from the convergence of $\|\varphi_n\|_{q+1} \to 0$. Therefore it is important to have a countably infinite rather than a finite number of norms; in the case of a finite number of norms, $a^\dagger$ is not a continuous operator, since the topology generated by a finite number of norms is equivalent to the topology generated by one norm. In particular, this implies that $a^\dagger$ cannot be a continuous operator with respect to the Hilbert space topology.

We have shown that a and $a^\dagger$, and therewith the elements of the algebra of observables, are $\tau_{\mathbf{\Phi}}$-continuous operators on the linear topological space Ψ. Their $\tau_{\mathbf{\Phi}}$-continuous extensions to $\mathbf{\Phi}$ are then unique. We denote the $\tau_{\mathbf{\Phi}}$-extensions of the operators a, $a^\dagger$, P, Q,

$H, \ldots$ to $\mathbf{\Phi}$ also by a, $a^\dagger$, P, Q, $H, \ldots$ Domain questions do not arise when we perform the algebraic operations, because the operators are defined on the whole space $\mathbf{\Phi}$, and because $\mathbf{\Phi}$ remains invariant under their action. It is worthwhile noting that the $\tau_{\mathbf{\Phi}}$-extension to $\mathbf{\Phi}$ of any operator A is the same as the Hilbert space extension of A to $\mathbf{\Phi}$.

The second aspect of the Dirac formalism, the existence of a complete set of eigenvectors, follows from the nuclear spectral theorem (see Section 3.5 below). In order to be able to apply this theorem to our example, we need to prove that the topology $\tau_{\mathbf{\Phi}}$ is nuclear.

Before introducing the notion of nuclear topology, we need the following definition: a bounded self-adjoint operator B defined on a Hilbert space $\mathcal{H}$ is Hilbert-Schmidt if B can be written as

$$B = \sum_{k=1}^{\infty} \lambda_k P_k \,, \tag{3.3.72}$$

where the P_k are projection operators (cf. Section 2.5.1) onto finite dimensional spaces $\mathcal{H}_k$ and $\sum_{k=1}^{\infty}(|\lambda_k| \dim \mathcal{H}_k)^2 < \infty$. Instead of giving the original definition of nuclear space (cf. Section 2.6.1), we shall use a theorem by Roberts (see [10]) which gives a necessary and sufficient condition for a space to be nuclear: a linear topological space $\mathbf{\Phi}$ is nuclear if there exists an e.s.a. $\tau_{\mathbf{\Phi}}$-continuous operator $A \in \mathcal{A}$, whose inverse is Hilbert-Schmidt.

It is now very easy to see that our $\mathbf{\Phi}$ is nuclear because N, and therefore $N + I$, is e.s.a., the spectrum of $(N + I)^{-1}$ is $(n + 1)^{-1}$, $n = 0, 1, 2, \ldots$, R_n is one dimensional and $\sum_{n=0}^{\infty} 1/(n + 1)^2 < \infty$. Thus $N + I$ is the operator that fulfills the above definition.

Having established that $\mathbf{\Phi}$ is nuclear, we can now adduce the nuclear spectral theorem to show that the essentially self-adjoint operators P and Q each has a complete set of eigenvectors in the sense of Dirac. Unlike the compact operators, for which such a set of vectors can be found from among the elements of the corresponding Hilbert space, the eigenvectors given by the nuclear spectral theorem neither reside in the space $\mathbf{\Phi}$ nor in $\mathcal{H}$. Instead, these vectors acquire mathematical sense as elements of the topological dual of $\mathbf{\Phi}$, and therewith the more precise terminology *generalized eigenvectors*. Before presenting the nuclear spectral theorem in Section 3.5 we shall discuss the dual space of $\mathbf{\Phi}$, the subject of the next section.

3.4 The RHS of the Harmonic Oscillator

3.4.1 The Conjugate Space

As mentioned above, the generalized eigenvectors of the Dirac basis vector expansion will be described by continuous antilinear functionals over the space $\mathbf{\Phi}$. This is the notion that we are about to present (see also Section 2.3.4).

An antilinear functional F on the linear space $\mathbf{\Phi}$ is a function $F(\varphi)$ from $\mathbf{\Phi}$ into the complex plane $\mathbb{C}$ which satisfies

$$F(\alpha\varphi + \beta\psi) = \overline{\alpha} F(\varphi) + \overline{\beta} F(\psi) \;, \quad \forall \varphi, \psi \in \mathbf{\Phi} \,, \; \forall \alpha, \beta, \in \mathbb{C} \,. \tag{3.4.1}$$

In the bra-ket notation $F(\varphi) = \langle\varphi|F\rangle$, Eq. (3.4.1) reads

$$\langle\alpha\varphi + \beta\psi|F\rangle = \overline{\alpha}\langle\varphi|F\rangle + \overline{\beta}\langle\psi|F\rangle\,. \tag{3.4.2}$$

In the space $\mathbf{\Phi}$, on which the topology $\tau_{\mathbf{\Phi}}$ is defined, we can use the notion of continuity with respect to this topology to introduce the concept of continuous mapping: a function F is continuous if the image of every convergent sequence is also convergent,

$$\varphi_n \xrightarrow[n\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \implies F(\varphi_n) \xrightarrow[n\to\infty]{\tau_{\mathbb{C}}} F(\varphi)\,, \tag{3.4.3}$$

where $\xrightarrow{\tau_{\mathbf{\Phi}}}$ indicates convergence with respect to the topology $\tau_{\mathbf{\Phi}}$ and $\xrightarrow{\tau_{\mathbb{C}}}$ means convergence in the sense of complex numbers.

A continuous antilinear functional F on $\mathbf{\Phi}$ is a function from $\mathbf{\Phi}$ into $\mathbb{C}$ that is antilinear and continuous. One can prove that a functional F on the countably Hilbert space $\mathbf{\Phi}$ is $\tau_{\mathbf{\Phi}}$-continuous iff there exist a positive constant K and a norm $\|\cdot\|_q$ among the collection of norms (3.3.36) that obey

$$|F(\varphi)| < K\|\varphi\|_q\,, \quad \forall\,\varphi \in \mathbf{\Phi}\,. \tag{3.4.4}$$

We now consider the collection of all continuous antilinear functionals over $\mathbf{\Phi}$, which is denoted by $\mathbf{\Phi}^\times$. The sum of two functionals and the multiplication of a functional by a number are defined by:

$$(\alpha F_1 + \beta F_2)(\varphi) = \alpha F_1(\varphi) + \beta F_2(\varphi)\,, \quad \forall\varphi \in \mathbf{\Phi}\,,\ \forall\alpha,\beta \in \mathbb{C}\,, \tag{3.4.5}$$

or in bra-ket notation

$$\langle\varphi|\alpha F_1 + \beta F_2\rangle = \alpha\langle\varphi|F_1\rangle + \beta\langle\varphi|F_2\rangle\,. \tag{3.4.6}$$

One can prove that if $F_1, F_2 \in \mathbf{\Phi}^\times$, i.e., if F_1 and F_2 satisfy (3.4.1) and (3.4.3), then $\alpha F_1 + \beta F_2$ is also in $\mathbf{\Phi}^\times$. Thus, $\mathbf{\Phi}^\times$ is a linear space under the operations defined by (3.4.5).

The dual space of the Hilbert space $\mathcal{H}$ can be constructed in a similar way. A function F from $\mathcal{H}$ into $\mathbb{C}$ is a $\tau_{\mathcal{H}}$-continuous antilinear functional if

1. F is antilinear,

$$F(\alpha f + \beta g) = \overline{\alpha}F(f) + \overline{\beta}F(g)\,, \quad \forall f,g \in \mathcal{H}\,,\ \forall\alpha,\beta \in \mathbb{C}\,. \tag{3.4.7}$$

2. F is $\tau_{\mathcal{H}}$-continuous,

$$f_n \xrightarrow{\tau_{\mathcal{H}}} f \implies F(f_n) \xrightarrow{\tau_{\mathbb{C}}} F(f)\,. \tag{3.4.8}$$

The adjoint space $\mathcal{H}^\times$ of $\mathcal{H}$ is the collection of all $\tau_{\mathcal{H}}$-continuous antilinear functionals over $\mathcal{H}$. The space $\mathcal{H}^\times$ can be endowed with a linear structure if the sum of two functionals and the multiplication of a functional by a number are defined as in (3.4.5).

From the relation $\mathbf{\Phi} \subset \mathcal{H}$, it can be shown that

$$\mathcal{H}^\times \subset \mathbf{\Phi}^\times\,. \tag{3.4.9}$$

Let $F \in \mathcal{H}^\times$. If $\{f_n\}$ is any sequence of elements of $\mathcal{H}$ that converges to $f \in \mathcal{H}$ with respect to $\tau_\mathcal{H}$, then $F(f_n)$ converges to $F(f)$,

$$f_n \xrightarrow{\tau_\mathcal{H}} f \implies F(f_n) \xrightarrow{\tau_\mathcal{H}} F(f)\,. \tag{3.4.10}$$

Let φ_n be a sequence of elements of $\mathbf{\Phi}$ that converges to $\varphi \in \mathbf{\Phi}$ with respect to $\tau_\mathbf{\Phi}$. Since $\varphi_n \xrightarrow{\tau_\mathbf{\Phi}} \varphi$ implies that $\varphi_n \xrightarrow{\tau_\mathcal{H}} \varphi$, if follows from (3.4.10) that $F(\varphi_n) \xrightarrow{\tau_\mathcal{H}} F(\varphi)$. Therefore,

$$\varphi_n \xrightarrow{\tau_\mathbf{\Phi}} \varphi \implies F(\varphi_n) \xrightarrow{\tau_\mathcal{H}} F(\varphi)\,, \tag{3.4.11}$$

which proves that $F \in \mathbf{\Phi}^\times$.

3.4.2 Construction of the Rigged Hilbert Space

We are now in a position to construct the Rigged Hilbert Space for the Harmonic Oscillator. We begin this construction considering the antilinear functional on $\mathcal{H}$ defined by

$$F_f(g) := (g, f)\,, \quad \forall g \in \mathcal{H}\,, \tag{3.4.12}$$

where f is a fixed element of $\mathcal{H}$. It is easy to see that F_f, which is determined by the vector $f \in \mathcal{H}$, fulfills the condition (3.4.7) if the function $(\,\cdot\,,\,\cdot\,)$ fulfills the conditions for a scalar product. Further, $F_f \in \mathcal{H}^\times$, i.e., it also fulfills (3.4.8). In order to prove this, we take a sequence g_n of elements of $\mathcal{H}$ that converges to $g \in \mathcal{H}$ with respect to $\tau_\mathcal{H}$. In a Hilbert space, the $\tau_\mathcal{H}$-convergence implies that

$$(g_n, h) \xrightarrow{\tau_\mathbb{C}} (g, h) \tag{3.4.13}$$

for each $h \in \mathcal{H}$. This scalar product convergence for each $h \in \mathcal{H}$ is called the weak convergence of g_n to g, in contrast to the norm convergence $g_n \xrightarrow{\tau_\mathcal{H}} g$ (called also strong convergence in $\mathcal{H}$). Applying Eq. (3.4.13) to f of (3.4.12), it follows that $F_f(g_n) \to F_f(g)$. Thus, Eq. (3.4.12) defines a $\tau_\mathcal{H}$-continuous antilinear functional for every $f \in \mathcal{H}$. Furthermore, the converse is also true (see Frechet-Riesz Theorem in Section 2.3.4), i.e., for every antilinear $\tau_\mathcal{H}$-continuous functional $F^{(\mathcal{H})} \in \mathcal{H}^\times$ there exists a unique vector $f_F \in \mathcal{H}$ such that

$$\langle g | F^{(\mathcal{H})} \rangle = F^{(\mathcal{H})}(g) = (g, f_F)\,, \quad \text{for every } g \in \mathcal{H}\,. \tag{3.4.14}$$

Therefore we can *identify* the Hilbert space $\mathcal{H}$ and its conjugate space $\mathcal{H}^\times$ by equating the functional $F^{(\mathcal{H})} \in \mathcal{H}^\times$ with the vector $f_F \in \mathcal{H}$ given by (3.4.14)

$$\mathcal{H}^\times \ni F^{(\mathcal{H})} \equiv f_F \in \mathcal{H}\,. \tag{3.4.15}$$

Then we have that

$$\Psi \subset \mathbf{\Phi} \subset \mathcal{H} \simeq \mathcal{H}^\times\,. \tag{3.4.16}$$

For $\tau_\mathcal{H}$-continuous functionals $F^{(\mathcal{H})}$ the symbols $\langle\,\cdot\,|\,\cdot\,\rangle$ and $(\,\cdot\,,\,\cdot\,)$ are equivalent after the identification $F^{(\mathcal{H})} \equiv f_F$. This identification is possible because the action of the functional $F^{(\mathcal{H})}$ at any vector $g \in \mathcal{H}$ is equal to the scalar product of g with f_F:

$$\langle g | F^{(\mathcal{H})} \rangle = \langle g | f_F \rangle = (g, f_F)\,. \tag{3.4.17}$$

In the bra-ket notation, the identification $F^{(\mathcal{H})} \equiv f_F$ is written as $|F^{(\mathcal{H})}\rangle \equiv |f_F)$ or even as $|F\rangle \equiv |f)$. However, for the class of $\tau_{\mathbf{\Phi}}$-continuous functionals F the symbol $\langle\varphi|F\rangle$ (the action of the functional F at the point φ) is equal to (φ, F) (the scalar product of φ and F) only if $F \in \mathcal{H}^\times$. That is,

$$\langle\varphi|F\rangle = \langle\varphi|F^{(\mathcal{H})}\rangle = (\varphi, F) \quad \text{only if } F \equiv F^{(\mathcal{H})} \in \mathcal{H}^\times . \tag{3.4.18}$$

From Eqs. (3.4.9) and (3.4.16), it follows that

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times . \tag{3.4.19}$$

This triplet of spaces is the Rigged Hilbert space (RHS) or the Gelfand Triplet for the Harmonic oscillator.

In the space $\mathbf{\Phi}^\times$, one can introduce various topologies and therewith various meanings of sequence convergence (cf. Section 2.4.2). An example is the weak topology, that is denoted by $\tau^\times$ or by τ_W (cf. Section 2.4.2). This topology leads to a meaning of sequence convergence that is analogous to the weak convergence in $\mathcal{H}$: a sequence of functionals $\{F_\gamma\}_{\gamma=1}^\infty \subset \mathbf{\Phi}^\times$ converges (weakly) to a functional F with respect to $\tau^\times$ if

$$\langle\varphi|F_\gamma\rangle \to \langle\varphi|F\rangle , \quad \text{for every } \varphi \in \mathbf{\Phi} . \tag{3.4.20}$$

However, this notion of sequence convergence does not specify the weak topology completely, i.e., $\tau^\times$ is not first countable.

Once $\mathbf{\Phi}^\times$ is equipped with the topology $\tau^\times$, we can construct its dual space, that is denoted by $\mathbf{\Phi}^{\times\times}$. The elements of $\mathbf{\Phi}^{\times\times}$ are the $\tau^\times$-continuous antilinear functionals $\widetilde{\varphi}$ on $\mathbf{\Phi}^\times$, i.e., the mappings $\widetilde{\varphi}$ from $\mathbf{\Phi}^\times$ into $\mathbb{C}$ that satisfy

1. $\widetilde{\varphi}$ is linear,

$$\widetilde{\varphi}(\alpha F_1 + \beta F_2) = \overline{\alpha}\widetilde{\varphi}(F_1) + \overline{\beta}\widetilde{\varphi}(F_2) , \quad \forall F_1, F_2 \in \mathbf{\Phi}^\times \text{ and } \forall \alpha, \beta \in \mathbb{C} , \tag{3.4.21}$$

   or in bra-ket notation

$$\langle \alpha F_1 + \beta F_2|\widetilde{\varphi}\rangle = \overline{\alpha}\langle F_1|\widetilde{\varphi}\rangle + \overline{\beta}\langle F_2|\widetilde{\varphi}\rangle . \tag{3.4.22}$$

2. $\widetilde{\varphi}$ is continuous with respect to $\tau^\times$.

The space $\mathbf{\Phi}^{\times\times}$ is also a linear topological space if addition and multiplication are defined by

$$\langle F|\alpha\widetilde{\varphi}_1 + \beta\widetilde{\varphi}_2\rangle = \alpha\langle F|\widetilde{\varphi}_1\rangle + \beta\langle F|\widetilde{\varphi}_2\rangle \tag{3.4.23}$$

and the (weak) convergence is defined by

$$\widetilde{\varphi}_\gamma \xrightarrow{\tau^{\times\times}} \widetilde{\varphi} \Leftrightarrow \langle F|\widetilde{\varphi}_\gamma\rangle \to \langle F|\widetilde{\varphi}\rangle \quad \text{for every } F \in \mathbf{\Phi}^\times . \tag{3.4.24}$$

One can prove that to each element $\varphi \in \mathbf{\Phi}$ there corresponds an antilinear continuous functional $\widetilde{\varphi}$ in $\mathbf{\Phi}^{\times\times}$ defined by

$$\widetilde{\varphi}(F) = \overline{F(\varphi)} , \tag{3.4.25}$$

or in the Dirac's notation

$$\langle F|\widetilde{\varphi}\rangle = \overline{\langle \varphi|F\rangle}\,. \tag{3.4.26}$$

Thus, we can identify every element $\widetilde{\varphi} \in \mathbf{\Phi}^{\times\times}$ with an element $\varphi \in \mathbf{\Phi}$ through (3.4.26) and vice versa. Further, it can be shown that the convergence defined by (3.4.24) is the same as the convergence with respect to $\tau_{\mathbf{\Phi}}$. Therefore, the spaces $\mathbf{\Phi}^{\times\times}$ and $\mathbf{\Phi}$ are, from a linear topological point of view, the same and can be identified

$$\mathbf{\Phi}^{\times\times} \simeq \mathbf{\Phi}\,. \tag{3.4.27}$$

The Hilbert space $\mathcal{H}$ certainly satisfies (3.4.27) because it already satisfies $\mathcal{H}^{\times} \simeq \mathcal{H}$. Since the functionals over $\mathcal{H}$ are given by (3.4.12), the Hilbert space relation that corresponds to the relation (3.4.26) is

$$(f,h) = \overline{(h,f)}\,, \tag{3.4.28}$$

which is a property of the scalar product.

3.4.3 Continuous Linear Operators on the Rigged Hilbert Space

The operators of the algebra of observables were assumed to be defined on the linear scalar product space Ψ. Later on, they were extended to the space $\mathbf{\Phi}$ in a unique way. We now extend their actions to the dual space $\mathbf{\Phi}^{\times}$. For every operator A on $\mathbf{\Phi}$, one can define the conjugate operator (also called the dual operator) $A^{\times}$ on $\mathbf{\Phi}^{\times}$ by

$$(A^{\times}F)(\varphi) := F(A\varphi)\,, \quad \forall\varphi \in \mathbf{\Phi}\,,\ \forall F \in \mathbf{\Phi}^{\times}\,, \tag{3.4.29}$$

or in bra-ket notation

$$\langle \varphi|A^{\times}|F\rangle = \langle A\varphi|F\rangle\,. \tag{3.4.30}$$

If A is a $\tau_{\mathbf{\Phi}}$-continuous operator on $\mathbf{\Phi}$, then $A^{\times}$ is a $\tau^{\times}$-continuous operator on $\mathbf{\Phi}^{\times}$. In particular, this implies that

$$A^{\times}F_{\gamma} \xrightarrow{\tau^{\times}} A^{\times}F \quad \text{whenever} \quad F_{\gamma} \xrightarrow{\tau^{\times}} F\,. \tag{3.4.31}$$

We have defined the notion of continuous operator through the notion of sequence convergence. This is possible only in spaces where the first axiom of countability is satisfied. The Hilbert space and the space $\mathbf{\Phi}$ are such spaces. In these cases, every continuous operator is bounded and every bounded operator is continuous. If the spaces are not first countable, the notion of continuity of an operator cannot be fully specified by the notion of sequence convergence. This is why in the space $\mathbf{\Phi}^{\times}$—that is not first countable—operators $A^{\times}$ that fulfill (3.4.31) are not necessarily bounded.

If a $\tau_{\mathbf{\Phi}}$-continuous operator A is also symmetric, then we have in correspondence to the relation (3.4.19) between the spaces the relation

$$A \subset \overline{A} \subset A^{\dagger} \subset A^{\times} \tag{3.4.32}$$

between the operators. When the operator A is also e.s.a., Eq. (3.4.32) becomes

$$A \subset \overline{A} = A^{\dagger} \subset A^{\times}\,. \tag{3.4.33}$$

In particular, the adjoint operators $P^{\times}$, $Q^{\times}$, $H^{\times}$ of the operators P, Q, H are $\tau^{\times}$-continuous operators on $\mathbf{\Phi}^{\times}$ and satisfy (3.4.33).

3.5 Basis Systems, Eigenvector Decomposition and the Gelfand-Maurin Theorem

The next section is presented a heuristic motivation for Dirac basis vector expansion. The mathematical details are covered in Section 3.5.2.

3.5.1 Basis Systems and Eigenvector Decomposition—a Heuristic Introduction

The simplest example of basis system and eigenvector decomposition is given by the three-dimensional space $\mathbb{R}^3$. In $\mathbb{R}^3$ it is customary to choose a system of three orthonormal vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ satisfying

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}\,, \quad i,j = 1,2,3\,, \tag{3.5.1}$$

where $\mathbf{e}_i \cdot \mathbf{e}_j$ is the scalar product of $\mathbf{e}_i$ and $\mathbf{e}_j$ and δ_{ij} is the Kronecker delta defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j\,. \end{cases} \tag{3.5.2}$$

The basis system fulfilling (3.5.1) can be chosen somewhat arbitrarily. But it is convenient to choose it in such a way that the particular physical problem under consideration takes its simplest mathematical form. For example, if one describes a three-dimensional rigid body with moment of inertia tensor $\mathbb{I}$, then it is useful to choose the basis system $\{\mathbf{e}_i\}$ such that

$$\mathbf{e}_i \cdot \mathbb{I} \cdot \mathbf{e}_j = \mathrm{I}_{(j)}\delta_{ij}, \tag{3.5.3}$$

i.e., to choose the $\{\mathbf{e}_i\}$ to be eigenvectors of the (rank 2) tensor $\mathbb{I}$. Every vector $\mathbf{v} \in \mathbb{R}^3$ can be expanded with respect to this basis system of eigenvectors of $\mathbb{I}$,

$$\mathbf{v} = \sum_{i=1}^{3} \mathbf{e}_i\, v_i\,, \tag{3.5.4}$$

where the $v_i = \mathbf{e}_i \cdot \mathbf{v}$ are the *coordinates* (or *components*) of the vector $\mathbf{v}$ with respect to the basis $\{\mathbf{e}_i\}$ of eigenvectors of the symmetric tensor $\mathbb{I}$.

In analogy to the three-dimensional space $\mathbb{R}^3$, one introduces a system of basis vectors in a general linear space $\mathbf{\Phi}$. If $\mathbf{\Phi}$ is an N-dimensional linear space, then there are N linearly independent vectors $\{e_i\}_{i=1}^N$ that form an orthonormal basis system for $\mathbf{\Phi}$. We denote these basis vectors e_i also by $|e_i)$. The scalar products of the elements of the basis system are written in one of the following ways:

$$e_i \cdot e_j \equiv (e_i, e_j) \equiv (e_i|e_j) = \delta_{ij}, \qquad i,j = 1,2,\ldots,N\,. \tag{3.5.5}$$

As the basis system for the space $\mathbf{\Phi}$, it is often extremely convenient to choose the eigenvectors of an operator A which represents an important observable (most frequently one

chooses the energy operator H, the position operator Q or the momentum operator P). Therefore, one seeks a set of basis vectors $e_i \in \mathbf{\Phi}$ which also fulfill

$$Ae_i = a_i e_i \tag{3.5.6}$$

for some $a_i \in \mathbb{C}$. These eigenvectors are often labeled by their eigenvalues a_i and denoted by

$$e_i \equiv |a_i)\,. \tag{3.5.7}$$

It can be proven that if A is a Hermitian operator on an N-dimensional space $\mathbf{\Phi}$, then there exists an orthonormal basis system of eigenvectors of A,

$$A|a_i) = a_i|a_i)\,, \qquad i = 1, 2, \ldots, N\,, \tag{3.5.8}$$

$$(a_i|a_j) = \delta_{ij}\,, \qquad i, j = 1, 2, \ldots, N\,, \tag{3.5.9}$$

such that every vector $\varphi \in \mathbf{\Phi}$ can be written as

$$\varphi = \sum_{i=1}^{N} |a_i)(a_i|\varphi)\,. \tag{3.5.10}$$

This result is the spectral theorem for a Hermitian operator A defined on a finite dimensional scalar product space $\mathbf{\Phi}$. Eq. (3.5.10) is called the *spectral decomposition* of the vector φ or the *eigenvector expansion* of φ with respect to the basis system $\{|a_i)\}$. The complex numbers

$$\varphi_i \equiv (a_i|\varphi) \tag{3.5.11}$$

are the *components* of the vector φ with respect to the basis $\{|a_i)\}$. The set of a_i's (which are real if A is Hermitian) is called the *spectrum* of A.

In general, the dimension of the linear space $\mathbf{\Phi}$ is not finite. In this case, the above result cannot be applied, and a proper generalization to the infinite dimensional case is needed. In this infinite dimensional case, there are two possibilities depending on the spectrum of the observable upon consideration. When the possible measurements of an observable are elements of a discrete set of numbers, then only a discrete set of eigenvalues is necessary. In this case, only an infinite dimensional generalization of (3.5.8)-(3.5.10) is needed. However, there seem to be observables in physics whose possible measurements are elements of a continuous set of numbers (e.g., the momentum and position can, in many cases, take any real value). In this second case, we need not only the infinite dimensional generalization of (3.5.8)-(3.5.10) but also the continuous infinite dimensional generalization. This generalization is the Dirac basis vector expansion (cf. [1]) or, in mathematical terms, the Gelfand-Maurin Theorem (cf. [5]). This theorem is valid under certain conditions on the space $\mathbf{\Phi}$. Since the eigenvector decomposition is essential in quantum physics, we will only consider spaces for which this theorem holds.

To explain the Gelfand-Maurin Theorem in detail requires much more mathematics. These mathematics are provided in Section 3.5.2. In this section, we just give an intuitive statement, which can be accepted in analogy to (3.5.10).

We consider the cases of an infinite discrete number of eigenvalues and a continuous set of eigenvalues in parallel. The self-adjoint operator with discrete spectrum will be called H. Its spectrum will consist of the infinitely many real eigenvalues E_n, $n = 0, 1, 2, \ldots$ The self-adjoint operator with continuous spectrum will be denoted by Q.[2] The spectrum of Q will be the continuous interval of real numbers $[m, M]$. Then the (heuristic) spectral theorem asserts:

There exists a system of eigenvectors, $|E_n)$ in the discrete case and $|x\rangle$ in the continuous case,

$$H|E_n) = E_n|E_n), \quad n = 0, 1, 2, \ldots, \tag{3.5.12}$$

$$Q|x\rangle = x|x\rangle, \quad -\infty < m \leq x \leq M < +\infty, \tag{3.5.13}$$

such that *every* $\varphi \in \mathbf{\Phi}$ can be expanded in terms of these eigenvectors,

$$\varphi = \sum_{n=0}^{\infty} |E_n)(E_n|\varphi), \tag{3.5.14}$$

$$\varphi = \int_m^M dx|x\rangle\langle x|\varphi\rangle\,, \tag{3.5.15}$$

and $\varphi = 0$ if and only if all its components are zero, i.e., $(E_n|\varphi) = 0$ for all E_n or $\langle x|\varphi\rangle = 0$ for all x.[3] A system of eigenvectors $|E_n)$ or $|x\rangle$ with these properties is called *complete* or a *basis system*. The $|x\rangle$ are called *kets*, the $\langle x|$ are called *bras* and the $\langle x|\varphi\rangle$ are called bra-kets (see [1]). The bra-ket $\langle x|\varphi\rangle$ is a generalization of the usual scalar product.

Thus the spectral theorem asserts the existence of a complete system of eigenvectors of a self-adjoint operator. $(E_n|\varphi)$ or $\langle x|\varphi\rangle$ are called the coordinates or components of φ with respect to the basis system $\{|E_n)\}$ or $\{|x\rangle\}$. They can be thought of, in analogy to the N-dimensional case stated in Eq. (3.5.11), as the scalar products of the eigenvectors with the vector φ

$$(E_n|\varphi) = (|E_n), \varphi)\,, \tag{3.5.16}$$

$$\langle x|\varphi\rangle = (|x\rangle, \varphi)\,. \tag{3.5.17}$$

Thus the $(E_n|\varphi)$ are the discrete infinite dimensional generalization of the φ_i in (3.5.11), and the $\langle x|\varphi\rangle$ are the continuous infinite dimensional generalizations of the φ_i.

Whereas the $|E_n)$ are proper eigenvectors, i.e., they are normalizable, the $|x\rangle$ are not. This is why the $|x\rangle$ are called generalized eigenvectors or *eigenkets* and denoted by corner-kets $|\cdot\rangle$, in contrast to the normalizable eigenvectors $|E_n)$, that are denoted by round-kets $|\cdot)$. Though we can manipulate the corner-kets as if they were proper eigenvectors,

[2]For instance, H can be the Hamiltonian for the harmonic oscillator and Q the position operator for the harmonic oscillator.

[3]The simple nondegenerate form (3.5.14), (3.5.15) is valid if the operator A (H or Q) is cyclic, i.e., if there exists an $f \in \mathbf{\Phi}$ such that $\{A^n f \equiv f_{(n)}\}$ spans the entire space $\mathbf{\Phi}$. This means that any $\varphi \in \mathbf{\Phi}$ can be written as $\varphi = \sum_n f_{(n)} c_{(n)}$, where $c_{(n)}$ are complex numbers. Degenerate spectra, which occur when more than one quantum number is needed, will be discussed in Section 3.7.2.

mathematically there is an important difference between the discrete basis vectors $|E_n)$ and the continuous basis vectors $|x\rangle$: the $|E_n)$ are in $\mathbf{\Phi}$ while the $|x\rangle$ are in $\mathbf{\Phi}^\times$, the space of continuous antilinear functionals over $\mathbf{\Phi}$. Further, $(E_n|\varphi)$ is indeed the scalar product of the normalized vector $|E_n)$ with φ, whereas $\langle x|\varphi\rangle$ is the action of the functional $|x\rangle$ at the vector φ.

If an operator H has discrete spectrum E_n, $n = 0, 1, 2 \ldots$, then all the corresponding eigenvectors $|E_n)$ enter into the discrete basis vector expansion (3.5.14) and there are no other eigenvectors that enter into this basis vector expansion. If an operator Q has a continuous spectrum, then in general—and this depends upon the properties of the space $\mathbf{\Phi}$—there are more generalized eigenvectors of Q (i.e., more kets which fulfill (3.5.13)) than appear in the eigenvector expansion (3.5.15). Whereas the discrete eigenvalues of a self-adjoint operator are always real, the generalized eigenvalues of a self-adjoint operator need not be real. They can be real or complex, and even if they are real, they do not necessarily belong to the spectrum, i.e., appear in the integral (3.5.15). However, for a self-adjoint operator there is always a real subset of the set of generalized eigenvalues such that the set of corresponding eigenvectors is complete.

The most general form of the spectral theorem for an operator A representing a physical observable is a combination of (3.5.14) and (3.5.15)

$$\varphi = \sum_i |a_i)(a_i|\varphi) + \int da|a\rangle\langle a|\varphi\rangle\,, \tag{3.5.18}$$

where the sum runs over the discrete spectrum of A and the integral runs over the continuous spectrum of A.[4] This is the case for the Hamiltonian of the hydrogen atom. It is possible that some or all of the values a_i appearing in the sum also appear in the integral. In that case, they are called discrete eigenvalues embedded in the continuous spectrum. If this happens for a_k, then $|a_k)$ is still orthogonal to all the $|a\rangle$ including $|a_k\rangle$

$$(a_k|a\rangle = 0\,, \quad (a_k|a_k\rangle = 0\,. \tag{3.5.19}$$

To see that the coordinates $(E_n|\varphi)$ are indeed what their notation indicates, namely the scalar product of the vector φ with the basis vector $|E_n)$, we calculate the scalar product of (3.5.14) with the eigenvector $|E_m)$:

$$(|E_m), \varphi) = \sum_{n=0}^{\infty} (|E_m), |E_n))(E_n|\varphi)\,. \tag{3.5.20}$$

[4]The nuclear spectral theorem for an arbitrary self-adjoint operator actually does not assert (3.5.18) but rather (3.5.43) with a general measure $d\mu(x)$, and it does not say anything about the spectral measure $d\mu(x)$ in addition to the assertion of its existence. However, all operators used in this dissertation are of the special kind that either $d\mu(x) = \rho(x)dx$ with $\rho(x)$ a positive smooth measurable function (such operators are said to have an absolutely continuous spectrum) or $d\mu(x) = \sum_i \delta(x - x_i)dx$ (these are the operators with discrete spectrum), or they have both an absolutely continuous and a discrete spectrum. So (3.5.18), after a normalization change (3.5.45), is the most general form used in this dissertation.

Since $|E_m)$ and $|E_n)$ are eigenvectors of the same Hermitian operator H,

$$(|E_m), |E_n)) = 0 \quad \text{if } E_n \neq E_m \,. \tag{3.5.21}$$

For $E_n = E_m$ we normalize them

$$(|E_n), |E_n)) = \| \, |E_n) \, \|^2 = 1 \,. \tag{3.5.22}$$

We combine (3.5.21) and (3.5.22) and obtain

$$(|E_m), |E_n)) = (E_m|E_n) = \delta_{E_n E_m} = \delta_{nm} \,, \quad n, m = 0, 1, 2, \ldots . \tag{3.5.23}$$

Thus, the eigenvectors of the self-adjoint operator H have the property (3.5.5) as required for orthonormal basis vectors. Inserting (3.5.23) into (3.5.20) one obtains

$$(|E_m), \varphi) = \sum_{n=0}^{\infty} \delta_{mn} (E_n|\varphi) = (E_m|\varphi) \,. \tag{3.5.24}$$

This is the expected identity (3.5.16).

The spectral theorem (3.5.14) leads to other spectral decompositions: one can omit the arbitrary vector $\varphi \in \mathbf{\Phi}$ on both sides of (3.5.14) and obtain the *spectral resolution of the identity operator I*

$$I = \sum_{n=0}^{\infty} |E_n)(E_n| \,, \tag{3.5.25}$$

where the quantities $|E_n)(E_n|$ are called *projection operators*. One can also apply the operator H to both sides of (3.5.14)

$$H\varphi = \sum_{n=0}^{\infty} H|E_n)(E_n|\varphi) = \sum_{n=0}^{\infty} E_n|E_n)(E_n|\varphi) \,, \tag{3.5.26}$$

and then omit the arbitrary vector φ on both sides

$$H = \sum_{n=0}^{\infty} E_n|E_n)(E_n| \,. \tag{3.5.27}$$

This identity between the operator H and the weighted sum of projection operators $|E_n)(E_n|$ is called the *spectral resolution* of the self-adjoint operator H with a discrete spectrum.

The scalar product of any two elements $\varphi, \psi \in \mathbf{\Phi}$ can be written in terms of the components of these vectors along the basis vectors $|E_n)$ as

$$(\psi, \varphi) = \sum_{n=0}^{\infty} (\psi|E_n)(E_n|\varphi) = \sum_{n=0}^{\infty} \overline{(E_n|\psi)} \, (E_n|\varphi) \,. \tag{3.5.28}$$

In particular, if one chooses $\psi = \varphi$, then one obtains

$$\|\varphi\|^2 = (\varphi, \varphi) = \sum_{n=0}^{\infty} (\varphi|E_n)(E_n|\varphi) = \sum_{n=0}^{\infty} |(E_n|\varphi)|^2. \tag{3.5.29}$$

Equation (3.5.28) is the analog to the formula

$$\mathbf{v} \cdot \mathbf{x} = \sum_{i,j=1}^{3} v_i \, \mathbf{e}_i \cdot \mathbf{e}_j \, x_j = \sum_{i=1}^{3} v_i \, x_i \tag{3.5.30}$$

for the ordinary scalar product in $\mathbb{R}^3$.

In the three-dimensional space $\mathbb{R}^3$, a vector $\mathbf{v}$ is specified by its components (v_1, v_2, v_3) with respect to the basis system $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. Moreover, any sequence of three real numbers (v_1, v_2, v_3) determines a vector $\mathbf{v}$. In the discrete infinite dimensional case, any vector φ is also completely specified by its components $(E_n|\varphi)$ with respect to a given basis $|E_n)$. But, unlike the three-dimensional case, the sequence of components

$$((E_0|\varphi), (E_1|\varphi), (E_2|\varphi), \ldots, (E_n|\varphi), \ldots) \tag{3.5.31}$$

is not arbitrary but has to fulfill

$$\sum_{n=0}^{\infty} |(E_n|\varphi)|^2 < \infty \,, \tag{3.5.32}$$

i.e., it must be *square summable* (cf. Eq. (3.5.29)). The sequence (3.5.31) is called the *realization* of φ by the sequence of its components. In the case of a Hilbert space $\mathcal{H}$, each $\varphi \in \mathcal{H}$ is associated to a sequence of components (3.5.31) that fulfills (3.5.32), and $\mathcal{H}$ is said to be realized by the space of infinite square summable sequences.

The elements of the space $\mathbf{\Phi}$ are usually required to satisfy further conditions besides (3.5.32). The $\varphi \in \mathbf{\Phi}$ must be such that every operator A representing a physical observable is defined on the whole space $\mathbf{\Phi}$. This implies that $A\varphi$ must be well defined for each $\varphi \in \mathbf{\Phi}$, i.e., $(A\varphi, A\varphi)$ must be finite. If the observable under consideration is represented by the operator H, then H and all of its powers must be well defined on $\mathbf{\Phi}$, i.e., $(H^p\varphi, H^p\varphi)$ must be finite for each $p = 0, 1, 2, \ldots$ This leads to

$$\begin{aligned} (H^p\varphi, H^p\varphi) &= \sum_{n=0}^{\infty} (\varphi|H^p|E_n)(E_n|H^p|\varphi) \\ &= \sum_{n=0}^{\infty} E_n^{2p} |(E_n|\varphi)|^2 < \infty \qquad \text{for any } p = 0, 1, 2, \ldots \end{aligned} \tag{3.5.33}$$

Thus, not only $\{(E_n|\varphi)\}_{n=0}^{\infty}$ but also $\{E^p(E_n|\varphi)\}_{n=0}^{\infty}$, $p = 1, 2, \ldots$, have to be square summable for any $\varphi \in \mathbf{\Phi}$. When each element of a space $\mathbf{\Phi}$ is associated to a sequence

$$\varphi \leftrightarrow (\,(E_0|\varphi), (E_1|\varphi), \ldots, (E_n|\varphi), \ldots) \tag{3.5.34}$$

which fulfills (3.5.33), we say that $\mathbf{\Phi}$ is realized by the space of *rapidly decreasing* infinite sequences.

We now turn to the continuous spectrum case and repeat the above considerations for this case. We calculate the scalar product of φ with the generalized eigenvector $|x\rangle$ [5] using Eq. (3.5.15)

$$(|x\rangle, \varphi) = \int_{-\infty}^{+\infty} dy\, (|x\rangle, |y\rangle)\, \langle y|\varphi\rangle\,, \tag{3.5.35}$$

where we have assumed that the continuous spectrum runs over the whole real line (which is the case for e.g. the position operator Q of the harmonic oscillator). Using the definition

$$\langle x|y\rangle \equiv (|x\rangle, |y\rangle)\,, \tag{3.5.36}$$

Eq. (3.5.35) can be rewritten as

$$(|x\rangle, \varphi) = \int_{-\infty}^{+\infty} dy\, \langle x|y\rangle\langle y|\varphi\rangle\,. \tag{3.5.37}$$

In analogy to the N-dimensional case (3.5.10), $\langle x|\varphi\rangle$ is the component of the vector φ along the direction of the basis vector $|x\rangle$, while $(|x\rangle, \varphi)$ is the "scalar product" of φ with the basis vector $|x\rangle$. This analogy also suggests that the component of φ along $|x\rangle$ should be given by the "scalar product" of φ with $|x\rangle$, i.e., it should be of the form $\langle x|\varphi\rangle \equiv (|x\rangle, \varphi)$. Then, one would have

$$\langle x|\varphi\rangle = \int_{-\infty}^{+\infty} dy\, \langle x|y\rangle\, \langle y|\varphi\rangle\,. \tag{3.5.38}$$

The components $\langle y|\varphi\rangle$ are functions of the continuous variable y in the same way as the scalar products $(E_n|\varphi)$ are functions of the discrete variable E_n. Equation (3.5.38) therefore says that the mathematical quantity $\langle x|y\rangle$ has the property that it maps the function $\varphi(y) = \langle y|\varphi\rangle$ by integration into $\varphi(x) = \langle x|\varphi\rangle$, its value at the fixed point x. There is no well-behaved (or even a locally integrable) function $\langle x|y\rangle$ which has the property (3.5.38).

Quantities like $\langle x|y\rangle$, which are defined by integration, are called *distributions* or *generalized functions* (see, for example, [67]). The distribution $\langle x|y\rangle$ *defined* by (3.5.38) is called the *Dirac delta function* (though it is not a function). It is denoted in analogy to (3.5.23) by

$$\langle x|y\rangle = \delta(x-y)\,. \tag{3.5.39}$$

$\delta(x-y)$ is the continuous analog to $\delta_{E_nE_m}$: the Kronecker delta is usually defined by (3.5.2), but it could as well have been defined as the function that maps any sequence $\{(E_n|\varphi)\}$ by summation into $(E_m|\varphi)$, the m-th component of the sequence,

$$(E_m|\varphi) = \sum_{n=0}^{\infty} \delta_{E_mE_n}(E_n|\varphi)\,. \tag{3.5.40}$$

[5] More precisely, we should say that we calculate the value $(|x\rangle, \varphi)$ of the functional $|x\rangle$ at the vector $\varphi \in \mathbf{\Phi}$.

Defining the Kronecker delta by (3.5.40) gives a clearer analogy to (3.5.38).

The $|x\rangle$ are not dimensionless. They have the dimension $1/\sqrt{\dim(dx)}$. For example, if dx has the dimension cm, then $\langle x'|x\rangle$ has the dimension cm^{-1}, and $|x\rangle$ has the dimension $\mathrm{cm}^{-1/2}$.

The eigenvectors $|E_n)$ are normalized according to (3.5.23). The normalization (3.5.39) for the generalized eigenvectors $|x\rangle$ is called δ-function normalization.

Instead of the generalized eigenvectors with δ-function normalization (3.5.39), one can also choose generalized eigenvectors of Q with a different normalization. One can define a new set of generalized eigenvectors by

$$|x\}_\rho := |x\rangle \frac{1}{\sqrt{\rho(x)}}\,, \tag{3.5.41}$$

where $\rho(x)$ is a real nonnegative and integrable function. These new kets are still eigenvectors of the operator Q,

$$Q|x\}_\rho = x|x\}_\rho\,. \tag{3.5.42}$$

Now instead of (3.5.15), the eigenfunction expansion in terms of the $|x\}_\rho$ kets reads

$$\varphi = \int d\mu(x)\; |x\}_\rho \; {}_\rho\{x|\varphi\rangle\,, \tag{3.5.43}$$

where $d\mu(x) = \rho(x)\,dx$. In order for the new components of φ (the ${}_\rho\{x|\varphi\rangle$) to be the scalar product of φ with the new eigenvectors $|x\}_\rho$, i.e., in order that

$${}_\rho\{x|\varphi\rangle = \int d\mu(y)\; {}_\rho\{x|y\}_\rho \; {}_\rho\{y|\varphi\rangle\,, \tag{3.5.44}$$

one has to demand

$$d\mu(y)\; {}_\rho\{x|y\}_\rho = dy\,\langle x|y\rangle = dy\,\delta(x-y)\,. \tag{3.5.45}$$

So, the normalization of the new generalized eigenvectors is

$${}_\rho\{x|y\}_\rho = \Big(\frac{d\mu(y)}{dy}\Big)^{-1}\delta(x-y) = \rho^{-1}(y)\delta(x-y). \tag{3.5.46}$$

Thus, when the integration contains the weight function $\rho(x)$, the generalized eigenvector normalization will contain the factor $\rho^{-1}(x)$.

The most appropriate choice for $\rho(x)$ depends upon the property of the operator Q and its relation to the other operators of the problem. The choice $\rho(x) = 1$ is not always the most convenient. For instance, it may be convenient to choose $\rho(x)$ in such a way that the measure $d\mu(x)$ in (3.5.43) is invariant under some important symmetry transformation of the physical system.

The scalar product of $\varphi \in \mathbf{\Phi}$ with $\psi \in \mathbf{\Phi}$ is given in the notation of (3.5.38) by

$$(\psi,\varphi) = \langle\psi|\varphi\rangle = \int_{-\infty}^{+\infty} dx\,\langle\psi|x\rangle\,\langle x|\varphi\rangle\,. \tag{3.5.47}$$

In the same way

$$(\varphi, \psi) = \int_{-\infty}^{+\infty} dx \, \langle \varphi | x \rangle \, \langle x | \psi \rangle \, . \tag{3.5.48}$$

Taking complex conjugates on both sides of (3.5.48), we get

$$\overline{(\varphi, \psi)} = \int_{-\infty}^{+\infty} dx \, \overline{\langle \varphi | x \rangle} \, \overline{\langle x | \psi \rangle} \, . \tag{3.5.49}$$

But the scalar product fulfills

$$(\psi, \varphi) = \overline{(\varphi, \psi)} \, . \tag{3.5.50}$$

Thus, comparing (3.5.47) and (3.5.49) we see that the following relation is natural:

$$\langle x | \psi \rangle = \overline{\langle \psi | x \rangle} \, , \quad \psi \in \mathbf{\Phi} \, , \ |x\rangle \in \mathbf{\Phi}^{\times} \, . \tag{3.5.51}$$

Using the notation

$$\langle x | \varphi \rangle \equiv \varphi(x) \tag{3.5.52}$$

and (3.5.51), one can write (3.5.47) in the form

$$(\psi, \varphi) = \int_{-\infty}^{+\infty} dx \, \overline{\psi(x)} \, \varphi(x) \, . \tag{3.5.53}$$

In particular, if one chooses $\psi = \varphi$, one obtains

$$\|\varphi\|^2 = (\varphi, \varphi) = \int_{-\infty}^{+\infty} dx \, \overline{\varphi(x)} \, \varphi(x) = \int_{-\infty}^{+\infty} dx \, |\varphi(x)|^2 . \tag{3.5.54}$$

This implies that the components of a vector $\varphi \in \mathbf{\Phi}$ with respect to the continuous basis system $|x\rangle$ cannot be given by any arbitrary function $\varphi(x)$. Rather, they can be given only by those functions for which the integral on the right-hand side of Eq. (3.5.54) exists, i.e., the functions $\varphi(x)$ must be at least square integrable.

The association of φ with its components

$$\mathbf{\Phi} \ni \varphi \leftrightarrow \langle x | \varphi \rangle = \varphi(x) \tag{3.5.55}$$

is called the *realization* of the space $\mathbf{\Phi}$ by the space of functions $\varphi(x)$. The function $\varphi(x) = \langle x | \varphi \rangle$ is called the *wave function* of the vector φ; in particular, if Q is the position operator, then $\varphi(x)$ is called the *position wave function*.

If the integrals in (3.5.53) and (3.5.54) are ordinary Riemann integrals, then the linear space of functions $\varphi(x)$ is not complete with respect to the norm defined by (3.5.54). This means that there will be sequences of functions $\psi_n(x)$ that are Cauchy sequences,

$$\|\psi_n - \psi_m\|^2 = \int_{-\infty \, \text{Riemann}}^{+\infty} dx \, |\psi_n(x) - \psi_m(x)|^2 \to 0 \quad \text{as } n, m \to \infty \, , \tag{3.5.56}$$

but for which there exists no function $\psi(x)$ which is the limit element of that sequence,

$$\|\psi_n - \psi\|^2 = \int_{-\infty\,\text{Riemann}}^{+\infty} dx\, |\psi_n(x) - \psi(x)|^2 \to 0 \quad \text{as } n \to \infty\,. \tag{3.5.57}$$

In order to obtain a complete space of functions with respect to the scalar product (3.5.53), one has to replace the Riemann integrals in (3.5.56) and in (3.5.57) by Lebesgue integrals. Then, for any sequence of (Lebesgue) square integrable functions $\psi_n(x)$ satisfying

$$\|\psi_n - \psi_m\|^2 = \int_{-\infty\,\text{Lebesgue}}^{+\infty} dx\, |\psi_n(x) - \psi_m(x)|^2 \to 0 \quad \text{as } n, m \to \infty\,, \tag{3.5.58}$$

there is always a (Lebesgue) square integrable function $\psi(x)$ satisfying

$$\|\psi_n - \psi\|^2 = \int_{-\infty\,\text{Lebesgue}}^{+\infty} dx\, |\psi_n(x) - \psi(x)|^2 \to 0 \quad \text{as } n \to \infty\,. \tag{3.5.59}$$

The (complete) space of Lebesgue square integrable functions is denoted by $L^2(\mathbb{R})$. Just like the space of infinite square summable sequences, the space $L^2(\mathbb{R})$ of square integrable functions is a realization of the Hilbert space.

The elements of the space $\mathbf{\Phi}$ of physical states φ are required, in addition to be square normalizable, to be such that the operator Q and all of its powers be well defined on every $\varphi \in \mathbf{\Phi}$. Then one must have

$$\|Q^p\varphi\|^2 = (Q^p\varphi, Q^p\varphi) = \int_{-\infty}^{+\infty} dx\, x^{2p} |\varphi(x)|^2 < \infty\,, \quad p = 0, 1, 2, \ldots \tag{3.5.60}$$

Thus, the functions $\varphi(x)$ that belong to the realization that fulfills (3.5.60) must decrease faster than any power of $1/x$. If other operators are also to be defined everywhere on $\mathbf{\Phi}$, further conditions will have to be imposed on the components $\langle x|\varphi\rangle$ of $\varphi \in \mathbf{\Phi}$. Consequently, the realization of $\mathbf{\Phi}$ by a space of functions must be a subset of $L^2(\mathbb{R})$.

For instance, we can define a linear operator P on the space $\mathbf{\Phi}$ by giving a prescription for its action on each function $\varphi(x)$ which realizes a vector $\varphi \in \mathbf{\Phi}$. Let this operator be defined by

$$\langle x|\varphi\rangle \to \langle x|P\varphi\rangle := \frac{1}{i}\frac{d}{dx}\langle x|\varphi\rangle \tag{3.5.61}$$

for every $\varphi \in \mathbf{\Phi}$. We also define, according to (3.5.13), the operator Q on $\mathbf{\Phi}$ by

$$\langle x|\varphi\rangle \to \langle x|Q\varphi\rangle := x\,\langle x|\varphi\rangle \tag{3.5.62}$$

for each $\varphi \in \mathbf{\Phi}$. If we demand that Q^p and P^p, $p = 0, 1, 2, \ldots$, are well defined at every $\varphi \in \mathbf{\Phi}$, then the functions $\varphi(x)$ must be infinitely differentiable, rapidly decreasing functions, i.e., in addition to (3.5.60) the $\varphi(x)$ must be in $C^\infty(\mathbb{R})$ and must satisfy

$$\|P^p\varphi\|^2 = (P^p\varphi, P^p\varphi) = \int_{-\infty}^{+\infty} dx \left|\frac{d^p\varphi(x)}{dx^p}\right|^2 < \infty\,, \quad p = 0, 1, 2, \ldots \tag{3.5.63}$$

The requirement that $Q^q P^p \varphi$, $q, p = 0, 1, 2, \ldots$, is well defined leads to the conditions

$$\|Q^q P^p \varphi\|^2 = \int_{-\infty}^{+\infty} dx \left| x^q \frac{d^p \varphi(x)}{dx^p} \right|^2 < \infty \,, \quad p, q = 0, 1, 2, \ldots \,. \tag{3.5.64}$$

This means that the realization of the space $\mathbf{\Phi}$ is the linear space of infinitely differentiable complex-valued functions which together with their derivatives vanish at infinite more rapidly than any power of $1/x$. This space is the *Schwartz space* $\mathcal{S}(\mathbb{R})$, and we call these functions *well behaved*. Conditions (3.5.64) are equivalent to

$$\lim_{x \to \pm\infty} x^n \frac{d^m}{dx^m} \varphi(x) = 0 \,, \quad n, m = 0, 1, 2, \ldots \tag{3.5.65}$$

The space $\mathcal{S}(\mathbb{R})$ is not complete with respect to the norm convergence defined through (3.5.54). In fact, its completion with respect to this norm is the space $L^2(\mathbb{R})$. However, $\mathcal{S}(\mathbb{R})$ is a complete countably Hilbert space with respect to the topology generated by the countable number of scalar products

$$(\psi, \varphi)_p := (\psi, (P^2 + Q^2 + \frac{1}{2} I)^p \varphi) = \int_{-\infty}^{\infty} dx\, \overline{\psi(x)} \left(-\frac{d^2}{dx^2} + x^2 + \frac{1}{2} \right)^p \varphi(x) \,, \quad p = 0, 1, 2, \ldots \tag{3.5.66}$$

A sequence $\varphi_n \in \mathcal{S}(\mathbb{R})$ converges to $\varphi \in \mathcal{S}(\mathbb{R})$ with respect to this topology if

$$\|\varphi_n - \varphi\|_p \xrightarrow[n \to \infty]{} 0 \,, \quad p = 0, 1, 2, \ldots \,, \tag{3.5.67}$$

where $\|\varphi\|_p = \sqrt{(\varphi, \varphi)_p}$.

In Section 3.6.3, we shall show that the Schwartz space is the realization of the space $\mathbf{\Phi}$ for the harmonic oscillator.

The Lebesgue integral, though mathematically well defined, is not easy to handle in practical computations, while Riemann integrations are easy to calculate. In physics, the Riemann integral is the one that is exclusively used to perform computations. The Hilbert space uses Lebesgue integration, whereas the space $\mathbf{\Phi}$ uses Riemann integration. This makes $\mathbf{\Phi}$ a much simpler space to work with and much more suitable for representing the physical wave functions than the Hilbert space. As an example, the integrals (3.5.54) in $L^2(\mathbb{R})$ are Lebesgue integrals, whereas the integrals (3.5.66) in $\mathcal{S}(\mathbb{R})$ are Riemann integrals. This makes $\mathcal{S}(\mathbb{R})$ a much easier space to handle than $L^2(\mathbb{R})$.

3.5.2 Gelfand-Maurin Theorem

We are now in a position to address the Gelfand-Maurin Theorem, which provides the mathematical justification for the heuristic Dirac basis vector expansion.

Before stating the Gelfand-Maurin Theorem, let us review the situation in finite dimensional spaces Ψ and in the Hilbert space $\mathcal{H}$.

A nonzero vector h in Ψ or in $\mathcal{H}$ is called an *eigenvector* of an operator A defined on Ψ or on $\mathcal{H}$ if there exists a complex number λ, called the *eigenvalue*, such that

$$Ah = \lambda h \,. \tag{3.5.68}$$

Theorem Every self-adjoint operator A defined on an N-dimensional scalar product space Ψ has a complete system of orthonormal eigenvectors $h_i = |\lambda_i) \in \Psi$, $i = 1, 2, \ldots, N$,

$$A|\lambda_i) = \lambda_i|\lambda_i)\,, \tag{3.5.69}$$
$$(\lambda_i|\lambda_j) = \delta_{ij}\,, \tag{3.5.70}$$

such that every $h \in \Psi$ can be expanded as

$$h = \sum_{i=1}^{N} |\lambda_i)(\lambda_i|h)\,. \tag{3.5.71}$$

The set $\mathrm{Sp}(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_N\}$ of the eigenvalues of A is called the spectrum of A.

For an infinite dimensional Hilbert space $\mathcal{H}$ this statement is no longer true. For example, it is well known that the differential operator

$$P\varphi(x) = -i\frac{d\varphi}{dx}(x) \tag{3.5.72}$$

and the multiplication operator

$$Q\varphi(x) = x\varphi(x) \tag{3.5.73}$$

have no eigenvectors in $L^2(\mathbb{R})$. However, there is a class of operators in the Hilbert space called *compact operators* for which the generalization of (3.5.69)-(3.5.71) holds.

A bounded operator A on a Hilbert space $\mathcal{H}$ is said to be *compact* if for every bounded sequence $\{h_n\} \subset \mathcal{H}$, $\{Ah_n\}$ has a subsequence convergent in $\mathcal{H}$. A self-adjoint compact operator A on an infinite dimensional Hilbert space $\mathcal{H}$ has only a discrete spectrum which coincides with the set of its eigenvalues, $\mathrm{Sp}(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n, \ldots\}$. In this case, the statements (3.5.69)-(3.5.71) for operators on finite dimensional spaces carry over to the infinite dimensional case.

Theorem For any compact self-adjoint operator A defined on a Hilbert space $\mathcal{H}$, there exists an orthonormal set of eigenvectors $h_i \equiv |\lambda_i)$, $\lambda_i \in \mathrm{Sp}(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n, \ldots\}$,

$$A|\lambda_i) = \lambda_i|\lambda_i)\,, \tag{3.5.74}$$
$$(\lambda_i|\lambda_j) = \delta_{ij}\,, \tag{3.5.75}$$

such that every $h \in \mathcal{H}$ can be expanded as

$$h = \sum_{i=1}^{\infty} |\lambda_i)(\lambda_i|h)\,, \tag{3.5.76}$$

where each eigenvalue λ_i is repeated according to its (finite) multiplicity.

The observables that usually appear in Quantum Mechanics are described by unbounded operators defined on some dense subdomains of the Hilbert space. In this case, the (Hilbert

space) spectrum of the operator is not discrete in general, but has a continuous part (cf. Section 2.5.3). For example, P and Q in (3.5.72) and (3.5.73) each has a continuous spectrum which coincides with the real line. When the spectrum of an operator has a continuous part, the spectral decompositions (3.5.71) and (3.5.76) are no longer valid because there are no vectors in the Hilbert space that are eigenvectors corresponding to eigenvalues in the continuous part of the spectrum. In order to extend (3.5.71) and (3.5.76) to the case where the spectrum has a continuous part, we need the Gelfand-Maurin Theorem which is stated below.

Dirac formalism is the way physicists handle continuous spectrum. For instance, the operators P and Q, as defined in (3.5.72) and (3.5.73), have a continuous spectrum that covers the whole real line but do not have any eigenvector in $\mathcal{H}$. Nevertheless, physicists, following Dirac, always associate an eigenket to each element of the continuous spectrum of P and of Q,

$$P|p\rangle = p|p\rangle\,, \quad p \in \mathbb{R}\,, \tag{3.5.77}$$

$$Q|q\rangle = q|q\rangle\,, \quad q \in \mathbb{R}\,, \tag{3.5.78}$$

and use the assumption that these eigenvectors form a "complete" system in the sense that every φ can be written as

$$\varphi = \int_{-\infty}^{+\infty} dp\, |p\rangle\langle p|\varphi\rangle\,, \tag{3.5.79}$$

$$\varphi = \int_{-\infty}^{+\infty} dq\, |q\rangle\langle q|\varphi\rangle\,. \tag{3.5.80}$$

When we omit φ in (3.5.79) and in (3.5.80), we obtain the *resolution of the identity*

$$I = \int_{-\infty}^{+\infty} dp\, |p\rangle\langle p|\,, \tag{3.5.81}$$

$$I = \int_{-\infty}^{+\infty} dq\, |q\rangle\langle q|\,. \tag{3.5.82}$$

However, the kets $|p\rangle$ and $|q\rangle$ are not in the Hilbert space, and the eigenvalues p and q are not proper eigenvalues. The eigenkets corresponding to elements in the continuous spectrum of an operator acquire mathematical meaning as generalized eigenvectors corresponding to generalized eigenvalues in the sense of the following definition:

Definition Let A be a $\tau_{\mathbf{\Phi}}$-continuous operator on $\mathbf{\Phi}$ and $A^\times$ its dual extension to $\mathbf{\Phi}^\times$. A *generalized eigenvector* of the operator A corresponding to the *generalized eigenvalue* λ is an antilinear functional $F \in \mathbf{\Phi}^\times$ such that

$$F(A\varphi) = \lambda F(\varphi)\,, \quad \forall \varphi \in \mathbf{\Phi}\,, \tag{3.5.83}$$

or in bra-ket notation

$$\langle A\varphi|F\rangle = \langle \varphi|A^\times F\rangle = \lambda\langle\varphi|F\rangle\,. \tag{3.5.84}$$

Equations (3.5.83) and (3.5.84) are often written as

$$A^\times F = \lambda F \quad \text{or} \quad A^\times |F\rangle = \lambda |F\rangle \,, \tag{3.5.85}$$

respectively. Following Dirac, the ket in (3.5.85) is often labeled by its eigenvalue, $|F\rangle \equiv |\lambda\rangle$. Then we write

$$A^\times |\lambda\rangle = \lambda |\lambda\rangle \,. \tag{3.5.86}$$

If A is essentially self-adjoint, we may also write

$$A|\lambda\rangle = \lambda |\lambda\rangle \,. \tag{3.5.87}$$

Let us assume that A has a generalized eigenvector in the Hilbert space, i.e., $F \equiv f$ in equation (3.5.84) is an element of $\mathcal{H}$. Then (3.5.84) reads

$$(A\varphi, f) = (\varphi, A^\dagger f) = \lambda(\varphi, f) \tag{3.5.88}$$

for every $\varphi \in \mathbf{\Phi}$. Since $\mathbf{\Phi}$ is $\tau_{\mathcal{H}}$-dense in $\mathcal{H}$, (3.5.88) implies that

$$A^\times F \equiv A^\dagger f = \lambda f \,. \tag{3.5.89}$$

Thus, a generalized eigenvector which is also an element of the Hilbert space is an ordinary eigenvector of the Hilbert space adjoint operator corresponding to the same eigenvalue.

To avoid complications which are inessential for our main purposes and inapplicable for the particular problem of the one-dimensional harmonic oscillator, we restrict ourselves here to cyclic operators.

Definition An operator A defined on a subdomain $\mathcal{D}(A)$ of a Hilbert space $\mathcal{H}$ is *cyclic* if there exists a vector $f \in \mathcal{D}(A)$ such that $\{A^k f\}_{k=0}^\infty$ spans the entire Hilbert space.

For instance, the operators P and Q in (3.5.72) and (3.5.73) are cyclic because the sets

$$\{Q^k \phi_0 \,, \quad k = 0, 1, 2, \ldots\} \tag{3.5.90}$$

and

$$\{P^k \phi_0 \,, \quad k = 0, 1, 2, \ldots\} \,, \tag{3.5.91}$$

where ϕ_0 is the zero-th Hermite polynomial, both span $\mathcal{H}$.

If A has a continuous spectrum, the spectral decomposition (3.5.76) is not possible in the Hilbert space. However, a generalization of (3.5.76), called the *Gelfand-Maurin Theorem* or the *Nuclear Spectral Theorem*, is possible in the Rigged Hilbert Space.

Theorem (Gelfand-Maurin Theorem or Nuclear Spectral Theorem) Let $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ be a Rigged Hilbert Space and A a cyclic, e.s.a., $\tau_{\mathbf{\Phi}}$-continuous operator. Then, for each λ in the spectrum of A, there exists a generalized eigenvector $F_\lambda \equiv |\lambda\rangle$,

$$A^\times |\lambda\rangle = \lambda |\lambda\rangle \,, \quad \lambda \in \mathrm{Sp}(A) \,, \tag{3.5.92}$$

i.e.,

$$\langle A\varphi|\lambda\rangle = \langle\varphi|A^{\times}|\lambda\rangle = \lambda\langle\varphi|\lambda\rangle\,, \quad \forall\varphi\in\mathbf{\Phi}\,. \tag{3.5.93}$$

Furthermore, there is some uniquely defined positive measure $d\mu(\lambda)$ on $\mathrm{Sp}(A)$ such that for every $\varphi,\psi\in\mathbf{\Phi}$

$$(\psi,\varphi) = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\langle\psi|\lambda\rangle\langle\lambda|\varphi\rangle\,, \tag{3.5.94}$$

where

$$\langle\lambda|\varphi\rangle = \overline{\langle\varphi|\lambda\rangle}\,. \tag{3.5.95}$$

Furthermore, if $f(\lambda)$ is a well-behaved function on $\mathrm{Sp}(A)$, then

$$(\psi, f(A)\varphi) = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\langle\psi|\lambda\rangle\langle\lambda|\varphi\rangle f(\lambda) \tag{3.5.96}$$

If we set $\psi=\varphi$ in (3.5.94), we see that if all the components $\langle\lambda|\varphi\rangle$ of the spectral decomposition of φ with respect to the operator A vanish, then $\|\varphi\|=0$, i.e., $\varphi=0$. Because of this property, the set of generalized eigenvectors $|\lambda\rangle$ occurring in (3.5.92) is called *complete* in analogy to the completeness of the system of ordinary eigenvectors in a Hilbert space.

In general, an e.s.a. operator has more generalized eigenvectors than those that appear in the spectral decomposition (3.5.94). In particular, a generalized eigenvalue may be complex.

The spectral decomposition provided by the Gelfand-Maurin theorem needs not be unique and it is also valid in many cases when $\mathbf{\Phi}$ is not a nuclear space.

The statement of the Gelfand-Maurin Theorem is still too general for the purposes of Quantum Mechanics. For the cases of physical interest, the measure $d\mu(\lambda)$ that appears in this theorem has a discrete and an absolutely continuous part, i.e., it can be written as

$$d\mu(\lambda) = \sum_{\substack{\text{discrete}\\ \text{spectrum}}} \mu(\lambda_i)\delta(\lambda-\lambda_i) + \rho(\lambda)d\lambda\,. \tag{3.5.97}$$

After a delta-normalization given by (3.5.41), equations (3.5.94) and (3.5.97) yield

$$(\psi,\varphi) = \sum_{\substack{\text{discrete}\\ \text{spectrum}}} (\psi|\lambda_i)(\lambda_i|\varphi) + \int_{\substack{\text{continuous}\\ \text{spectrum}}} d\lambda\,\langle\psi|\lambda\rangle\langle\lambda|\varphi\rangle\,, \quad \varphi,\psi\in\mathbf{\Phi}\,. \tag{3.5.98}$$

Eq. (3.5.98) is the form in which the Gelfand-Maurin theorem is used in physics because it is precisely the Dirac basis vector expansion. This expansion treats the elements of the discrete spectrum and the elements of the continuous spectrum of the operator A on the same footing: there is always an eigenvector corresponding to each element of the spectrum of the operator. If this element belongs to the discrete spectrum, then the corresponding eigenket is an ordinary eigenvector (i.e., it is square normalizable). If the element is in the continuous part of the spectrum, then the corresponding eigenket is a generalized eigenvector

(i.e., it is a functional). It is worthwhile noting that the spectral decomposition (3.5.98) is only valid for elements ψ, φ in the space $\mathbf{\Phi}$, but not for every element h in the Hilbert space $\mathcal{H}$.

The Gelfand-Maurin Theorem provides a mathematical rephrasing of several formal expressions used in Quantum Mechanics. For instance, omission of ψ in (3.5.98) leads to the spectral decomposition of any wave function $\varphi \in \mathbf{\Phi}$,

$$\varphi = \sum_i |\lambda_i)(\lambda_i|\varphi) + \int d\lambda |\lambda\rangle\langle\lambda|\varphi\rangle \,. \tag{3.5.99}$$

In the same way, we can obtain the spectral resolution of the identity operator

$$I = \sum_i |\lambda_i)(\lambda_i| + \int d\lambda \, |\lambda\rangle\langle\lambda| \tag{3.5.100}$$

and of the operator itself

$$A = \sum_i \lambda_i \, |\lambda_i)(\lambda_i| + \int d\lambda \, \lambda \, |\lambda\rangle\langle\lambda| \,. \tag{3.5.101}$$

As an example, Eq. (3.5.79) is a particular case of (3.5.94) with $\mathrm{Sp}(P) = \mathbb{R}$, $\lambda = p \in \mathbb{R}$ and $d\mu(\lambda) = dp$, the Lebesgue measure on $\mathbb{R}$, and similarly for the position operator.

3.6 Gelfand-Maurin Theorem Applied to the Harmonic Oscillator

In this section, we will apply the Gelfand-Maurin Theorem to the operators of the algebra of observables of the harmonic oscillator. We will show that the defining algebraic assumptions (3.2.1)-(3.2.4) and the $\tau_{\mathbf{\Phi}}$-continuity of the algebra of observables lead to the Schrödinger representation in the Schwartz space $\mathcal{S}(\mathbb{R})$. The operators P, Q and H will be realized by the standard differential operators and the space $\mathbf{\Phi}$ will be realized by the Schwartz space.

3.6.1 Spectral Theorem Applied to the Energy Operator

We now recall the spectral properties of H. These spectral properties were derived in the construction of the RHS for the harmonic oscillator.

The spectrum of H is the discrete set

$$\mathrm{Sp}(H) = \{E_n = \hbar\omega(n + \frac{1}{2}) \,,\ n = 0, 1, 2, \ldots\} \,. \tag{3.6.1}$$

Corresponding to each eigenvalue E_n, there is an eigenvector $\phi_n \equiv |n)$ of H:

$$H|n) = E_n|n) \,. \tag{3.6.2}$$

The eigenvectors $|n)$ are proper eigenvectors, i.e., $|n) \in \mathbf{\Phi}$, rather than generalized eigenvectors, i.e., elements of $\mathbf{\Phi}^\times$. These eigenvectors form a basis system for $\mathbf{\Phi}$, i.e., every $\varphi \in \mathbf{\Phi}$ can be written as

$$\varphi = \sum_{n=0}^{\infty} |n)(n|\varphi) \,, \tag{3.6.3}$$

where the components $(n|\varphi) \in \mathbb{C}$ satisfy

$$\sum_{n=0}^{\infty} (n+1)^p \, |(n|\varphi)|^2 < \infty \tag{3.6.4}$$

for every $p = 0, 1, 2, \ldots$

3.6.2 Spectral Theorem Applied to the Position and Momentum Operators

We now want to calculate the spectra of the operators Q and P and the generalized eigenvectors that correspond to the elements of these spectra. These generalized eigenvectors will be continuous antilinear functionals over the space $\mathbf{\Phi}$ constructed in Section 3.3.

We first determine whether the Gelfand-Maurin Theorem of Section 3.5.2 can be applied to the operators Q and P. The space $\mathbf{\Phi}$, whose topology is defined by the countable number of scalar products

$$(\varphi, \psi)_p = (\varphi, (N+I)^p \psi) \,, \tag{3.6.5}$$

was proved to be a nuclear space (cf. Section 3.3.5). The operators position Q and momentum P were proved to be $\tau_{\mathbf{\Phi}}$-continuous (cf. Section 3.3.5). Q and P are cyclic operators, since the sets

$$\{Q^n \phi_0 \mid n = 0, 1, 2, \ldots\} \tag{3.6.6}$$

and

$$\{P^n \phi_0 \mid n = 0, 1, 2, \ldots\} \,, \tag{3.6.7}$$

where ϕ_0 is the zeroth eigenvector of the Hamiltonian operator, both span the whole of $\mathcal{H}$. Therefore, we can apply the Gelfand-Maurin to these operators. This theorem assures the existence of a complete set of generalized eigenvectors of the operators Q and P,

$$Q^\times |x\rangle = x|x\rangle \,, \quad x \in \mathrm{Sp}(Q) \,, \tag{3.6.8}$$

$$P^\times |p\rangle = p|p\rangle \,, \quad p \in \mathrm{Sp}(P) \,, \tag{3.6.9}$$

and either of these two sets can be used for the spectral decomposition of any vector φ in $\mathbf{\Phi}$:

$$\varphi = \int_{\mathrm{Sp}(Q)} d\mu(x) \, |x\rangle \langle x|\varphi\rangle \,, \tag{3.6.10}$$

or

$$\varphi = \int_{\mathrm{Sp}(P)} d\mu(p) \, |p\rangle \langle p|\varphi\rangle \,, \tag{3.6.11}$$

where $d\mu(x)$ and $d\mu(p)$ are measures on $\mathrm{Sp}(Q)$ and $\mathrm{Sp}(P)$, respectively.

It is well known that the spectrum of both P and Q is the real line. However, it is not so widely known that the derivation of this is far from being trivial (see [68] and references therein). The approach of a physicist is usually the reverse of the one described here, namely a physicist finds the defining assumptions (3.2.1)-(3.2.4) of the harmonic oscillator from the spectra of Q and P, which are conjectured from experimental data to be the real line. We shall derive these spectra in the present section. We will see that $d\mu(x) = dx$, $\mathrm{Sp}(Q) = \mathbb{R}$, $d\mu(p) = dp$ and $\mathrm{Sp}(P) = \mathbb{R}$. We shall see that the set of *generalized* eigenvalues of Q (of P) agrees with the spectrum of Q (of P) when we choose for the space $\mathbf{\Phi}$ in the RHS the countably Hilbert space defined by the countable number of scalar products (3.6.5). However, since the set of generalized eigenvalues depends upon the choice of the space $\mathbf{\Phi}$, we could choose a different countably Hilbert space and obtain also complex generalized eigenvalues of the essentially self-adjoint operator Q (or P).

We begin by examining for which values $x \in \mathbb{C}$ the equation

$$Q^\times|x\rangle = x|x\rangle \tag{3.6.12}$$

can be fulfilled, i.e., for which complex numbers x the equation

$$\langle Q\varphi|x\rangle = \langle\varphi|Q^\times|x\rangle = x\langle\varphi|x\rangle \tag{3.6.13}$$

holds for every $\varphi \in \mathbf{\Phi}$. Since every $\varphi \in \mathbf{\Phi}$ can be expanded in terms of the basis of eigenvectors $\phi_n = |n)$ of H as in (3.6.3), it will be sufficient to know for which x the equation

$$(n|Q^\times|x\rangle = x(n|x\rangle \tag{3.6.14}$$

holds for every $|n)$.

From (3.2.5), (3.2.6) and (3.2.27) it follows that

$$\begin{aligned} Q|n) &= \sqrt{\frac{\hbar}{2\mu\omega}}(a + a^\dagger)|n) \\ &= \sqrt{\frac{\hbar}{2\mu\omega}}\left(\sqrt{n}|n-1) + \sqrt{n+1}|n+1)\right) . \end{aligned} \tag{3.6.15}$$

Taking the "scalar product" of this equation with $|x\rangle$ we obtain

$$(n|Q^\times|x\rangle = \sqrt{\frac{\hbar}{2\mu\omega}}(\sqrt{n}(n-1|x\rangle + \sqrt{n+1}(n+1|x\rangle)\,. \tag{3.6.16}$$

Equation (3.6.16) is mathematically well defined even though we used the term "scalar product" of $Q|n)$ with $|x\rangle$, which is not well defined since $|x\rangle \in \mathbf{\Phi}^\times$. The precise meaning of (3.6.16) is as follows: since $|n) \in \mathbf{\Phi}$, so is $\varphi \equiv Q|n)$, because Q leaves $\mathbf{\Phi}$ invariant. Therefore, we can consider the value of the functional $|x\rangle \equiv F_x \in \mathbf{\Phi}^\times$ at

the point $\varphi \in \mathbf{\Phi}$, $F_x(\varphi) = \langle\varphi|F_x\rangle$. According to (3.4.25), this is related to the value of the functional $\widetilde{\varphi} \in \mathbf{\Phi}^{\times\times} \equiv \mathbf{\Phi}$ at the point $F_x \in \mathbf{\Phi}^{\times}$ by

$$F_x(\varphi) = \overline{\widetilde{\varphi}(F_x)}\,, \tag{3.6.17}$$

or in bra-ket notation

$$\langle\varphi|F_x\rangle = \overline{\langle F_x|\widetilde{\varphi}\rangle} \equiv \overline{\langle F_x|\varphi\rangle}\,, \tag{3.6.18}$$

where the identification $\mathbf{\Phi}^{\times\times} \ni \widetilde{\varphi} \equiv \varphi \in \mathbf{\Phi}$ was used. Returning to $\varphi \equiv Q|n) = Q\phi_n$, (3.6.18) is written as

$$\overline{\langle x|Q|n)} = \overline{\langle x|Q\phi_n\rangle} = \langle Q\phi_n|x\rangle = (n|Q^{\times}|x\rangle\,. \tag{3.6.19}$$

This is the quantity that appears on the left hand side of (3.6.16). The quantities $(n-1|x\rangle$ and $(n+1|x\rangle$ are similarly defined by choosing $\varphi = |n-1)$ and $\varphi = |n+1)$ respectively.

On the other hand, taking the scalar product of (3.6.12) with $|n)$, (more precisely, the action of the functional $Q^{\times}|x\rangle$ at $|n)$) we obtain

$$(n|Q^{\times}|x\rangle = x\,(n|x\rangle\,. \tag{3.6.20}$$

Comparing (3.6.16) with (3.6.20) yields

$$x\,(n|x\rangle = \sqrt{\frac{\hbar}{2\mu\omega}}\left(\sqrt{n}(n-1|x\rangle + \sqrt{n+1}(n+1|x\rangle\right)\,, \tag{3.6.21}$$

or with $n+1 = m$,

$$\sqrt{m}(m|x\rangle = \sqrt{\frac{2\mu\omega}{\hbar}}x(m-1|x\rangle - \sqrt{m-1}(m-2|x\rangle\,. \tag{3.6.22}$$

Since Eq. (3.6.15) is valid for $n = 1, 2, \ldots$, Eq. (3.6.22) is valid for $m = 2, 3, \ldots$ For $n = 0$ $(m = 1)$, we obtain instead of (3.6.15)

$$Q|0) = \sqrt{\frac{\hbar}{2\mu\omega}}\,\sqrt{0+1}\,|0+1) = \sqrt{\frac{\hbar}{2\mu\omega}}\,|1)\,, \tag{3.6.23}$$

and instead of (3.6.22)

$$\sqrt{1}\,(1|x\rangle = \sqrt{\frac{2\mu\omega}{\hbar}}\,x\,(0|x\rangle\,. \tag{3.6.24}$$

Thus we see that (3.6.22) is a recurrence relation for $(m|x\rangle$: if $(0|x\rangle$ is known, we can determine $(1|x\rangle$ by (3.6.24) and then determine $(2|x\rangle$ by (3.6.22). With $(1|x\rangle$ and $(2|x\rangle$ we can determine $(3|x\rangle$ by (3.6.22), and so on.

To find out what the transition coefficients $(m|x\rangle$ are, we introduce

$$y \equiv \sqrt{\frac{\mu\omega}{\hbar}}\,x \tag{3.6.25}$$

and

$$f_n(y) \equiv \sqrt{2^n n!}\,\frac{(n|x\rangle}{(0|x\rangle}\,, \tag{3.6.26}$$

which is defined for all x such that $(0|x\rangle \neq 0$ (if $(0|x\rangle = 0$, then by (3.6.22) and (3.6.24) $(n|x\rangle = 0$ for all n). Then from (3.6.22) it follows that

$$\sqrt{\frac{m}{2^m m!}}\,f_m(y) = \sqrt{\frac{2}{2^{m-1}(m-1)!}}\,y\,f_{m-1}(y) - \sqrt{\frac{m-1}{2^{m-2}(m-2)!}}\,f_{m-2}(y)\,, \tag{3.6.27}$$

or

$$f_m(y) = 2yf_{m-1}(y) - 2(m-1)f_{m-2}(y) \tag{3.6.28}$$

From (3.6.24) we have

$$f_1(y) = 2yf_0(y)\,, \tag{3.6.29}$$

and from (3.6.26)

$$f_0(y) = 1\,. \tag{3.6.30}$$

Equations (3.6.28)-(3.6.30) are the recurrence relations for the Hermite functions and have solutions for any complex number y. Thus for any complex value x there is a solution $(n|x\rangle$ of the recurrence relation (3.6.22). Since Q is an e.s.a. operator, the (Hilbert space) spectrum of Q must be real (cf. Section 2.5.3). Therefore the generalized eigenvalues that appear in the integral decomposition (3.6.10) must be real, and we need to consider only the solutions $f_m(y)$ for $y \in \mathbb{R}$.

For real values of y, the solutions $f_m(y)$ of (3.6.28)-(3.6.30) are the Hermite polynomials:

$$f_n(y) = H_n(y) = (-1)^n e^{y^2}\frac{d^n(e^{-y^2})}{dy^n}\,. \tag{3.6.31}$$

Thus from (3.6.26) we can obtain the transition coefficient $(n|x\rangle$ for every real value of x for which $(0|x\rangle$ is defined. We restrict ourselves to those solutions of (3.6.22) for which $(0|x\rangle$ is finite, because $|(0|x\rangle|^2$, the probability for obtaining the value x in a measurement of Q in the ground state $\Lambda_0 = |\phi_0)(\phi_0|$, is assumed to be finite.

Combining (3.6.25), (3.6.26) and (3.6.31), we have

$$(n|x\rangle = \frac{1}{\sqrt{2^n n!}}(0|x\rangle H_n\Big(\sqrt{\frac{\mu\omega}{\hbar}}x\Big) \tag{3.6.32}$$

for $-\infty < x < +\infty$.

Since every $\varphi \in \mathbf{\Phi}$ can be expanded as

$$\varphi = \sum_{n=0}^{\infty} |n)(n|\varphi)\,, \tag{3.6.33}$$

the $|x\rangle$ can be defined at each φ by

$$\langle x|\varphi\rangle = \sum_{n=0}^{\infty}\langle x|n)(n|\varphi)\,. \tag{3.6.34}$$

The quantities $\langle x|\varphi\rangle \equiv \varphi(x)$ are called the *position wave functions* or the *wave functions in the position representation*. The quantities $\langle x|n) \equiv \phi_n(x)$ are called the *energy eigenfunctions*, since they fulfill

$$\langle x|H|n) = E_n \langle x|n) \,. \tag{3.6.35}$$

Because of Eq. (3.6.34), the energy eigenfunctions $\langle x|n)$ can be viewed also as "transition elements" between the x- and the n-representation.

If we consider the expansion

$$\phi_n = \int_{\mathrm{Sp}(Q)} d\mu(x)\, |x\rangle\langle x|\phi_n) \tag{3.6.36}$$

of the energy eigenvectors ϕ_n in terms of the eigenkets of Q as a functional acting on the generalized eigenvector $F_{x'} = |x'\rangle \in \mathbf{\Phi}^\times$, $x' \in \mathrm{Sp}(Q)$, then according to (3.6.18) we obtain from (3.6.36)

$$\widetilde{\phi}_n(F_{x'}) = \langle x'|\phi_n\rangle = \int_{\mathrm{Sp}(Q)} d\mu(x)\, \langle x'|x\rangle\langle x|\phi_n\rangle \,. \tag{3.6.37}$$

Thus $d\mu(x)\, \langle x'|x\rangle$ must be the Dirac measure, i.e., the distribution defined by (3.6.37) must have the property of the Dirac delta-function

$$d\mu(x)\, \langle x'|x\rangle = dx\, \delta(x'-x) \,. \tag{3.6.38}$$

We now calculate the scalar product of $\phi_n = |n)$ and $\phi_m = |m)$ using (3.6.36)

$$\delta_{mn} = (\phi_m, \phi_n) = (m|n) = \int_{\mathrm{Sp}(Q)} d\mu(x)\, (m|x\rangle\, \langle x|n) \,. \tag{3.6.39}$$

We shall make use of

$$\langle x|n) = \overline{(n|x\rangle} \,. \tag{3.6.40}$$

We insert (3.6.32) and (3.6.40) into (3.6.39) and obtain

$$\sqrt{\frac{1}{2^n 2^m n! m!}} \int_{\mathrm{Sp}(Q)} d\mu(x)\ |(0|x\rangle|^2\ H_m(\sqrt{\frac{\mu\omega}{\hbar}}x) H_n(\sqrt{\frac{\mu\omega}{\hbar}}x) = \delta_{mn} \,. \tag{3.6.41}$$

Comparing (3.6.41) with the orthogonality relations for the Hermite polynomials,

$$\frac{1}{n! 2^n \sqrt{\pi}} \int_{-\infty}^{+\infty} dy\ e^{-y^2} H_m(y) H_n(y) = \delta_{nm} \,, \tag{3.6.42}$$

and taking into account that the Hermite polynomials are only orthogonal polynomials if associated with the interval $-\infty < y < +\infty$ and the weight e^{-y^2} (one can define $H_n(y)$ by (3.6.42) and derive (3.6.28)-(3.6.30) for real y) we conclude

$$d\mu(x)\, |(0|x\rangle|^2 = dx \sqrt{\frac{\mu\omega}{\pi\hbar}} e^{-(\mu\omega/\hbar)x^2} \tag{3.6.43}$$

and

$$\mathrm{Sp}(Q) = \{x \mid -\infty < x < +\infty\}\,. \tag{3.6.44}$$

If we agree to normalize the generalized eigenvectors such that

$$\langle x'|x\rangle = \delta(x'-x)\,, \tag{3.6.45}$$

then according to (3.6.38)

$$d\mu(x) = dx\,. \tag{3.6.46}$$

From (3.6.43) and (3.6.46) we conclude

$$|(0|x\rangle|^2 = \sqrt{\frac{\mu\omega}{\pi\hbar}}e^{-(\mu\omega/\hbar)x^2}\,. \tag{3.6.47}$$

Thus, up to an arbitrary phase factor (which we choose to be unity),

$$(0|x\rangle = \left(\frac{\mu\omega}{\pi\hbar}\right)^{1/4} e^{-(\mu\omega/2\hbar)x^2}\,. \tag{3.6.48}$$

With this and (3.6.32) we obtain the transition coefficients $(n|x\rangle$ between the x- and n-basis, i.e., the harmonic-oscillator energy wave eigenfunctions $\phi_n(x)$:

$$(n|x\rangle = \left(\frac{\mu\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right)e^{-(\mu\omega/2\hbar)x^2} = \langle x|n) = \phi_n(x)\,. \tag{3.6.49}$$

We now repeat for the operator P the procedure that we have gone through for the operator Q. The generalized eigenvectors of P will be denoted by $|p\rangle$:

$$P^\times|p\rangle = p|p\rangle\,. \tag{3.6.50}$$

The action of P on $|n)$ is, using (3.2.5), (3.2.6) and (3.2.27),

$$\begin{aligned} P|n) &= -i\sqrt{\frac{\hbar\mu\omega}{2}}(a-a^\dagger)|n) \\ &= -i\sqrt{\frac{\hbar\mu\omega}{2}}\left(\sqrt{n}|n-1) - \sqrt{n+1}|n+1)\right)\,. \end{aligned} \tag{3.6.51}$$

If we apply the functional $|p\rangle \in \mathbf{\Phi}^\times$ on the vector $P|n) \in \mathbf{\Phi}$ and use (3.6.50), we obtain

$$p\langle p|n) = -i\sqrt{\frac{\hbar\mu\omega}{2}}\left(\sqrt{n}\langle p|n-1) - \sqrt{n+1}\langle p|n+1)\right)\,, \tag{3.6.52}$$

or

$$p(n|p\rangle = i\sqrt{\frac{\hbar\mu\omega}{2}}\left(\sqrt{n}(n-1|p\rangle - \sqrt{n+1}(n+1|p\rangle\right)\,. \tag{3.6.53}$$

If we introduce the new quantities $(n|p\}$ defined by

$$(n|p\} := i^{-n}(n|p\rangle\,, \tag{3.6.54}$$

then

$$i(n-1|p\rangle = i^n(n-1|p\}\,, \tag{3.6.55}$$

$$-i(n+1|p\rangle = i^n(n+1|p\}\,, \tag{3.6.56}$$

so (3.6.53) may be written as

$$p(n|p\} = \sqrt{\frac{\hbar\mu\omega}{2}}\left(\sqrt{n}(n-1|p\} + \sqrt{n+1}(n+1|p\}\right)\,. \tag{3.6.57}$$

We see that this is exactly the same recurrence relation as in (3.6.21), with $x\sqrt{\mu\omega/\hbar}$ replaced by $p/\sqrt{\mu\omega\hbar}$. Thus by the same argument as for $(n|x\rangle$, we find (using (3.6.54)) that

$$(n|p\rangle = i^n\Big(\frac{1}{\pi\mu\omega\hbar}\Big)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\Big(\frac{1}{\sqrt{\hbar\mu\omega}}p\Big)e^{-p^2/2\mu\omega\hbar}\,. \tag{3.6.58}$$

Therefore, the eigenvectors $|n)$ of the energy operator H for the harmonic oscillator have the very particular property that the transition coefficients (3.6.49) between these vectors and the x-basis have the same functional form as the transition coefficients (3.6.58) between these vectors and the p-basis except for a phase factor.

By the same argument as above for the operator Q, we conclude that the spectrum of P is continuous,

$$\mathrm{Sp}(P) = \{p\,|\ -\infty < p < \infty\}\,, \tag{3.6.59}$$

and that if we normalize the generalized eigenvectors $|p\rangle$ according to

$$\langle p'|p\rangle = \delta(p'-p)\,, \tag{3.6.60}$$

then the measure $d\mu(p)$ is the Lebesgue measure on the real line,

$$d\mu(p) = dp\,. \tag{3.6.61}$$

The transition coefficients $\langle p|n)$ in

$$|n) = \int_{-\infty}^{+\infty} dp\,|p\rangle\langle p|n) \tag{3.6.62}$$

are called the *energy wave eigenfunctions in the momentum representation* and are denoted by

$$\widehat{\phi}_n(p) \equiv \langle p|n)\,. \tag{3.6.63}$$

Also, for any arbitrary vector φ the transition coefficient

$$\widehat{\varphi}(p) = \langle p|\varphi\rangle \tag{3.6.64}$$

in

$$\varphi = \int_{-\infty}^{+\infty} dp\, |p\rangle\langle p|\varphi\rangle \tag{3.6.65}$$

is called the *momentum wave function* or the *wave function in the momentum representation* of φ. We have used the notation $\widehat{\varphi}(p) = \langle p|\varphi\rangle$ instead of the notation $\varphi(p) = \langle p|\varphi\rangle$ because the function $\widehat{\varphi}(p)$ of p is in general different to the function $\varphi(x) = \langle x|\varphi\rangle$ of x. Therefore, to avoid confusion, we label the two different functions $\widehat{\varphi}(p)$ and $\varphi(x)$ by two different symbols.

3.6.3 Realizations of the RHS of the Harmonic Oscillator by Spaces of Functions

Thus far, we have obtained the matrix elements of Q in the x-representation,

$$\langle x|Q|n) = x\langle x|n)\,, \quad \langle x|Q|\varphi\rangle = x\langle x|\varphi\rangle\,, \tag{3.6.66}$$

and the matrix elements of P in the p-representation,

$$\langle p|P|n) = p\langle p|n)\,, \quad \langle p|P|\varphi\rangle = p\langle p|\varphi\rangle\,. \tag{3.6.67}$$

We now want to calculate $\langle x|P|\varphi\rangle$, the matrix elements of P in the x-representation, and $\langle p|Q|\varphi\rangle$, the matrix elements of Q in the p-representation. We do this in two steps:

1. We introduce the new mathematical objects $\langle x|p\rangle$ and $\langle p|x\rangle$. They are generalizations of the scalar product, but are the "scalar products" between the eigenvectors $|x\rangle \in \mathbf{\Phi}^\times$ and $|p\rangle \in \mathbf{\Phi}^\times$. Thus, they are something like the $\langle x|y\rangle$ in (3.5.39) of Section 3.5, i.e., distributions that are defined by integration. Like the $(n|x\rangle$ and the $(n|p\rangle$ in (3.6.36) and (3.6.62), the $\langle x|p\rangle$ (and $\langle p|x\rangle$) are transition coefficients between basis systems. But whereas $\langle x|n)$ are transition coefficients between the continuous basis system $\{|x\rangle\}$ and the discrete basis system $\{|n)\}$, the $\langle x|p\rangle$ are the transition coefficients between the continuous basis system $\{|x\rangle\}$ and the continuous basis system $\{|p\rangle\}$.

2. We compute $\langle x|P|\varphi\rangle$ and $\langle p|Q|\varphi\rangle$ using the expressions for $\langle x|p\rangle$ and $\langle p|x\rangle$.

The mathematical object $\langle p|x\rangle$ appears when we take the "scalar product" of

$$\phi_n = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|n) \tag{3.6.68}$$

with $|p\rangle$ (or, more precisely, we consider ϕ_n as a functional at the generalized eigenvector $|p\rangle \in \mathbf{\Phi}^\times,\ p \in \mathrm{Sp}(P)$, and use (3.6.68)):

$$\langle p|n) = \int_{-\infty}^{+\infty} dx\, \langle p|x\rangle\langle x|n)\,. \tag{3.6.69}$$

On the other hand, the mathematical object $\langle x|p\rangle$ appears when we take the scalar product of

$$\phi_n = \int_{-\infty}^{+\infty} dp\, |p\rangle\langle p|n) \tag{3.6.70}$$

with $\langle x|$ (or, more precisely, we consider ϕ_n as a functional acting on the generalized eigenvector $|x\rangle \in \mathbf{\Phi}^\times$, $x \in \mathrm{Sp}(Q)$, and use (3.6.70)):

$$\langle x|n) = \int_{-\infty}^{+\infty} dp\, \langle x|p\rangle\langle p|n)\,. \tag{3.6.71}$$

In (3.6.69) and (3.6.71), $\langle x|n)$ and $\langle p|n)$ are given by (3.6.49) and (3.6.58), respectively.

The Hermite polynomials have the property

$$i^n e^{-\eta^2/2} H_n(\eta) = \int_{-\infty}^{+\infty} d\xi\, \frac{e^{i\xi\eta}}{\sqrt{2\pi}}\, e^{-\xi^2/2} H_n(\xi)\,, \tag{3.6.72}$$

where $\eta = \frac{p}{\sqrt{\hbar\mu w}}$ and $\xi = \sqrt{\frac{\mu w}{\hbar}}\, x$. Inserting (3.6.49) and (3.6.58) into this relation, it follows that

$$(n|p\rangle = \int_{-\infty}^{+\infty} dx\, \frac{e^{ixp/\hbar}}{\sqrt{2\pi\hbar}}\, (n|x\rangle\,, \tag{3.6.73}$$

or taking the complex conjugate

$$\langle p|n) = \int_{-\infty}^{+\infty} dx\, \frac{e^{-ixp/\hbar}}{\sqrt{2\pi\hbar}}\, \langle x|n)\,. \tag{3.6.74}$$

Comparing (3.6.74) with (3.6.69), we find that the $\langle p|x\rangle$ are given by

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-ixp/\hbar}\,. \tag{3.6.75}$$

In the same way one obtains from (3.6.71) and (3.6.72)

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ixp/\hbar}\,. \tag{3.6.76}$$

Eqs. (3.6.75) and (3.6.76) together give

$$\langle x|p\rangle = \overline{\langle p|x\rangle}. \tag{3.6.77}$$

It is now simple to calculate the matrix element of P in the basis of generalized eigenvectors of Q using (3.6.76):

$$\begin{aligned}\langle x|P|\varphi\rangle &= \int_{-\infty}^{+\infty} dp\, p\, \langle x|p\rangle\langle p|\varphi\rangle = \int_{-\infty}^{+\infty} dp\, p \frac{e^{ixp/\hbar}}{\sqrt{2\pi\hbar}}\, \langle p|\varphi\rangle \\ &= \int_{-\infty}^{+\infty} dp\, \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle\langle p|\varphi\rangle = \frac{\hbar}{i}\frac{d}{dx}\int_{-\infty}^{+\infty} dp\, \langle x|p\rangle\langle p|\varphi\rangle\,.\end{aligned} \tag{3.6.78}$$

Thus

$$\langle x|P|\varphi\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|\varphi\rangle\,. \tag{3.6.79}$$

In the same way using (3.6.75) one obtains

$$\langle p|Q|\varphi\rangle = -\frac{\hbar}{i}\frac{d}{dp}\langle p|\varphi\rangle\,. \tag{3.6.80}$$

Therewith, we have shown that the operators Q and P are "realized" in the space of position wave functions $\langle x|\varphi\rangle = \varphi(x)$ by the multiplication operator

$$Q\varphi(x) = x\varphi(x) \tag{3.6.81}$$

and by the differentiation operator

$$P\varphi(x) = \frac{\hbar}{i}\frac{d}{dx}\varphi(x)\,, \tag{3.6.82}$$

respectively. These are the standard expressions that are usually assumed to represent the position and momentum operators. We have derived them here from the Heisenberg commutation relation $[P,Q] = -i\hbar I$, the relation $H = \frac{1}{2\mu}P^2 + \frac{\mu\omega^2}{2}Q^2$, and the *additional* assumption of the existence of an eigenvector of H.

We shall now derive the position representation of the energy operator H, i.e., we shall calculate the matrix element $\langle x|H|n\rangle$. In this position representation, the energy eigenvalue equation

$$H\phi_n = E_n\phi_n \tag{3.6.83}$$

is called the *time-independent Schrödinger equation.* The Hamiltonian for the harmonic oscillator is given by

$$H = \frac{1}{2\mu}P^2 + \frac{\mu\omega^2}{2}Q^2\,. \tag{3.6.84}$$

Let us take the matrix element of H between $\langle x|$ and $|n\rangle$ (or, more precisely, the action of of the functional $\langle x|$ at the point $H|n\rangle$):

$$\langle x|H|n\rangle = \frac{1}{2\mu}\langle x|P^2|n\rangle + \frac{\mu\omega^2}{2}\langle x|Q^2|n\rangle\,. \tag{3.6.85}$$

From (3.6.79), it follows that

$$\begin{aligned}\langle x|P^2|n\rangle &= \langle x|P^2|\phi_n\rangle \\ &= \frac{\hbar}{i}\frac{d}{dx}\langle x|P|\phi_n\rangle \\ &= \left(\frac{\hbar}{i}\right)^2\frac{d^2}{dx^2}\langle x|\phi_n\rangle \\ &= \left(\frac{\hbar}{i}\right)^2\frac{d^2}{dx^2}\langle x|n\rangle\,.\end{aligned} \tag{3.6.86}$$

From (3.6.66),

$$\langle x|Q^2|n\rangle = x^2\langle x|n\rangle\,. \tag{3.6.87}$$

Inserting (3.6.86) and (3.6.87) into (3.6.85), we have for the matrix element of the energy operator

$$\begin{aligned}\langle x|H|n\rangle &= -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}\langle x|n\rangle + \frac{\mu\omega^2}{2}x^2\langle x|n\rangle \\ &= \Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{\mu\omega^2}{2}x^2\Big)\langle x|n\rangle\,. \end{aligned}\tag{3.6.88}$$

Therefore, the Schrödinger representation of the eigenvalue equation (3.6.83) reads

$$\Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{\mu\omega^2}{2}x^2\Big)\phi_n(x) = E_n\phi_n(x)\,, \tag{3.6.89}$$

where $\langle x|n\rangle = \phi_n(x)$ is given in terms of the n-th Hermite polynomial as in (3.6.49). Eq. (3.6.89) is the time-independent Schrödinger equation. This equation, that is usually taking as the starting point in the study of the harmonic oscillator, has been derived here from the algebraic assumptions (3.2.1)-(3.2.4).

So far we have discussed the action of the operators Q, P and H on the wave functions $\varphi(x) = \langle x|\varphi\rangle$ without specifying the particular properties of these functions. We shall now show that as a consequence of the properties of the space $\mathbf{\Phi}$, it follows that the position realization of $\mathbf{\Phi}$ is the Schwartz space $\mathcal{S}(\mathbb{R})$ (cf. Section 2.4.1):

Since the space $\mathbf{\Phi}$ remains stable under the action of the algebra of observables, $\mathbf{\Phi}$ remains stable under the action of any power of P and Q. This means that the quantities

$$(\varphi, Q^n\varphi) = \int_{-\infty}^{+\infty} dx\, x^n\, |\varphi(x)|^2 < \infty\,, \quad n = 0, 1, 2, \ldots, \tag{3.6.90}$$

$$(\varphi, P^m\varphi) = (-i\hbar)^m \int_{-\infty}^{+\infty} dx\, \overline{\varphi(x)}\, \frac{d^m}{dx^m}\varphi(x) < \infty\,, \quad m = 0, 1, 2, \ldots, \tag{3.6.91}$$

$$(\varphi, Q^nP^m\varphi) = (-i\hbar)^m \int_{-\infty}^{+\infty} dx\, \overline{\varphi(x)}\, x^n\, \frac{d^m}{dx^m}\varphi(x) < \infty\,, \quad n, m = 0, 1, 2, \ldots \tag{3.6.92}$$

must be well defined for every $\varphi \in \mathbf{\Phi}$. This implies that the functions $\varphi(x) = \langle x|\varphi\rangle$ in the realization space must be infinitely differentiable and that the functions and their derivatives must decay at infinity faster than any power of x. Therefore, $\varphi(x) \in \mathcal{S}(\mathbb{R})$. Moreover, the topology on $\mathbf{\Phi}$ is equivalent to the topology on $\mathcal{S}(\mathbb{R})$. To show that equivalence, we recall that the topology on $\mathbf{\Phi}$ is described by the following prescription for sequence convergence: a sequence $\varphi_k \in \mathbf{\Phi}$ converges to $\varphi \in \mathbf{\Phi}$ if

$$\|\varphi_k - \varphi\|_p \to 0\,, \quad p = 0, 1, 2, \ldots, \tag{3.6.93}$$

where $\|\varphi\|_p = \sqrt{(\varphi, (N+I)^p)}$. In the realization of $\mathbf{\Phi}$, the conditions (3.6.93) are equivalent to the following: a sequence $\varphi_k(x) = \langle x|\varphi_k\rangle$, which is the realization of the $\tau_{\mathbf{\Phi}}$-convergent

sequence $\varphi_k \to \varphi$, converges to $\varphi(x) = \langle x|\varphi\rangle$ if the $x^n \frac{d^m}{dx^m}\varphi_k(x)$ converge uniformly on every bounded region to $x^n \frac{d^m}{dx^m}\varphi(x)$ for each $n, m = 0, 1, 2, \ldots$ Therefore the topology of the realization of $\mathbf{\Phi}$ is equivalent to the topology of the Schwartz space.

Since the space $\mathbf{\Phi}$ is realized by the Schwartz space $\mathcal{S}(\mathbb{R})$, the dual space $\mathbf{\Phi}^\times$ is realized by the space of tempered distributions $\mathcal{S}(\mathbb{R})^\times$. The realization of the generalized eigenvector $|x\rangle$ of Q is the Dirac delta function (see Eq. (3.6.45)), which is a distribution that belongs to $\mathcal{S}(\mathbb{R})^\times$,

$$\mathbf{\Phi}^\times \ni |x\rangle \longleftrightarrow \langle x'|x\rangle = \delta(x'-x) \in \mathcal{S}(\mathbb{R})^\times \,. \tag{3.6.94}$$

The realization of the generalized eigenvector $|p\rangle$ of P is the exponential function e^{ixp}, which is also a distribution,[6]

$$\mathbf{\Phi}^\times \ni |p\rangle \longleftrightarrow \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ixp/\hbar} \in \mathcal{S}(\mathbb{R})^\times \,. \tag{3.6.95}$$

To say that $\delta(x'-x)$ and $\frac{1}{\sqrt{2\pi\hbar}}e^{ixp/\hbar}$ are distributions in $\mathcal{S}(\mathbb{R})^\times$ means that they only make sense as kernels of integrals that involve functions $\varphi(x) \in \mathcal{S}(\mathbb{R})$,

$$\int_{-\infty}^{+\infty} dx' \delta(x'-x)\varphi(x') = \varphi(x)\,, \quad \varphi(x) \in \mathcal{S}(\mathbb{R})\,, \tag{3.6.96}$$

$$\int_{-\infty}^{+\infty} dp \frac{1}{\sqrt{2\pi\hbar}} e^{ixp/\hbar}\widehat{\varphi}(p) = \varphi(x)\,, \quad \varphi(x) \in \mathcal{S}(\mathbb{R})\,, \tag{3.6.97}$$

or in bra-ket notation

$$\int_{-\infty}^{+\infty} dx' \langle x|x'\rangle\langle x'|\varphi\rangle = \langle x|\varphi\rangle\,, \tag{3.6.98}$$

$$\int_{-\infty}^{+\infty} dp\, \langle x|p\rangle\langle p|\varphi\rangle = \langle x|\varphi\rangle\,. \tag{3.6.99}$$

Finally, it is clear that the Hilbert space $\mathcal{H}$ is realized by the space of Lebesgue square integrable functions $L^2(\mathbb{R}, dx)$.

Summarizing, each vector φ in the vector space $\mathbf{\Phi}$ can be fully characterized by its components with respect to the continuous basis system of eigenvectors $|x\rangle$ of Q,

$$\varphi = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|\varphi\rangle\,. \tag{3.6.100}$$

Thus to the vector φ corresponds the function $\langle x|\varphi\rangle = \varphi(x)$ and to the vector $P\varphi$ corresponds the function $\langle x|P|\varphi\rangle \equiv P\varphi(x)$. Equation (3.6.79) then states that in the realization of the space of vectors φ by the space of wave functions $\langle x|\varphi\rangle = \varphi(x)$, the momentum operator is realized by the differential operator times $\hbar/i$,

$$P \longleftrightarrow -i\hbar\frac{d}{dx}\,, \tag{3.6.101}$$

[6]The exponential function is not square integrable.

Eq. (3.6.66) states that the position operator is realized by the operator of multiplication by x

$$Q \longleftrightarrow x\,, \tag{3.6.102}$$

and Eq. (3.6.88) states that the energy operator is realized by the differential operator

$$H \longleftrightarrow \Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{\mu\omega^2}{2}x^2\Big)\,. \tag{3.6.103}$$

The realization of the space $\mathbf{\Phi}$ for the harmonic oscillator given by the association

$$\mathbf{\Phi} \ni \varphi \longleftrightarrow \varphi(x) = \langle x|\varphi\rangle \in \mathcal{S}(\mathbb{R}) \tag{3.6.104}$$

between the vector φ and its "continuous components" $\langle x|\varphi\rangle = \varphi(x)$ establishes an equivalence between two Rigged Hilbert Spaces, the RHS of the harmonic oscillator

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \tag{3.6.105}$$

and the RHS of Schwartz space functions

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dx) \subset \mathcal{S}^\times(\mathbb{R})\,. \tag{3.6.106}$$

This realization is called the *Schrödinger (position) representation* or the *x-representation.*

We stress that the Schrödinger representation could not be derived from the Heisenberg commutation relation

$$[P, Q] = -i\hbar I \tag{3.6.107}$$

and the relation

$$H = \frac{1}{2\mu}P^2 + \frac{\mu\omega^2}{2}Q^2 \tag{3.6.108}$$

alone, but required an additional assumption: the operator H has at least one proper eigenvector in the space of states.

It is usually very useful to show the realizations of the abstract mathematical objects (RHS, operators, functions, eigenvectors) through a diagram. For instance, the position representation of the operator Q is visualized by the following diagram:

<u>x-representation diagram for the operator Q</u>

$$\begin{array}{ccccccccccc}
Q, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^\times & \ni & |x\rangle \\
\updownarrow & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\
x, & \varphi(x) = \langle x|\varphi\rangle & \in & \mathcal{S}(\mathbb{R}) & \subset & L^2(\mathbb{R}, dx) & \subset & \mathcal{S}(\mathbb{R})^\times & \ni & \langle x'|x\rangle = \delta(x - x')
\end{array} \tag{3.6.109}$$

On the top line of the diagram (3.6.109), we have the abstract objects. On the bottom line, we have the x-realizations of all these abstract objects: Q is realized by the multiplication

operator, φ is realized by the position wave function $\varphi(x)$, $\mathbf{\Phi}$ by the Schwartz space $\mathcal{S}(\mathbb{R})$, $\mathcal{H}$ by the Hilbert space of square integrable functions $L^2(\mathbb{R}, dx)$, $\mathbf{\Phi}^\times$ by the space of tempered distributions $\mathcal{S}(\mathbb{R})^\times$ and $|x\rangle$ by the Dirac delta function $\delta(x - x')$.

In a similar way, we can construct the position representation diagram for the momentum operator P,

x-representation diagram for the operator P

$$\begin{array}{ccccccccccc}
P, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^\times & \ni & |p\rangle \\
\updownarrow & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\
-i\hbar\frac{d}{dx}, & \varphi(x) = \langle x|\varphi\rangle & \in & \mathcal{S}(\mathbb{R}) & \subset & L^2(\mathbb{R}, dx) & \subset & \mathcal{S}(\mathbb{R})^\times & \ni & \langle x|p\rangle = \frac{e^{ixp/\hbar}}{\sqrt{2\pi\hbar}}
\end{array} \tag{3.6.110}$$

As in the diagram (3.6.109), the top line of (3.6.110) contains the abstract mathematical objects and the bottom line contains their x-realizations.

The x-diagram for the energy operator reads

x-representation diagram for the operator H

$$\begin{array}{ccccccccccc}
H, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^\times & \ni & |n\rangle \\
\updownarrow & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\
\frac{-\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{\mu\omega^2}{2}x^2, & \varphi(x) & \in & \mathcal{S}(\mathbb{R}) & \subset & L^2(\mathbb{R}, dx) & \subset & \mathcal{S}(\mathbb{R})^\times & \ni & \phi_n(x)
\end{array} \tag{3.6.111}$$

The momentum representation leads to similar considerations. The operator P is realized by the multiplication operator (see Eq. (3.6.67))

$$P\widehat{\varphi}(p) = p\widehat{\varphi}(p)\,, \tag{3.6.112}$$

and the operator Q by the differentiation operator (see Eq. (3.6.80))

$$Q\widehat{\varphi}(p) = -\frac{\hbar}{i}\frac{d}{dp}\widehat{\varphi}(p)\,. \tag{3.6.113}$$

The space $\mathbf{\Phi}$ is realized by the Schwartz space of functions $\widehat{\varphi}(p)$. In the p-representation, the generalized eigenvector $|x\rangle$ is realized by the exponential function

$$\mathbf{\Phi}^\times \ni |x\rangle \longleftrightarrow \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}\,, \tag{3.6.114}$$

and the eigenvector $|p\rangle$ by the Dirac delta function

$$\mathbf{\Phi}^\times \ni |p\rangle \longleftrightarrow \langle p'|p\rangle = \delta(p' - p)\,. \tag{3.6.115}$$

As a consequence of (3.6.114),

$$\widehat{\varphi}(p) = \langle p|\varphi\rangle = \int_{-\infty}^{+\infty} dx\, \langle p|x\rangle\langle x|\varphi\rangle = \int_{-\infty}^{+\infty} dx\, \frac{1}{\sqrt{2\pi\hbar}} e^{-ixp/\hbar}\varphi(x)\,, \tag{3.6.116}$$

Therefore, we can transform from the position representation $\varphi(x)$ into the momentum representation $\widehat{\varphi}(p)$ using (3.6.95) and (3.6.116). Note that Eqs. (3.6.95) and (3.6.116) show that the x- and the p-representation are related by the Fourier transform.

We can also construct diagrams similar to those constructed for the position representation. For instance, the p-representation of the position operator leads to

<u>p-representation diagram for the operator Q</u>

$$\begin{array}{ccccccccccc}
Q, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^{\times} & \ni & |x\rangle \\
\updownarrow & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\
\frac{-\hbar}{i}\frac{d}{dp}, & \widehat{\varphi}(p) = \langle p|\varphi\rangle & \in & \mathcal{S}(\mathbb{R}) & \subset & L^2(\mathbb{R}, dp) & \subset & \mathcal{S}(\mathbb{R})^{\times} & \ni & \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}
\end{array} \tag{3.6.117}$$

For the momentum operator we have:

<u>p-representation diagram for the operator P</u>

$$\begin{array}{ccccccccccc}
P, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^{\times} & \ni & |p\rangle \\
\updownarrow & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\
p, & \widehat{\varphi}(p) = \langle p|\varphi\rangle & \in & \mathcal{S}(\mathbb{R}) & \subset & L^2(\mathbb{R}, dp) & \subset & \mathcal{S}(\mathbb{R})^{\times} & \ni & \langle p'|p\rangle = \delta(p' - p)
\end{array} \tag{3.6.118}$$

Finally, the p-representation diagram for the energy operator reads

<u>p-representation diagram for the operator H</u>

$$\begin{array}{ccccccccccc}
H, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^{\times} & \ni & |n) \\
\updownarrow & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\
-\frac{\hbar^2\mu\omega^2}{2}\frac{d^2}{dp^2} + \frac{1}{2\mu}p^2, & \widehat{\varphi}(p) & \in & \mathcal{S}(\mathbb{R}) & \subset & L^2(\mathbb{R}, dp) & \subset & \mathcal{S}(\mathbb{R})^{\times} & \ni & \langle p|n) = \widehat{\phi}_n(p)
\end{array} \tag{3.6.119}$$

For the sake of completeness, we recall the energy representation $\varphi(n) = (n|\varphi\rangle$. In this representation, the variable $n \equiv E_n$ is discrete, and the realization of the vectors φ are given

by sequences of complex numbers $\varphi(n) = (n|\varphi\rangle$ rather than by functions. The Hilbert space $\mathcal{H}$ is realized by the sequence of square integrable functions (3.3.51) and the space $\mathbf{\Phi}$ by the space of rapidly decreasing sequences (3.3.52). The matrix elements of the operators H, Q and P are

$$(n|H|m) = E_n\,\delta_{nm}\,, \tag{3.6.120}$$

$$(m|Q|n) = \sqrt{\frac{\hbar}{2\mu\omega}}\left(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right)\,, \tag{3.6.121}$$

and

$$(m|P|n) = -i\sqrt{\frac{\hbar\mu\omega}{2}}\left(\sqrt{n}\,\delta_{m,n-1} - \sqrt{n+1}\,\delta_{m,n+1}\right)\,, \tag{3.6.122}$$

respectively. In this representation, these operators are visualized as infinite matrices whose entries are given by the equations (3.6.120)-(3.6.122).

3.6.4 Summary

In the preceding sections, we have constructed the Rigged Hilbert Space for the one-dimensional harmonic oscillator. We started out with the algebra of observables $\mathcal{A}$ generated by P, Q and H. These operators fulfill the algebraic relations

$$[P,Q] = -i\hbar I\,, \qquad H = \frac{1}{2\mu}P^2 + \frac{\mu w^2}{2}Q^2\,. \tag{3.6.123}$$

The elements of $\mathcal{A}$ were assumed to be symmetric operators defined on a linear space Ψ,

$$(A\varphi,\psi) = (\varphi,A\psi)\,, \quad \varphi,\psi\in\Psi\,, \quad A\in\mathcal{A}\,, \tag{3.6.124}$$

where $(\,\cdot\,,\,\cdot\,)$ is the scalar product that provides the probabilities. This space Ψ was assumed to remain stable under the action of the elements of $\mathcal{A}$. We made the crucial additional assumption that the operator H has at least one eigenvector[7] ϕ_0 in the space Ψ,

$$H\phi_0 = \frac{1}{2}\hbar\omega\phi_0\,. \tag{3.6.125}$$

From this one eigenvector we defined the vectors

$$|n) = \frac{1}{\sqrt{n!}}(a^\dagger)^n\phi_0\,, \quad n = 0,1,2,\ldots, \tag{3.6.126}$$

which fulfill

$$H|n) = \hbar\omega(n+1/2)|n)\,. \tag{3.6.127}$$

[7]This is equivalent to the assumption that H is essentially self-adjoint on the invariant dense subspace of the algebra $\mathcal{A}$.

These eigenvectors span the linear space Ψ. With respect to the scalar product on Ψ, the eigenvectors $|n)$ are orthonormal to each other,

$$(n|m) = \delta_{nm} \,. \tag{3.6.128}$$

The space Ψ was completed to the Hilbert space $\mathcal{H}$ using the topology generated by the norm

$$\|\varphi\| = \sqrt{(\varphi, \varphi)} \,. \tag{3.6.129}$$

The (complete) Hilbert space $\mathcal{H}$ is

$$\mathcal{H} = \{\varphi = \sum_{n=0}^{\infty} |n)(n|\varphi) \mid \quad \sum_{n=0}^{\infty} |(n|\varphi)|^2 < \infty\} \,. \tag{3.6.130}$$

The operators in the algebra of observables were extended from Ψ into larger subdomains of $\mathcal{H}$. However, these extensions are not continuous with respect to the Hilbert space topology, and the domains do not remain stable under the action of the operators. In order to find a common invariant subdomain $\mathbf{\Phi}$ for the algebra $\mathcal{A}$ that is endowed with a topology that makes these observables continuous operators, we introduced the sequence of scalar products

$$(\varphi, \psi)_p = (\varphi, (N + I)^p \psi) \,, \quad p = 0, 1, 2, \ldots \tag{3.6.131}$$

The completion of Ψ with respect to the topology generated by these scalar products is the space

$$\mathbf{\Phi} = \{\varphi = \sum_{n=0}^{\infty} |n)(n|\varphi) \mid \quad \sum_{n=0}^{\infty} (n+1)^p \, |(n|\varphi)|^2 < \infty \,, \quad p = 0, 1, 2, \ldots\} \,. \tag{3.6.132}$$

The elements of the algebra $\mathcal{A}$ were extended continuously into $\mathbf{\Phi}$. The space $\mathbf{\Phi}$ remains stable under the action of these extensions and all these extensions are continuous with respect to the topology on $\mathbf{\Phi}$. Therefore, all the algebraic calculations needed in physics involving the elements of the algebra of observables are allowed.

The operators P and Q are essentially self-adjoint[8] and have a continuous spectrum that coincides with the real line. In order to associate an eigenvector to each element of the spectrum of these operators, we introduced the adjoint space $\mathbf{\Phi}^\times$ and constructed the RHS

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \,. \tag{3.6.133}$$

In this RHS, the Gelfand-Maurin Theorem holds. This theorem assured the existence of a complete system of generalized eigenvectors of Q

$$Q^\times |x\rangle = x|x\rangle \,, \quad |x\rangle \in \mathbf{\Phi}^\times \,, \tag{3.6.134}$$

[8] As a consequence of H being essentially self-adjoint.

such that any $\varphi \in \mathbf{\Phi}$ was expanded in terms of these generalized eigenvectors of Q,

$$\varphi = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|\varphi\rangle\,. \tag{3.6.135}$$

Eq. (3.6.135) is the mathematical rephrasing of the heuristic Dirac basis vector expansion.

Using the spectral decomposition (3.6.135), we derived the x-realization of the abstract φ by functions $\varphi(x)$ in the Schwartz space,

$$\mathbf{\Phi} \ni \varphi \longleftrightarrow \varphi(x) = \langle x|\varphi\rangle \in \mathcal{S}(\mathbb{R})\,. \tag{3.6.136}$$

In particular, to every eigenvector $|n)$ of H there corresponds a function $\langle x|n) = \phi_n(x)$,

$$|n) \longleftrightarrow \langle x|n) = \phi_n(x)\,, \tag{3.6.137}$$

given in terms of the Hermite polynomials. The x-representation of the operator Q is the multiplication operator

$$Q\varphi \longleftrightarrow x\varphi(x)\,, \tag{3.6.138}$$

the x-representation of the operator P is given by the differentiation operator

$$P\varphi \longleftrightarrow \frac{\hbar}{i}\frac{d}{dx}\varphi(x)\,, \tag{3.6.139}$$

and the x-representation of the Hamiltonian is

$$H\varphi \longleftrightarrow \Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{\mu\omega^2}{2}x^2\Big)\varphi(x)\,. \tag{3.6.140}$$

The realization of $\mathbf{\Phi}$ given by the association between the vector φ and its "continuous components" $\varphi(x)$ yields the realization of the abstract RHS

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \tag{3.6.141}$$

by the RHS of Schwartz space functions

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dx) \subset \mathcal{S}^\times(\mathbb{R})\,. \tag{3.6.142}$$

The generalized eigenvector $|x\rangle$ of Q is realized by the Dirac delta function

$$\mathbf{\Phi}^\times \ni |x\rangle \longleftrightarrow \langle x'|x\rangle = \delta(x'-x) \in \mathcal{S}(\mathbb{R})^\times\,, \tag{3.6.143}$$

and the generalized eigenvector $|p\rangle$ of P by the exponential function

$$\mathbf{\Phi}^\times \ni |p\rangle \longleftrightarrow \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ixp/\hbar} \in \mathcal{S}(\mathbb{R})^\times\,. \tag{3.6.144}$$

Therewith, we have derived the Schrödinger representation of the harmonic oscillator from the algebraic assumptions (3.6.123)-(3.6.125). We remark again that the Schrödinger

representation is only one of the many possible representations of (3.6.123), and that it is the additional assumption (3.6.125) which singles out the Schrödinger representation among all the possible representations.[9]

From a mathematical point of view, the RHS formulation extends the Hilbert space formulation and justifies the mathematically undefined operations that physicists are accustomed to in their calculations. In particular, using the Rigged Hilbert Space formalism we are able to reproduce the main features of the Dirac formalism.

3.7 A Remark Concerning Generalizations

3.7.1 Realization of the Abstract RHS by Spaces of Functions

The realization of the RHS of the harmonic oscillator by the RHS of Schwartz functions suggests that any RHS associated to the spectral decomposition of an operator can be realized by spaces of functions.

Let A be an operator defined on the RHS $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ and

$$\varphi = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, |\lambda\rangle\langle\lambda|\varphi\rangle \tag{3.7.1}$$

be the spectral decomposition of $\varphi \in \mathbf{\Phi}$ provided by the Gelfand-Maurin Theorem. The quantity $\langle\lambda|\varphi\rangle$ which appears in this spectral decomposition may be regarded as a complex function of the real variable $\lambda \in \mathrm{Sp}(A)$, i.e., we can define

$$\begin{aligned} \varphi(\cdot) : \mathrm{Sp}(A) &\longmapsto \mathbb{C} \\ \lambda &\longmapsto \varphi(\lambda) := \langle\lambda|\varphi\rangle\,. \end{aligned} \tag{3.7.2}$$

(In this section, we shall write $\varphi(\cdot)$ when we want to speak about a function and $\varphi(\lambda)$ when we want to speak about the value of this function at a particular point λ). If we write

$$(\varphi,\varphi) = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, \langle\varphi|\lambda\rangle\, \langle\lambda|\varphi\rangle = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, |\langle\lambda|\varphi\rangle|^2\,, \tag{3.7.3}$$

we immediately realize that $\varphi(\cdot)$ in (3.7.2) must be a square integrable function with respect to $d\mu(\lambda)$. We shall denote the space of functions fulfilling (3.7.3) as $L^2(\mathrm{Sp}(A), d\mu(\lambda))$. The scalar product on $L^2(\mathrm{Sp}(A), d\mu(\lambda))$ is defined as

$$(\varphi(\cdot), \psi(\cdot))_{L^2} := \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, \overline{\varphi(\lambda)}\, \psi(\lambda)\,. \tag{3.7.4}$$

[9] There are several equivalent forms of the assumption (3.6.125):
(a) The assumption that H is essentially self adjoint.
(b) The assumption that P, Q, and I are the generators of a group, the Weyl group (subgroup of the symmetry group of non-relativistic space-time, the Galilei group).

If φ, $\psi \in \mathbf{\Phi}$, we have

$$(\varphi(\cdot), \psi(\cdot))_{L^2} = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, \langle\varphi|\lambda\rangle\, \langle\lambda|\psi\rangle = (\varphi, \psi)\,. \tag{3.7.5}$$

Thus the mapping $\varphi \leftrightarrow \varphi(\cdot)$ that takes $\varphi \in \mathcal{H}$ into the function $\varphi(\cdot) \in L^2(\mathrm{Sp}(A), d\mu(\lambda))$ preserves the scalar products,

$$(\varphi, \psi)_{\mathcal{H}} = (\varphi(\cdot), \psi(\cdot))_{L^2}\,. \tag{3.7.6}$$

Further, this mapping is obviously linear, because $\langle\lambda|\alpha\varphi + \beta\psi\rangle = \alpha\langle\lambda|\varphi\rangle + \beta\langle\lambda|\psi\rangle$ for $\alpha, \beta \in \mathbb{C}$. Thus, this mapping can be represented by means of a linear operator $U^\dagger$ such that

$$\begin{aligned} U^\dagger : \mathbf{\Phi} &\longmapsto L^2(\mathrm{Sp}(A), d\mu(\lambda)) \\ \varphi &\longmapsto U^\dagger\varphi = \varphi(\cdot)\,. \end{aligned} \tag{3.7.7}$$

Since $U^\dagger$ preserves scalar products, $U^\dagger$ is an isometry (cf. Section 2.5.2). Moreover, it can be proved that the image of $\mathbf{\Phi}$ by $U^\dagger$ is dense in $L^2(\mathrm{Sp}(A), d\mu(\lambda))$. Therefore, $U^\dagger$ has a unique extension to $\mathcal{H}$. This extension (which we also denote by $U^\dagger$) is a unitary operator from $\mathcal{H}$ onto $L^2(\mathrm{Sp}(A), d\mu(\lambda))$,

$$\begin{aligned} U^\dagger : \mathcal{H} &\longmapsto L^2(\mathrm{Sp}(A), d\mu(\lambda)) \\ f &\longmapsto U^\dagger f\,. \end{aligned} \tag{3.7.8}$$

It is important to remark that the equation $f(\lambda) = \langle\lambda|f\rangle$, i.e., the statement that the value of the function $f(\cdot)$ at the point λ equals the action of the functional $\langle\lambda|$ at f, holds only when f is an element of $\mathbf{\Phi}$. For a general f in $\mathcal{H}$, the corresponding $U^\dagger f \equiv f(\cdot)$ has no meaning as a function, but only as a class of equivalence of functions which differ on a set of zero Lebesgue measure.

We can endow $U^\dagger\mathbf{\Phi}$ with a topology τ_λ by transporting the topology of $\mathbf{\Phi}$ into $U^\dagger\mathbf{\Phi}$ via $U^\dagger$. Since $\mathbf{\Phi}$ is assumed to satisfy the first axiom of countability, so does $U^\dagger\mathbf{\Phi}$. Therefore, we can transport the topology $\tau_{\mathbf{\Phi}}$ on $\mathbf{\Phi}$ into $U^\dagger\mathbf{\Phi}$ by using the notion of sequence convergence. Then, we say that $\varphi_n(\cdot) \to \varphi(\cdot)$ with respect to τ_λ iff $\varphi_n \to \varphi$ with respect to $\tau_{\mathbf{\Phi}}$. With this definition, all topological properties are transferred from $\mathbf{\Phi}$ into $U^\dagger\mathbf{\Phi}$ by means of $U^\dagger$. In particular, $U^\dagger\mathbf{\Phi}$ is a τ_λ-complete nuclear space, and it is τ_λ-dense in $L^2(\mathrm{Sp}(A), d\mu(\lambda))$, i.e., for any $f(\cdot) \in L^2(\mathrm{Sp}(A), d\mu(\lambda))$ there exists a sequence of functions $\{\varphi_n(\cdot)\}_{n=1}^\infty$ in $U^\dagger\mathbf{\Phi}$ such that

$$\int_{\mathrm{Sp}(A)} d\mu(\lambda)\, |\varphi_n(\lambda) - f(\lambda)|^2 \xrightarrow[n\to\infty]{} 0\,. \tag{3.7.9}$$

Our next step is to extend the operator $U^\dagger$ on $\mathbf{\Phi}$ to an operator $U^\times$ on $\mathbf{\Phi}^\times$. This operator is defined by

$$\langle U^\dagger\varphi|U^\times F_\lambda\rangle := \langle\varphi|F_\lambda\rangle\,, \quad \varphi \in \mathbf{\Phi}\,,\ F_\lambda \in \mathbf{\Phi}^\times\,. \tag{3.7.10}$$

$U^\times$ is a well defined linear operator from $\mathbf{\Phi}^\times$ into $(U^\dagger\mathbf{\Phi})^\times$. To show this, we just need to prove that $U^\times F_\lambda$ is a continuous antilinear functional on $U^\dagger\mathbf{\Phi}$. The antilinearity follows from the definition (3.7.10), and the continuity from the fact that if $U^\dagger\varphi_n \to U^\dagger\varphi$, then

$$\langle U^\dagger\varphi_n|U^\times F_\lambda\rangle = \langle\varphi_n|\lambda\rangle \to \langle\varphi|\lambda\rangle = \langle U^\dagger\varphi|U^\times F_\lambda\rangle\,. \tag{3.7.11}$$

Therefore, $U^\times F_\lambda$ is an element of $(U^\dagger\mathbf{\Phi})^\times$.

The action of $U^\times$ extends the action of $U^\dagger$. This means that if $f \in \mathcal{H}$, then $U^\times f = U^\dagger f$. In fact,

$$\langle U^\dagger\varphi|U^\times f\rangle = \langle\varphi|f\rangle \equiv (\varphi, f) = (U^\dagger\varphi, U^\dagger f) \equiv \langle U^\dagger\varphi|U^\dagger f\rangle \tag{3.7.12}$$

for any $\varphi \in \mathbf{\Phi}$ or, equivalently, for any $U^\dagger\varphi \in U^\dagger\mathbf{\Phi}$. Therefore, the functionals $U^\times f$ and $U^\dagger f$ can be identified.

One can also prove that $U^\times : \mathbf{\Phi}^\times \to (U^\dagger\mathbf{\Phi})^\times$ is continuous when $\mathbf{\Phi}^\times$ is endowed with the $\tau^\times$ topology and $(U\mathbf{\Phi})^\times$ with the $\tau^\times_\lambda$ topology. Hence

$$U^\times\mathbf{\Phi}^\times = (U^\dagger\mathbf{\Phi})^\times \tag{3.7.13}$$

and both spaces have the same linear topological structure.

In summary, we have constructed a realization of the RHS

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \tag{3.7.14}$$

by the RHS of spaces of functions

$$U^\dagger\mathbf{\Phi} \subset L^2(\mathrm{Sp}(A), d\mu(\lambda)) \subset (U^\dagger\mathbf{\Phi})^\times \tag{3.7.15}$$

using the unitary operator $U^\dagger$ provided by the Gelfand-Maurin Theorem.

At this point, it is important to stress that the unitary operator $U^\dagger$ which yields the realization of $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ depends drastically on A (the operator providing the generalized eigenvectors). The dependence of the space $L^2(\mathrm{Sp}(A), d\mu(\lambda))$ on A is twofold: both $\mathrm{Sp}(A)$ and $d\mu(\lambda)$ depend on A. However, it is also possible that two different observables A and B (with two different $U^\dagger$'s) lead to the same space $L^2(\mathrm{Sp}(A), d\mu(\lambda))$. For instance, in the case of the harmonic oscillator we have seen that $A = Q$ and $B = P$ both lead to $L^2(\mathrm{Sp}(A), d\mu(\lambda)) = L^2(\mathbb{R})$. However, the Gelfand-Maurin theorem for Q gives a unitary operator $U^\dagger$ from $\mathcal{H}$ onto $L^2(\mathbb{R})$, and for P gives the operator $V^\dagger = \mathcal{F}U^\dagger$, where $\mathcal{F}$ is the Fourier transform operator.

Along with the realization of the vectors of the triplet $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$, we can also consider a realization of observables. If A is an operator on $\mathbf{\Phi}$, then $U^\dagger AU$ is the corresponding operator on $U^\dagger\mathbf{\Phi}$. We call $U^\dagger AU$ the *realization* of A on $U^\dagger\mathbf{\Phi}$.

As we did in the case of the harmonic oscillator, we show the realization of an abstract RHS through the following diagram:

$$\begin{array}{ccccccccccc}
A, & \varphi & \in & \mathbf{\Phi} & \subset & \mathcal{H} & \subset & \mathbf{\Phi}^\times & \ni & |\lambda\rangle \\
\downarrow & \downarrow & & U^\dagger\downarrow & & U^\dagger\downarrow & & U^\times\downarrow & & \\
U^\dagger AU, & U^\dagger\varphi = \varphi(\cdot) & \in & U^\dagger\mathbf{\Phi} & \subset & L^2(\mathrm{Sp}(A), d\mu(\lambda)) & \subset & \mathbf{\Phi}^\times & \ni & U^\times|\lambda\rangle
\end{array} \tag{3.7.16}$$

The top line of the diagram (3.7.16) contains the abstract mathematical objects, and the bottom line contains their realizations.

An abstract RHS and its realization are equivalent Rigged Hilbert Spaces—there is no linear topological property that distinguishes one from the other. This suggests the following definition:

Definition Two Rigged Hilbert Spaces $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ and $\mathbf{\Psi} \subset \mathcal{G} \subset \mathbf{\Psi}^\times$ are *equivalent* iff there exists a unitary operator $U^\dagger$ from $\mathcal{H}$ onto $\mathcal{G}$ such that

1. $U^\dagger\mathcal{H} = \mathcal{G}$, $U^\dagger\mathbf{\Phi} = \mathbf{\Psi}$.

2. $U^\dagger$ and U are continuous with respect to the topologies on $\mathbf{\Phi}$ and $\mathbf{\Psi}$.

As a consequence, $U^\dagger$ can be extended to an operator $U^\times : \mathbf{\Phi}^\times \to \mathbf{\Psi}^\times$ defined by

$$\langle U^\dagger\varphi | U^\times F\rangle = \langle\varphi|F\rangle\,. \tag{3.7.17}$$

This extension $U^\times$ is a bicontinuous bijective[10] linear mapping from $\mathbf{\Phi}^\times$ onto $\mathbf{\Psi}^\times$ and hence $U^\times\mathbf{\Phi}^\times = \mathbf{\Psi}^\times$.

The RHS spectral decomposition

$$\varphi = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\,|\lambda\rangle\langle\lambda|\varphi\rangle \tag{3.7.18}$$

of $\varphi \in \mathbf{\Phi}$ is a "continuous infinite dimensional" generalization of the Hilbert space spectral decomposition of a compact self-adjoint operator. However, there are some differences between these two spectral decompositions. The content of (3.7.18) is that any vector in $\mathbf{\Phi}$ can be written in terms of the generalized eigenvectors of A. Therefore, the eigenvectors of $A^\times$ form a "system of generators" for the space $\mathbf{\Phi}$. This system of generators is not a basis for $\mathbf{\Phi}$ in the usual Hilbert space sense for the following reasons:

1. The vectors $|\lambda\rangle$ do not, in general, belong to $\mathbf{\Phi}$ or to $\mathcal{H}$.

[10] One-to-one, onto, with continuous inverse.

2. The finite or countably infinite sum

$$\varphi = \sum_{n=0}^{\infty} c_n e_n = \sum_{n=0}^{\infty} (e_n, \varphi) e_n \tag{3.7.19}$$

in the Hilbert space spectral decomposition is replaced by an integral

$$\varphi = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, |\lambda\rangle \langle\lambda|\varphi\rangle \,. \tag{3.7.20}$$

In the Hilbert space spectral decomposition (3.7.19), c_n is the discrete coefficient (or weight) for e_n. The c_n can be viewed as the n-th component of φ with respect to the basis e_n. In the RHS spectral decomposition (3.7.20), $\varphi(\lambda) = \langle\lambda|\varphi\rangle$ is the continuous coefficient (or weight) for $|\lambda\rangle$. For a fixed $\lambda \in \mathrm{Sp}(A)$, $\varphi(\lambda) = \langle\lambda|\varphi\rangle$ can be viewed as the "λ-th" component of φ with respect to the system of generators $|\lambda\rangle$.

The decomposition (3.7.19) leads to a realization of the Hilbert space $\mathcal{H}$ by the space of sequences $\{c_n\}$ of complex numbers having the property $\sum_{n=0}^{\infty} |c_n|^2 < \infty$. Analogously, (3.7.20) leads to a realization of the space $\mathbf{\Phi}$ by the space of functions $\varphi(\lambda)$.

The Gelfand-Maurin Theorem allows us to spectrally decompose the scalar product of any two vectors φ, $\psi \in \mathbf{\Phi}$ as

$$(\psi, \varphi) = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, \langle\varphi|\lambda\rangle\langle\lambda|\psi\rangle \,. \tag{3.7.21}$$

In analogy to (3.7.21), we also spectrally decompose the action of any functional F at a vector φ,

$$\langle\varphi|F\rangle = \int_{\mathrm{Sp}(A)} d\mu(\lambda)\, \langle\varphi|\lambda\rangle\langle\lambda|F\rangle \,. \tag{3.7.22}$$

Hence, quantities of the type $\langle\lambda|F\rangle$ are distributions that are well defined only as a kernel of integration whenever we write the action of a functional F as an integral operator. As an example, the functional $|x\rangle$ that associates to any $\varphi \in \mathcal{S}(\mathbb{R})$ the value of the function at the point x,

$$\begin{aligned} |x\rangle : \mathcal{S}(\mathbb{R}) &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|x\rangle := \varphi(x) \,, \end{aligned} \tag{3.7.23}$$

can be written as an integral operator:

$$\langle\varphi|x\rangle = \int_{-\infty}^{+\infty} dx\, \langle\varphi|x'\rangle\langle x'|x\rangle \,. \tag{3.7.24}$$

The functional $|x\rangle$ in (3.7.23) is the Schwartz delta functional, whereas the distribution $\langle x'|x\rangle$ in (3.7.24) is the Dirac delta function,

$$\langle x'|x\rangle = \delta(x' - x) \,. \tag{3.7.25}$$

Therefore, the Dirac delta function appears when we spectrally decompose the action of the Schwartz delta function as an integral operator.

3.7.2 General Statement of the Gelfand-Maurin Theorem

The version of the Gelfand-Maurin Theorem stated in Section 3.5.2 is only suitable for cyclic operators. In general, the linear operators in the algebra of observables are not cyclic. Then more than one quantum number is needed to characterize pure states, and one needs a complete system of commuting operators to obtain a complete set of generalized eigenvectors.

Definition The collection of operators $\{A_k\}_{k=1}^N$ is a *system of commuting operators* if

1. $[A_i, A_k] = 0$ for all $i, k = 1, \ldots, N$,
2. $\sum_{k=1}^N A_k^2$ is essentially self-adjoint.

Let $\mathcal{A}$ be the algebra generated by a collection of operators $\{A_k\}_{k=1}^N$. Then the collection $\{A_k\}_{k=1}^N$ is said to be a *complete system* if there exists a vector $\varphi \in \mathbf{\Phi}$ such that the space

$$\{A\varphi \mid A \in \mathcal{A}\} \tag{3.7.26}$$

spans the Hilbert space $\mathcal{H}$.

The notions of generalized eigenvector and generalized eigenvalue of an operator can be extended to the case of a system $\{A_k\}_{k=1}^N$. An antilinear functional F on $\mathbf{\Phi}$ is a *generalized eigenvector* for a system $\{A_k\}_{k=1}^N$ if for every $k = 1, \ldots, N$ there exists a complex number $\lambda^{(k)}$ such that

$$A_k^\times F = \lambda^{(k)} F\,. \tag{3.7.27}$$

The numbers $\lambda \equiv (\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)})$ are called *generalized eigenvalues* corresponding to the generalized eigenvector $F \equiv |\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}\rangle$.

Theorem (Gelfand-Maurin Theorem) Let $\{A_k\}_{k=1}^N$ be a complete system of commuting, e.s.a., $\tau_{\mathbf{\Phi}}$-continuous operators on the Rigged Hilbert Space $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$. Then, there exists a set of generalized eigenvectors,

$$|\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}\rangle \in \mathbf{\Phi}^\times\,, \tag{3.7.28}$$

$$A_k^\times |\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}\rangle = \lambda^{(k)} |\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}\rangle\,, \tag{3.7.29}$$

$$\lambda^{(k)} \in \Lambda^{(k)} = \mathrm{Sp}(A_k)\,, \tag{3.7.30}$$

and a uniquely defined measure $d\mu(\lambda)$ on $\Lambda = \Lambda^{(1)} \times \Lambda^{(2)} \times \cdots \times \Lambda^{(N)}$, (where $\times$ denotes the Cartesian product), such that for every $\psi, \varphi \in \mathbf{\Phi}$

$$(\psi, \varphi) = \int_\Lambda d\mu(\lambda)\, \langle\psi|\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}\rangle\langle\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}|\varphi\rangle\,, \tag{3.7.31}$$

or omitting ψ,

$$\varphi = \int_\Lambda d\mu(\lambda)\, |\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(N)}\rangle\langle\lambda^{(1)}, \lambda^{(2)}, \ldots \lambda^{(N)}|\varphi\rangle\,. \tag{3.7.32}$$

This theorem gives the mathematical formulation of the famous Dirac conjecture if the starting point is a precisely defined algebra of observables.

The mathematical task that has to be accomplished if one starts out with a well defined algebra is to find a complete commuting system and its spectrum. The problem of determining when a system is complete is far from trivial. Already for the simplest cases of enveloping algebras of group representations the number of commuting observables is not independent of the particular commuting system.

The problem of the physicist is usually the reverse. From the experimental data one finds out how many quantum numbers are required, and what their possible values are. This gives a minimum number of operators for the complete commuting system because the "matrix elements" of the A_k's calculated from the properties of this algebra must agree with the experimental values of the corresponding observables.

3.7.3 Generalization of the Algebra of Operators

The construction of the nuclear space $\mathbf{\Phi}$ carried out for the harmonic oscillator can be immediately generalized to more general algebras of operators. The analog of the lemma (3.3.67) is

$$(\varphi, X(\Delta + I)^p X\varphi) \leq \kappa(\varphi, (\Delta + I)^{p+1}\varphi)\,, \tag{3.7.33}$$

where X is one of the generators X_i and $\Delta = \sum X_i^2$ is the Nelson operator (Laplacian). Eq. (3.7.33) holds for all enveloping algebras (lemma by Nelson). Therewith the continuity of the algebra in a linear topological space in which the topology is defined by the countable number of scalar products

$$(\varphi, \psi)_p = (\varphi, (\Delta + I)^p \psi) \tag{3.7.34}$$

follows immediately. Further, if Δ is e.s.a., then all symmetric generators are also e.s.a. (theorems by Nelson and Stinespring).

Eq. (3.7.33) is much stronger than what is required for the proof of the continuity of the generators. The continuity of the generators (and therewith of the whole algebra) can be proved if instead of $p + 1$ on the right hand side of (3.7.33) one has $p + n$, where n is any positive integer. Therefore, it appears that the continuity of the generators can already be proved for any finitely generated associative algebra.

The nuclearity is a much harder property to establish. It has been proven for the cases that the algebra is the enveloping algebra $E(G)$ of the following groups G:

1. G is nilpotent (because then $E(G)$ is isomorphic to the enveloping algebra generated by P_α, Q_α, $\alpha = 1, 2, \ldots m$, with $[P_\alpha, Q_\beta] = -\delta_{\alpha\beta} I$ for some m (a theorem by Kirillov in [69]) and we have just an m-dimensional generalization of the harmonic oscillator).

2. G is semi-simple (Bohm in [70]).

3. $G = A\Theta K$, where Θ stands for semidirect product, with A Abelian and K compact (B. Nagel in [71]).

4. G is the Poincare group, for some of the representations (see [71]).

3.7.4 Appendix: Continuity of the Algebra of the Harmonic Oscillator

In this appendix, we provide a proof for Eq. (3.3.67)

$$(\psi, a(N+I)^p a^\dagger \psi) \leq \kappa(\psi, (N+I)^{p+1}\psi)\,, \quad \forall \psi \in \Psi\,. \tag{3.7.35}$$

Before proceeding with the proof, we need some preliminary results. From the commutation relation (3.2.10), it follows that

$$(N+I)a^\dagger = a^\dagger(N+2I)\,, \tag{3.7.36}$$
$$a(N+I) = (N+2I)a\,. \tag{3.7.37}$$

It also holds that

$$(\psi, (N+I)\psi) \leq (\psi, (N+I)^2\psi)\,, \quad \forall \psi \in \Psi\,. \tag{3.7.38}$$

Eq. (3.7.38) comes from the fact that N is a positive operator, i.e., $(\psi, N\psi) \geq 0$ for each ψ in Ψ and then

$$\begin{aligned}(\psi, (N+I)^2\psi) - (\psi, (N+I)\psi) &= (N\psi, N\psi) + (\psi, N\psi) \\ &= \|N\psi\|^2 + (\psi, N\psi) \geq 0\,.\end{aligned} \tag{3.7.39}$$

From the positive definiteness of N, it also follows that if m and n are positive integers and $m \leq n$, then

$$(\psi, (N+I)^m\psi) \leq (\psi, (N+I)^n\psi)\,, \quad \forall \psi \in \Psi\,. \tag{3.7.40}$$

We are now going to prove Eq. (3.7.35) by induction. Eq. (3.7.35) is true for $p = 1$, because

$$\begin{aligned}(\psi, a(N+I)a^\dagger\psi) &= (\psi, aa^\dagger(N+2I)\psi) \\ &= (\psi, (N+I)(N+2I)\psi) \\ &= (\psi, (N+I)^2\psi) + (\psi, (N+I)\psi) \\ &\leq 2(\psi, (N+I)^2\psi)\,,\end{aligned} \tag{3.7.41}$$

where in the last step we have made use of Eq. (3.7.38).

We now assume that (3.7.35) is true for $p \leq q$, i.e.,

$$(\psi, a(N+I)^p a^\dagger\psi) \leq \kappa(\psi, (N+I)^{p+1}\psi)\,, \quad \forall \psi \in \Psi\,, \quad p = 1, 2, \ldots, q\,. \tag{3.7.42}$$

We have to prove that (3.7.35) is also true for $p = q+1$ using (3.7.42). So we calculate

$$\begin{aligned}(\psi, a(N+I)^{q+1}a^\dagger\psi) &= (\psi, a(N+I)(N+I)^{q-1}(N+I)a^\dagger\psi) \\ &= (\psi, (N+2I)a(N+I)^{q-1}a^\dagger(N+2I)\psi) \\ &= ((N+2I)\psi, a(N+I)^{q-1}a^\dagger(N+2I)\psi)\end{aligned} \tag{3.7.43}$$

$$
\begin{aligned}
&\leq \kappa((N+2I)\psi,(N+I)^q(N+2I)\psi) && (3.7.44)\\
&= \kappa[((N+I)\psi,\ (N+I)^q(N+I)\psi)+(\psi,(N+I)^q\psi)\\
&\quad +((N+I)\psi,(N+I)^q\psi)+(\psi,(N+I)^q(N+I)\psi)]\\
&= \kappa[(\psi,(N+I)^{q+2}\psi)+(\psi,(N+I)^q\psi)\\
&\quad +(\psi,(N+I)^{q+1}\psi)+(\psi,(N+I)^{q+1}\psi)]\\
&\leq 4\kappa(\psi,\ (N+I)^{q+2}\psi)\,, && (3.7.45)
\end{aligned}
$$

where we have used Eqs. (3.7.36)-(3.7.37) in step (3.7.43), Eq. (3.7.42) in step (3.7.44) and Eq. (3.7.40) in the last step.

Consequently, (3.7.35) has been shown to be fulfilled also for $p = q + 1$ and, therefore, it is true for any integer p.

Chapter 4

A Rigged Hilbert Space of the Square Barrier Potential

In this chapter, we construct a RHS of the square barrier Hamiltonian. In order to do it, we shall use the Sturm-Liouville theory. This theory provides the direct integral decomposition of the Hilbert space. From this direct integral decomposition, we shall construct the RHS.

CHARLIE [*Stopping* HAPPY's *movement and reply. To* BIFF] Nobody dast blame this man. You don't understand: Willy was a salesman. And for a salesman, there is no rock bottom to the life. He don't put a bolt to a nut, he don't tell you the law or give you medicine. He's a man way out there in the blue, riding on a smile and a shoeshine. And when they start not smiling back—that's an earthquake. And then you get yourself a couple of spots on your hat, and you're finished. Nobody dast blame this man. A salesman is got to dream, boy. It comes with the territory.

BIFF: Charley, the man didn't know who he was.

HAPPY[*infuriated*]: Don't say that!

BIFF: Why don't you come with me, Happy?

HAPPY: I'm not licked that easily. I'm staying right in this city, and I'm gonna beat this racket! [*He looks at* BIFF, *his chin set.*] The Loman Brothers!

BIFF: I know who I am, kid.

Arthur Miller, *Death of a Salesman*

4.1 Introduction

In the previous chapter, we have constructed the RHS of the harmonic oscillator. This system has a Hamiltonian whose spectrum is discrete, i.e., the solutions of the time independent Schrödinger equation corresponding to the harmonic oscillator are square normalizable. Because the spectrum of its Hamiltonian has no continuous part, the harmonic oscillator cannot have scattering states.

We now turn to study systems whose time independent Schrödinger equation has non-square normalizable solutions. That is, systems whose Hamiltonian has a continuous spectrum. We shall focus on the square barrier potential, because its Schrödinger equation can be solved explicitly. The square barrier potential will give us the long-sought example of the Rigged Hilbert Space generated by a Schrödinger Hamiltonian with continuous spectrum.

First, we review the gist of the Dirac formalism for the case of a Hamiltonian with continuous spectrum. The dynamical equation that governs the behavior of a quantum system at any time is the time dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\varphi(t) = H\varphi(t)\,, \tag{4.1.1}$$

where H denotes the Hamiltonian of the system and $\varphi(t)$ denotes the value of the wave function φ at time t. The Dirac formalism solves this equation formally as follows: for each energy E in the spectrum $\mathrm{Sp}(H)$ of the Hamiltonian, there exists a ket $|E\rangle$ that is an eigenvector of H,

$$H|E\rangle = E|E\rangle\,, \quad E \in \mathrm{Sp}(H)\,. \tag{4.1.2}$$

These eigenkets form a complete basis system that expands any wave function φ as

$$\varphi = \int dE\,|E\rangle\langle E|\varphi\rangle \equiv \int dE\,\varphi(E)|E\rangle\,. \tag{4.1.3}$$

The time dependent solution of Eq. (4.1.1) is obtained by Fourier-transforming the time independent solution (4.1.3),

$$\varphi(t) = \int dE\,e^{-iEt/\hbar}\,\varphi(E)\,. \tag{4.1.4}$$

If the spectrum of the Hamiltonian has a continuous part, and if the energy E belongs to this continuous part of the spectrum, then the corresponding eigenket $|E\rangle$ that solves Eq. (4.1.2) is not square integrable, i.e., $|E\rangle$ is not an element of the Hilbert space.

It is the purpose of this chapter to show that the Rigged Hilbert Space is the mathematical framework that supports the above formal manipulations. We will show that the expansion (4.1.3) is not valid for every element of the Hilbert space $\mathcal{H}$, but only for those φ that belong to the space of wave functions $\mathbf{\Phi} \subset \mathcal{H}$. We will also show that the kets $|E\rangle$ can be understood mathematically as continuous antilinear functionals over the space of wave functions $\mathbf{\Phi}$, i.e., $|E\rangle \in \mathbf{\Phi}^{\times}$.

According to the RHS mathematics, equation (4.1.2) means that

$$\langle H\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi\in\mathbf{\Phi}\,. \tag{4.1.5}$$

The action of H can be extended to the kets $|E\rangle$ in $\mathbf{\Phi}^\times$ as follows:

$$\langle\varphi|H^\times|E\rangle = \langle H\varphi|E\rangle\,, \quad \forall\varphi\in\mathbf{\Phi}\,. \tag{4.1.6}$$

Because H is continuous on $\mathbf{\Phi}$, the operator $H^\times$ is a uniquely defined extension of H. Using the definition (4.1.6), we rewrite Eq. (4.1.5) as

$$\langle\varphi|H^\times|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi\in\mathbf{\Phi}\,. \tag{4.1.7}$$

Omitting the arbitrary φ in this equation leads to

$$H^\times|E\rangle = E|E\rangle\,, \tag{4.1.8}$$

which is the same as Eq. (4.1.2). (Note that in Eq. (4.1.8) we have denoted the action of the Hamiltonian on the ket $|E\rangle$ by $H^\times$ and not just by H. We shall use this notation in order to stress that the Hamiltonian is acting on vectors that lie outside the Hilbert space.)

The statement of the Nuclear Spectral Theorem [5] only assures the existence of the generalized eigenvectors $|E\rangle$, but it does not say how to construct them or how to construct the space $\mathbf{\Phi}$, which is assumed to be given beforehand. In this chapter, we provide an example of a Hamiltonian with continuous spectrum where all the quantities are explicitly constructed. As mentioned above, this example is the three-dimensional square barrier potential. We shall use the Sturm-Liouville theory (Weyl theory) [30] to find the RHS of this potential.

By applying the Sturm-Liouville theory to the Schrödinger equation of the square barrier potential, we will obtain a domain $\mathcal{D}(H)$ on which the Hamiltonian is self-adjoint. The Green functions, the spectrum, and the unitary transformation that diagonalizes our Hamiltonian will be also computed. The diagonalization of the Hamiltonian will allow us to obtain the energy (spectral) representation and the direct integral decomposition of the Hilbert space induced by our Hamiltonian. We will see why this direct integral decomposition is not enough for the purposes of Quantum Mechanics and why the RHS is necessary. Next, we will construct the space $\mathbf{\Phi}$. The RHS

$$\mathbf{\Phi}\subset\mathcal{H}\subset\mathbf{\Phi}^\times \tag{4.1.9}$$

of the square barrier potential will follow. Dirac kets will be accommodated as elements of $\mathbf{\Phi}^\times$, and the Schwartz delta functional will appear in the energy (spectral) representation of the triplet (4.1.9). The Nuclear Spectral Theorem will be proved, and it will be shown that this theorem is just a restatement of the (heuristic) Dirac basis vector expansion (4.1.3).

4.2 Sturm-Liouville Theory Applied to the Square Barrier Potential

4.2.1 Schrödinger Equation in the Position Representation

In order to calculate the set of real generalized eigenvalues of the square barrier Hamiltonian (the physical spectrum) and their corresponding generalized eigenvectors, we solve equation (4.1.8) in the position representation,

$$\langle \vec{x}|H^{\times}|E\rangle = E\langle \vec{x}|E\rangle \,. \tag{4.2.1}$$

The expression of the Hamiltonian in the position representation is

$$\langle \vec{x}|H^{\times}|E\rangle = \left(\frac{-\hbar^2}{2m}\Delta + V(\vec{x})\right)\langle \vec{x}|E\rangle \,, \tag{4.2.2}$$

where Δ is the three-dimensional Laplacian and

$$V(\vec{x}) = V(r) = \begin{cases} 0 & 0 < r < a \\ V_0 & a < r < b \\ 0 & b < r < \infty \end{cases} \tag{4.2.3}$$

is the square barrier potential. Writing Eqs. (4.2.1) and (4.2.2) in spherical coordinates and restricting ourselves to the case of zero angular momentum, we obtain the radial time-independent Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right)\chi(r;E) = E\chi(r;E) \,. \tag{4.2.4}$$

Thus our Hamiltonian in the radial representation is given by the differential operator

$$h \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) \,. \tag{4.2.5}$$

Throughout this chapter, the symbol h will be used to denote the formal differential operator (4.2.5).

The Sturm-Liouville theory studies the differential operator

$$\frac{d}{dx}(p(x)\frac{d}{dx}) + q(x) \,, \tag{4.2.6}$$

where $p(x)$ and $q(x)$ are functions of the real variable x, x running over an interval of the real axis. In our example, x will be the radial coordinate r running over the interval $[0,\infty)$, $p(x)$ the constant $-\hbar^2/2m$ and $q(x)$ the square barrier potential (4.2.3). In this case, the Sturm-Liouville differential operator (4.2.6) coincides with the Schrödinger differential operator (4.2.5) and therefore we are allowed to apply the Sturm-Liouville theory to our problem.

Mathematically, all the information about the differential operator h provided by the Sturm-Liouville theory (resolvent, spectrum, spectral representation,...) is obtained from the generalized eigenvalue equation

$$h\chi(r,E) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right)\chi(r,E) = E\chi(r,E)\,, \quad E \in \mathbb{C}\,, \tag{4.2.7}$$

with various boundary conditions. As mentioned in the introduction, the "monoenergetic" eigensolutions of (4.2.7) are not in general square integrable, i.e., they are not in the Hilbert space. Those "monoenergetic" eigensolutions will be associated to antilinear functionals $F_E \in \mathbf{\Phi}^\times$ by

$$F_E(\varphi) \equiv \int_0^\infty dr\, \overline{\varphi(r)}\chi(r;E)\,. \tag{4.2.8}$$

These functionals are generalized eigenvectors of the Hamiltonian H,

$$H^\times F_E = EF_E\,, \tag{4.2.9}$$

or more precisely,

$$\langle\varphi|H^\times|F_E\rangle = \langle H\varphi|F_E\rangle = E\langle\varphi|F_E\rangle\,, \quad \forall\varphi \in \mathbf{\Phi}\,. \tag{4.2.10}$$

From a physical point of view, Eq. (4.2.7) is the time-independent Schrödinger equation. Different boundary conditions imposed upon it yield either Dirac kets, Lippmann-Schwinger kets or Gamow kets.

4.2.2 Self-Adjoint Extension

Our first objective will be to define a linear operator on a Hilbert space corresponding to the formal differential operator h and investigate its self-adjoint extensions. Among all the possibilities, we shall choose the self-adjoint extension that fits spherically symmetric potentials. Later sections will deal with the spectral properties of this self-adjoint extension and with the RHS induced by it.

The Hilbert space that is in the RHS of the square barrier potential is realized by the space $L^2([0,\infty),dr)$ of square integrable functions $f(r)$ defined on the interval $[0,\infty)$. In this section, we find a subdomain $\mathcal{D}(H)$ of this Hilbert space on which the differential operator h is self-adjoint. This domain must be a proper dense linear subspace of $L^2([0,\infty),dr)$. The action of h must be well-defined on $\mathcal{D}(H)$, and this action must remain in $L^2([0,\infty),dr)$. We need also a boundary condition that assures the self-adjointness of the Hamiltonian. Among all the possible boundary conditions that provide a self-adjoint extension (see Appendix 4.4.1), we choose $f(0) = 0$. These requirements can be written as

$$f(r) \in L^2([0,\infty),dr)\,, \tag{4.2.11a}$$

$$(hf)(r) \in L^2([0,\infty),dr)\,, \tag{4.2.11b}$$

$$f(r) \in AC^2[0,\infty)\,, \tag{4.2.11c}$$

$$f(0) = 0\,, \tag{4.2.11d}$$

where $AC^2[0,\infty)$ denotes the space of functions whose derivative is absolutely continuous (cf. Appendix 4.4.1). Condition (4.2.11a) just means that the wave functions are square normalizable. Condition (4.2.11b) assures that the action of h on any $f(r)$ is square integrable. Condition (4.2.11c) is the weakest condition sufficient for the second derivative of $f(r)$ to be well-defined. In our example, this condition implies that $f(r)$ and $f'(r)$ are continuous at $r=a$ and at $r=b$. Equation (4.2.11d) selects, among all the possible possible boundary conditions that provide a domain on which the differential operator h is self-adjoint (see Appendix 4.4.1), the self-adjoint extension needed in physics.

The reason why we choose (4.2.11d) is the following: in physics [1, 54, 72, 73], the set of boundary conditions imposed on the Schrödinger equation (4.2.7) always includes

$$\chi(0;E)=0\,, \tag{4.2.12a}$$

$$\chi(r;E),\ \text{and}\ \chi'(r;E)\ \text{are continuous at}\ r=a\ \text{and at}\ r=b\,. \tag{4.2.12b}$$

Condition (4.2.12b) is implied by (4.2.11c), so we just need to recover (4.2.12a). This is why we impose (4.2.11d).

The set of conditions (4.2.11) leads to the domain

$$\mathcal{D}(H)=\{f(r)\mid f(r),hf(r)\in L^2([0,\infty),dr),\ f(r)\in AC^2[0,\infty),\ f(0)=0\}\,. \tag{4.2.13}$$

In choosing (4.2.13) as the domain of our formal differential operator h, we define a linear operator H by

$$(Hf)(r):=hf(r)=\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)f(r)\,,\quad f(r)\in\mathcal{D}(H)\,. \tag{4.2.14}$$

4.2.3 Resolvent and Green Functions

The Green function is the kernel of integration needed to write the resolvent of H as an integral operator,

$$(E-H)^{-1}f(r)=\int_0^\infty G(r,s;E)f(s)\,ds\,. \tag{4.2.15}$$

In Dirac notation this equation reads

$$\langle r|(E-H)^{-1}|f\rangle=\int_0^\infty\langle r|(E-H)^{-1}|s\rangle\langle s|f\rangle\,ds\,, \tag{4.2.16}$$

and therefore

$$G(r,s;E)=\langle r|(E-H)^{-1}|s\rangle\,. \tag{4.2.17}$$

The so-called outgoing and incoming Green functions are defined by

$$G^{\pm}(r,s;E)=\lim_{\mu\to0^+}G(r,s;E\pm i\mu)\,. \tag{4.2.18}$$

The procedure to compute the Green function of our operator (4.2.14) is explained in [30] (see also [74]). For the sake of completeness, we include in Appendix 4.4.2 the statement

of the theorem that is used to calculate $G(r,s;E)$. The expression of the Green function will be given in terms of eigenfunctions of the differential operator h subject to different boundary conditions (cf. Theorem 1 in Appendix 4.4.2).

We shall consider three regions of the complex plane and compute the Green function for each region separately. In all our calculations, we will use the following branch of the square root function:

$$\sqrt{\cdot} : \{E \in \mathbb{C} \mid -\pi < \arg(E) \leq \pi\} \longmapsto \{E \in \mathbb{C} \mid -\pi/2 < \arg(E) \leq \pi/2\}\,. \tag{4.2.19}$$

Region $\Re(E) < 0$, $\Im(E) \neq 0$

For $\Re(E) < 0$, $\Im(E) \neq 0$, the Green function (see Theorem 1 in Appendix 4.4.2) is given by

$$G(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\, \frac{\widetilde{\chi}(r;E)\,\widetilde{\Theta}(s;E)}{2\widetilde{\mathcal{J}}_3(E)} & r < s \\ -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\, \frac{\widetilde{\chi}(s;E)\,\widetilde{\Theta}(r;E)}{2\widetilde{\mathcal{J}}_3(E)} & r > s \end{cases} \qquad \Re(E) < 0\,,\ \Im(E) \neq 0\,. \tag{4.2.20}$$

The eigenfunction $\widetilde{\chi}(r;E)$ satisfies the Schrödinger equation (4.2.7) and the boundary conditions

$$\widetilde{\chi}(0;E) = 0\,, \tag{4.2.21a}$$
$$\widetilde{\chi}(r;E) \in AC^2([0,\infty))\,, \tag{4.2.21b}$$
$$\widetilde{\chi}(r;E) \text{ is square integrable at } 0\,. \tag{4.2.21c}$$

The boundary conditions (4.2.21) can be written as

$$\widetilde{\chi}(0;E) = 0\,, \tag{4.2.22a}$$
$$\widetilde{\chi}(a-0;E) = \widetilde{\chi}(a+0;E)\,, \tag{4.2.22b}$$
$$\widetilde{\chi}'(a-0;E) = \widetilde{\chi}'(a+0;E)\,, \tag{4.2.22c}$$
$$\widetilde{\chi}(b-0;E) = \widetilde{\chi}(b+0;E)\,, \tag{4.2.22d}$$
$$\widetilde{\chi}'(b-0;E) = \widetilde{\chi}'(b+0;E)\,, \tag{4.2.22e}$$
$$\widetilde{\chi}(r;E) \text{ is square integrable at } 0\,, \tag{4.2.22f}$$

and lead to

$$\widetilde{\chi}(r;E) = \begin{cases} e^{\sqrt{-\frac{2m}{\hbar^2}E}r} - e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & 0 < r < a \\ \widetilde{\mathcal{J}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} + \widetilde{\mathcal{J}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} & a < r < b \\ \widetilde{\mathcal{J}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}E}r} + \widetilde{\mathcal{J}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & b < r < \infty\,. \end{cases} \tag{4.2.23}$$

The functions $\widetilde{\mathcal{J}}_1 - \widetilde{\mathcal{J}}_4$ are such that $\widetilde{\chi}(r;E)$ satisfies the boundary conditions (4.2.22), and their expressions are given in Eq. (4.4.12) of Appendix 4.4.2.

The eigenfunction $\widetilde{\Theta}(r;E)$ satisfies the Schrödinger equation (4.2.7) and the boundary conditions

$$\widetilde{\Theta}(r;E) \in AC^2([0,\infty))\,, \tag{4.2.24a}$$
$$\widetilde{\Theta}(r;E) \text{ is square integrable at } \infty\,. \tag{4.2.24b}$$

The boundary conditions (4.2.24) can be written as

$$\widetilde{\Theta}(a-0;E) = \widetilde{\Theta}(a+0;E)\,, \tag{4.2.25a}$$
$$\widetilde{\Theta}'(a-0;E) = \widetilde{\Theta}'(a+0;E)\,, \tag{4.2.25b}$$
$$\widetilde{\Theta}(b-0;E) = \widetilde{\Theta}(b+0;E)\,, \tag{4.2.25c}$$
$$\widetilde{\Theta}'(b-0;E) = \widetilde{\Theta}'(b+0;E)\,, \tag{4.2.25d}$$
$$\widetilde{\Theta}(r;E) \text{ is square integrable at } \infty\,, \tag{4.2.25e}$$

and lead to

$$\widetilde{\Theta}(r;E) = \begin{cases} \widetilde{\mathcal{A}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}E}r} + \widetilde{\mathcal{A}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & 0<r<a \\ \widetilde{\mathcal{A}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} + \widetilde{\mathcal{A}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{4.2.26}$$

The functions $\widetilde{\mathcal{A}}_1 - \widetilde{\mathcal{A}}_4$ are such that $\widetilde{\Theta}(r;E)$ satisfies the boundary conditions (4.2.25), and their expressions are given in Eq. (4.4.13) of Appendix 4.4.2.

Region $\Re(E)>0$, $\Im(E)>0$

When $\Re(E)>0$, $\Im(E)>0$, the expression of the Green function is

$$G(r,s;E) = \begin{cases} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(r;E)\,\Theta_+(s;E)}{2i\mathcal{J}_4(E)} & r<s \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(s;E)\,\Theta_+(r;E)}{2i\mathcal{J}_4(E)} & r>s \end{cases} \qquad \Re(E)>0,\ \Im(E)>0\,. \tag{4.2.27}$$

The eigenfunction $\chi(r;E)$ satisfies the Schrödinger equation (4.2.7) and the boundary conditions (4.2.21),

$$\chi(r;E) = \begin{cases} \sin(\sqrt{\frac{2m}{\hbar^2}E}r) & 0<r<a \\ \mathcal{J}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{J}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \mathcal{J}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{J}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{4.2.28}$$

The functions $\mathcal{J}_1 - \mathcal{J}_4$ are determined by the boundary conditions (4.2.22), and their expressions are listed in Eq. (4.4.16) of Appendix 4.4.2.

The eigenfunction $\Theta_+(r;E)$ satisfies the Schrödinger equation (4.2.7) and the boundary conditions (4.2.24),

$$\Theta_+(r;E) = \begin{cases} \mathcal{A}_1^+(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{A}_2^+(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & 0 < r < a \\ \mathcal{A}_3^+(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{A}_4^+(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a < r < b \\ e^{i\sqrt{\frac{2m}{\hbar^2}E}r} & b < r < \infty\,. \end{cases} \tag{4.2.29}$$

The functions $\mathcal{A}_1^+ - \mathcal{A}_4^+$ are determined by the boundary conditions (4.2.25), and their expressions are listed in Eq. (4.4.17) of Appendix 4.4.2.

Region $\Re(E) > 0$, $\Im(E) < 0$

In the region $\Re(E) > 0$, $\Im(E) < 0$, the Green function reads

$$G(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(r;E)\,\Theta_-(s;E)}{2i\mathcal{J}_3(E)} & r < s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(s;E)\,\Theta_-(r;E)}{2i\mathcal{J}_3(E)} & r > s \end{cases} \qquad \Re(E) > 0,\ \Im(E) < 0\,. \tag{4.2.30}$$

The eigenfunction $\chi(r;E)$ is given by (4.2.28). The eigenfunction $\Theta_-(r;E)$ satisfies the Schrödinger equation (4.2.7) and the boundary conditions (4.2.24),

$$\Theta_-(r;E) = \begin{cases} \mathcal{A}_1^-(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{A}_2^-(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & 0 < r < a \\ \mathcal{A}_3^-(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{A}_4^-(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a < r < b \\ e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b < r < \infty\,. \end{cases} \tag{4.2.31}$$

The functions $\mathcal{A}_1^- - \mathcal{A}_4^-$ are such that $\Theta_-(r;E)$ and its derivative are continuous at $r = a$ and at $r = b$. Their expressions are listed in Eq. (4.4.19) of Appendix 4.4.2.

4.2.4 Diagonalization of H and Eigenfunction Expansion

In the present section, we diagonalize our Hamiltonian H and construct the expansion of the wave functions in terms of the eigenfunctions of the differential operator h. In order to do so, we will compute the spectrum of H and then construct a unitary operator U that transforms from the position representation into the energy representation. We will see that the spectrum of H is the positive real line $[0,\infty)$. In the energy representation, H will act as the multiplication operator, the Hilbert space will be realized by $L^2([0,\infty), dE)$ and the domain of the Hamiltonian will be realized by the maximal domain on which the multiplication operator is well-defined. On our way, we shall take advantage of some results of the Sturm-Liouville theory that are proved in [30]. For the sake of completeness, we include in Appendix 4.4.3 the statements of the theorems that are used in this section.

Spectrum of H

We first compute the spectrum $\mathrm{Sp}(H)$ of the operator H by applying Theorem 4 of Appendix 4.4.3 (see also [30]). Since H is self-adjoint, its spectrum is real. This spectrum is the subset of the real line on which the Green function fails to be analytic. This non-analyticity of $G(r,s;E)$ will be built into the functions $\theta_{ij}^{\pm}(E)$ that appear in Theorem 4 of Appendix 4.4.3.

From the expression of the Green function computed above, it is clear that the subsets $(-\infty,0)$ and $(0,\infty)$ should be studied separately. We will denote either of these subsets by Λ.

Subset $\Lambda=(-\infty,0)$

We first take Λ from Theorem 4 of Appendix 4.4.3 to be $(-\infty,0)$. We choose a basis for the space of solutions of the equation $h\sigma=E\sigma$ that is continuous on $(0,\infty)\times\Lambda$ and analytically dependent on E as

$$\sigma_1(r;E)=\begin{cases}\widetilde{\mathcal{B}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}E}r}+\widetilde{\mathcal{B}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & 0<r<a\\ \widetilde{\mathcal{B}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r}+\widetilde{\mathcal{B}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b\\ e^{\sqrt{-\frac{2m}{\hbar^2}E}r} & b<r<\infty\,,\end{cases}\tag{4.2.32a}$$

$$\sigma_2(r;E)=\widetilde{\Theta}(r;E)\,.\tag{4.2.32b}$$

The functions $\widetilde{\mathcal{B}}_1-\widetilde{\mathcal{B}}_4$ are such that $\sigma_1(r;E)$ and its derivative are continuous at $r=a$ and at $r=b$. Their expressions are listed in Eq. (4.4.29) of Appendix 4.4.3.

Obviously,

$$\widetilde{\chi}(r;E)=\widetilde{\mathcal{J}}_3(E)\sigma_1(r;E)+\widetilde{\mathcal{J}}_4(E)\sigma_2(r;E)\,,\tag{4.2.33}$$

which along with Eq. (4.2.20) leads to

$$G(r,s;E)=-\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{1}{2}\left[\sigma_1(r;E)+\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)}\,\sigma_2(r;E)\right]\sigma_2(s;E)\,,\qquad r<s\,,\ \Re(E)<0\,,\Im(E)\neq 0\,.\tag{4.2.34}$$

Since

$$\overline{\sigma_2(s;\overline{E})}=\sigma_2(s;E)\,,\tag{4.2.35}$$

we can write Eq. (4.2.34) as

$$G(r,s;E)=-\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{1}{2}\left[\sigma_1(r;E)\overline{\sigma_2(s;\overline{E})}+\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)}\,\sigma_2(r;E)\overline{\sigma_2(s;\overline{E})}\right],\qquad r<s\,,\ \Re(E)<0\,,\Im(E)\neq 0\,.\tag{4.2.36}$$

On the other hand, by Theorem 4 in Appendix 4.4.3 we have

$$G(r,s;E) = \sum_{i,j=1}^{2} \theta_{ij}^{-}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} \qquad r<s\,. \tag{4.2.37}$$

By comparing Eqs. (4.2.36) and (4.2.37) we see that

$$\theta_{ij}^{-}(E) = \begin{pmatrix} 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2} \\ 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2}\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)} \end{pmatrix}, \quad \Re(E)<0\,,\ \Im(E)\neq 0\,. \tag{4.2.38}$$

The functions $\theta_{ij}^{-}(E)$ are analytic in a neighborhood of $\Lambda=(-\infty,0)$. Therefore, the interval $(-\infty,0)$ is in the resolvent set $\mathrm{Re}(H)$ of the operator H.

Subset $\Lambda=(0,\infty)$

Now we study the case $\Lambda=(0,\infty)$. In order to be able to apply Theorem 4 of Appendix 4.4.3, we choose the following basis for the space of solutions of $h\sigma=E\sigma$ that is continuous on $(0,\infty)\times\Lambda$ and analytically dependent on E:

$$\sigma_1(r;E) = \chi(r;E)\,, \tag{4.2.39a}$$

$$\sigma_2(r;E) = \begin{cases} \cos(\sqrt{\frac{2m}{\hbar^2}E}r) & 0<r<a \\ \mathcal{C}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{C}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \mathcal{C}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{C}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{4.2.39b}$$

The functions $\mathcal{C}_1-\mathcal{C}_4$, whose expressions are given in Eq. (4.4.30) of Appendix 4.4.3, are such that σ_2 and its derivative are continuous at $r=a$ and at $r=b$.

Eqs. (4.2.29), (4.2.31) and (4.2.39) lead to

$$\Theta_+(r;E) = -\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E) \tag{4.2.40}$$

and to

$$\Theta_-(r;E) = \frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\,, \tag{4.2.41}$$

where

$$W(E) = \mathcal{J}_4(E)\mathcal{C}_3(E) - \mathcal{J}_3(E)\mathcal{C}_4(E)\,. \tag{4.2.42}$$

By substituting Eq. (4.2.40) into Eq. (4.2.27) we get to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_4(E)}\left[-\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)>0\,,\ r>s\,. \tag{4.2.43}$$

By substituting Eq. (4.2.41) into Eq. (4.2.30) we get to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_3(E)}\,\left[\frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)<0\,,\; r>s\,, \qquad (4.2.44)$$

Since

$$\overline{\sigma_1(s;\overline{E})} = \sigma_1(s;E)\,, \qquad (4.2.45)$$

Eq. (4.2.43) leads to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_4(E)}\,\left[-\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)>0\,,\; r>s\,, \quad (4.2.46)$$

and Eq. (4.2.44) leads to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_3(E)}\,\left[\frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)<0\,,\; r>s\,, \quad (4.2.47)$$

The expression of the resolvent in terms of the basis σ_1, σ_2 can be written as (see Theorem 4 in Appendix 4.4.3)

$$G(r,s;E) = \sum_{i,j=1}^{2}\theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} \qquad r>s\,. \qquad (4.2.48)$$

By comparing (4.2.48) to (4.2.46) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{-\mathcal{C}_4(E)}{\mathcal{J}_4(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{1}{W(E)} & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\; \Im(E)>0\,, \qquad (4.2.49)$$

By comparing (4.2.48) to (4.2.47) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{\mathcal{C}_3(E)}{\mathcal{J}_3(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{1}{W(E)} & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\; \Im(E)<0\,, \qquad (4.2.50)$$

From Eqs. (4.2.49) and (4.2.50) we can see that the measures ρ_{12}, ρ_{21} and ρ_{22} in Theorem 4 of Appendix 4.4.3 are zero and that the measure ρ_{11} is given by

$$\begin{aligned}\rho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}\left[\theta_{11}^{+}(E-i\epsilon)-\theta_{11}^{+}(E+i\epsilon)\right]dE \\ &= \int_{E_1}^{E_2}\frac{1}{4\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{\mathcal{J}_3(E)\mathcal{J}_4(E)}\,dE\,, \qquad (4.2.51)\end{aligned}$$

which leads to

$$\rho(E) \equiv \rho_{11}(E) = \frac{1}{4\pi} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{|\mathcal{J}_4(E)|^2}\,, \quad E \in (0,\infty)\,. \tag{4.2.52}$$

The function $\theta_{11}^{+}(E)$ has a branch cut along $(0,\infty)$, and therefore $(0,\infty)$ is included in $\mathrm{Sp}(H)$. Since $\mathrm{Sp}(H)$ is a closed set, $\mathrm{Sp}(H) = [0,\infty)$. Thus the resolvent set of H is $\mathrm{Re}(H) = \mathbb{C} - [0,\infty)$.

Diagonalization and Eigenfunction Expansion

We are now in a position to diagonalize the Hamiltonian. By Theorem 2 of Appendix 4.4.3, there is a unitary map $\widetilde{U}$ defined by

$$\begin{aligned} \widetilde{U} : L^2([0,\infty), dr) &\longmapsto L^2((0,\infty), \rho(E)dE) \\ f(r) &\longmapsto \widetilde{f}(E) = (\widetilde{U}f)(E) = \int_0^\infty dr\, f(r)\overline{\chi(r;E)}\,, \end{aligned} \tag{4.2.53}$$

that brings $\mathcal{D}(H)$ onto the space

$$\mathcal{D}(\widetilde{E}) = \{\widetilde{f}(E) \in L^2((0,\infty), \rho(E)dE) \mid \int_0^\infty dE\, E^2 |\widetilde{f}(E)|^2 \rho(E) < \infty\}\,. \tag{4.2.54}$$

Eqs. (4.2.53) and (4.2.54) provide a ρ-diagonalization of H. If we seek a δ-diagonalization, i.e., if we seek eigenfunctions that are δ-normalized, then the measure $\rho(E)$ must be absorbed by the eigenfunctions and by the wave functions.[1] This is why we define

$$\sigma(r;E) := \sqrt{\rho(E)}\,\chi(r;E)\,, \tag{4.2.55}$$

which is the eigensolution of the differential operator h that is δ-normalized, and

$$\widehat{f}(E) := \sqrt{\rho(E)}\widetilde{f}(E)\,, \quad \widetilde{f}(E) \in L^2((0,\infty), \rho(E)dE)\,, \tag{4.2.56}$$

and construct the unitary operator

$$\begin{aligned} \widehat{U} : L^2((0,\infty)), \rho(E)dE) &\longmapsto L^2((0,\infty), dE) \\ \widetilde{f} &\longmapsto \widehat{f}(E) = \widehat{U}\widetilde{f}(E) := \sqrt{\rho(E)}\widetilde{f}(E)\,. \end{aligned} \tag{4.2.57}$$

The operator that δ-diagonalizes our Hamiltonian is $U := \widehat{U}\widetilde{U}$,

$$\begin{aligned} U : L^2([0,\infty)), dr) &\longmapsto L^2((0,\infty), dE) \\ f &\longmapsto Uf := \widehat{f}\,. \end{aligned} \tag{4.2.58}$$

[1] The meaning of the δ-normalization of the eigenfunctions will be explained in Section 4.2.9.

The action of U can be written as an integral operator,

$$\widehat{f}(E) = (Uf)(E) = \int_0^\infty dr f(r)\overline{\sigma(r;E)}\,, \quad f(r) \in L^2([0,\infty), dr)\,. \tag{4.2.59}$$

The image of $\mathcal{D}(H)$ under the action of U is

$$\mathcal{D}(\widehat{E}) := U\mathcal{D}(H) = \{\widehat{f}(E) \in L^2((0,\infty), dE) \mid \int_0^\infty E^2|\widehat{f}(E)|^2 dE < \infty\}\,. \tag{4.2.60}$$

Therefore, we have constructed a unitary operator

$$\begin{aligned} U : \mathcal{D}(H) \subset L^2([0,\infty), dr) &\longmapsto \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) \\ f &\longmapsto \widehat{f} = Uf \end{aligned} \tag{4.2.61}$$

that transforms from the position representation into the energy representation. The operator U diagonalizes our Hamiltonian in the sense that $\widehat{E} \equiv UHU^{-1}$ is the multiplication operator,

$$\begin{aligned} \widehat{E} : \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) &\longmapsto L^2((0,\infty), dE) \\ \widehat{f} &\longmapsto (\widehat{E}\widehat{f})(E) := E\widehat{f}(E)\,. \end{aligned} \tag{4.2.62}$$

The inverse operator of U is given by (see Theorem 3 of Appendix 4.4.3)

$$f(r) = (U^{-1}\widehat{f})(r) = \int_0^\infty dE\, \widehat{f}(E)\sigma(r,E)\,, \quad \widehat{f}(E) \in L^2((0,\infty), dE)\,. \tag{4.2.63}$$

The operator U^{-1} transforms from the energy representation into the position representation.

The expressions (4.2.59) and (4.2.63) provide the eigenfunction expansion of any square integrable function in terms of the eigensolutions $\sigma(r;E)$ of h.

The unitary operator U can be looked at as a sort of generalized Fourier transform: the Fourier transform connects the position and the momentum representations. U connects the position and the energy representations. The role played by the plane waves e^{-ipx} (which are generalized eigenfunctions of the operator $-id/dx$) is here played by the $\sigma(r;E)$ (which are generalized eigenfunctions of the differential operator h). Therefore $\sigma(r;E) \equiv \langle r|E\rangle$, which is the δ-normalized eigensolutions of the Schrödinger equation, can be viewed as "transition elements" between the r- and the E-representations.

The label f of the functions in the position representation is different from the label $\widehat{f}$ of the functions in the energy representation because they have different functional dependences. The same applies to the Hamiltonian H, the domains, etc. This is not the standard practice in the physics literature, where different representations are usually identified and labeled by the same symbol (see, for instance, [72, 54, 73, 15]).

We remark that the operator U that diagonalizes H is not unique. In fact, different eigenkets, i.e., different boundary conditions imposed upon (4.2.7), lead to different operators U.

4.2.5 The Need of the RHS

The Sturm-Liouville theory only provides a domain $\mathcal{D}(H)$ on which the Hamiltonian H is self-adjoint and a unitary operator U that diagonalizes H. This unitary operator induces a direct integral decomposition of the Hilbert space (see [4, 5]),

$$\begin{aligned} \mathcal{H} &\longmapsto U\mathcal{H} \equiv \widehat{\mathcal{H}} = \oplus \int_{\mathrm{Sp}(H)} \mathcal{H}(E) dE \\ f &\longmapsto Uf \equiv \{\widehat{f}(E)\}, \quad \widehat{f}(E) \in \mathcal{H}(E)\,, \end{aligned} \tag{4.2.64}$$

where $\mathcal{H}$ is realized by $L^2([0,\infty), dr)$, and $\widehat{\mathcal{H}}$ is realized by $L^2([0,\infty), dE)$. The Hilbert space $\mathcal{H}(E)$ associated to each energy eigenvalue of $\mathrm{Sp}(H)$ is realized by the Hilbert space of complex numbers $\mathbb{C}$. On $\widehat{\mathcal{H}}$, the operator H acts as the multiplication operator,

$$Hf \longmapsto UHf \equiv \{E\widehat{f}(E)\}\,, \quad f \in \mathcal{D}(H)\,. \tag{4.2.65}$$

The scalar product on $\widehat{\mathcal{H}}$ can be written as

$$\left(\widehat{f}, \widehat{g}\right)_{\widehat{\mathcal{H}}} = \int_{\mathrm{Sp}(H)} \left(\widehat{f}(E), \widehat{g}(E)\right)_E dE\,, \tag{4.2.66}$$

where the scalar product $(\,\cdot\,,\,\cdot\,)_E$ on $\mathcal{H}(E)$ is the usual scalar product on $\mathbb{C}$,

$$\left(\widehat{f}(E), \widehat{g}(E)\right)_E = \overline{\widehat{f}(E)}\,\widehat{g}(E)\,. \tag{4.2.67}$$

As we shall explain below, the direct integral decomposition does not shelter some of the basic requirements needed in Quantum Mechanics. These requirements can be sheltered by the RHS.

One of the most important principles of Quantum Mechanics is that the quantity $(\varphi, H\varphi)$ should fit the experimental expectation value of the observable H in the state φ. However, $(\varphi, H\varphi)$ is not defined for every element in $\mathcal{H}$, but only for those square normalizable wave functions that are also in $\mathcal{D}(H)$. Therefore, not every square normalizable function can represent a "physical wave function," but only those that are (at least) in $\mathcal{D}(H)$. Another fundamental assumption of quantum physics is that the quantity

$$\mathrm{disp}_\varphi H = (\varphi, H^2\varphi) - (\varphi, H\varphi)^2 \tag{4.2.68}$$

represents the dispersion of the observable H in the state φ, and that

$$\Delta_\varphi H \equiv \sqrt{\mathrm{disp}_\varphi H} \tag{4.2.69}$$

represents the uncertainty of the observable H in the state φ. Since (4.2.68) and (4.2.69) are only defined when φ is an element of $\mathcal{D}(H^2) \subset \mathcal{D}(H)$, not every element of $\mathcal{D}(H)$ can be assigned to a "physical wave function," but only those functions that are (at least) in

$\mathcal{D}(H^2)$. Therefore, we would like to find a subdomain $\mathbf{\Phi}$ included in $\mathcal{D}(H)$ on which the expectation values

$$(\varphi, H^n\varphi)\,, \quad n = 0, 1, 2, \ldots\,, \quad \varphi \in \mathbf{\Phi} \tag{4.2.70}$$

are well-defined.

Another important requirement of Quantum Mechanics is that algebraic operations such as the sum and multiplication of two operators are well-defined. In the HS formalism, these algebraic operations are not always well-defined because the domains on which these operators are self-adjoint do not remain stable under their actions in general. In fact, much of the trouble of the HS formalism comes from domain questions. In our case, the domain $\mathcal{D}(H)$ in (4.2.13) does not remain stable under H. We therefore would like to find a subdomain $\mathbf{\Phi}$ included in $\mathcal{D}(H)$ that remains stable under the action of H and all of its powers,

$$H^n : \mathbf{\Phi} \longmapsto \mathbf{\Phi}\,, \quad n = 0, 1, 2, \ldots \tag{4.2.71}$$

One can see that if Eq. (4.2.71) holds, then the expectation values (4.2.70) are well-defined for each φ in $\mathbf{\Phi}$, i.e., if the domain $\mathbf{\Phi}$ remains stable under the action of H, then the expectation values of H in any state $\varphi \in \mathbf{\Phi}$ are well-defined.

In Quantum Mechanics, it is always assumed that for each $E \in \mathrm{Sp}(H)$ there is a Dirac ket $|E\rangle$ such that

$$H^\times|E\rangle = E|E\rangle \tag{4.2.72}$$

and such that the Dirac basis vector expansion (4.1.3) holds. Equation (4.2.72) has no solution in the Hilbert space when E belongs to the continuous part of the spectrum of the Hamiltonian. In fact, Eq. (4.2.72) has to be related to the equation

$$\langle\vec{x}|H^\times|E\rangle = E\langle\vec{x}|E\rangle\,, \tag{4.2.73}$$

which in the radial representation reads

$$h\sigma(r; E) = E\sigma(r; E)\,, \tag{4.2.74}$$

where h is the differential operator (4.2.5) and $\sigma(r; E)$ is the delta-normalized eigenfunction (4.2.55). Since $\sigma(r; E) \equiv \langle r|E\rangle$ lies outside $L^2([0, \infty), dr)$, i.e.,

$$\int_0^\infty dr\,|\sigma(r; E)|^2 = \infty\,, \tag{4.2.75}$$

the corresponding eigenket $|E\rangle$, which is defined by

$$\begin{aligned} |E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r; E)dr\,, \end{aligned} \tag{4.2.76}$$

should also lie outside the Hilbert space. Actually, $|E\rangle$ is an element of $\mathbf{\Phi}^\times$.

In summary, what our mathematical framework should provide us with is:

1. a dense invariant domain on which all the powers of H and all the expectation values (4.2.70) are well-defined,
2. smooth enough wave functions so that Eq. (4.2.72) holds,
3. Dirac basis vector expansion must follow.

In the direct integral decomposition formalism, there is not enough room for either of these three requirements. This is why we introduce the RHS.

4.2.6 Construction of the Rigged Hilbert Space

The first step is to make all the powers of the Hamiltonian well-defined. In order to do so, we construct the maximal invariant subspace $\mathcal{D}$ of the operator H,

$$\mathcal{D} := \bigcap_{n=0}^{\infty} \mathcal{D}(H^n)\,. \tag{4.2.77}$$

The space $\mathcal{D}$ is the largest subspace of $\mathcal{D}(H)$ that remains stable under the action of the Hamiltonian H and all of its powers. It is easy to check that

$$\begin{aligned}\mathcal{D} = \{\varphi \in L^2([0,\infty), dr) \mid\ & h^n\varphi(r) \in L^2([0,\infty), dr),\ h^n\varphi(0) = 0, \varphi^{(n)}(a) = \varphi^{(n)}(b) = 0,\\ & n = 0, 1, 2, \ldots;\ \varphi(r) \in C^\infty([0,\infty))\}\,.\end{aligned} \tag{4.2.78}$$

The conditions $\varphi^{(n)}(a) = \varphi^{(n)}(b) = 0$ in (4.2.78) come from taking the discontinuities of the potential $V(r)$ at $r = a$ and at $r = b$ into consideration (see [10]).

The second step is to find a subspace $\mathbf{\Phi}$ on which the eigenkets $|E\rangle$ of H are well-defined as antilinear functionals. For each $E \in \mathrm{Sp}(H)$, we associate a ket $|E\rangle$ to the generalized eigenfunction $\sigma(r; E)$ through

$$\begin{aligned}|E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C}\\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r; E)dr = \overline{(U\varphi)(E)}\,.\end{aligned} \tag{4.2.79}$$

As actual computations show, the ket $|E\rangle$ in (4.2.79) is a generalized eigenfunctional of H if $\mathbf{\Phi}$ is included in the maximal invariant subspace of H,

$$\mathbf{\Phi} \subset \mathcal{D}\,. \tag{4.2.80}$$

Due to the non-square integrability of the eigenfunction $\sigma(r; E)$, we need to impose further restrictions on the elements of $\mathcal{D}$ in order to make the eigenfunctional $|E\rangle$ in Eq. (4.2.79) continuous,

$$\int_0^\infty dr\ |(r+1)^n(h+1)^m\varphi(r)|^2 < \infty, \quad n, m = 0, 1, 2, \ldots \tag{4.2.81}$$

The imposition of conditions (4.2.81) upon the space $\mathcal{D}$ leads to the space of test functions of the square barrier potential,

$$\mathbf{\Phi} = \{\varphi \in \mathcal{D} \,|\, \int_0^\infty dr\, |(r+1)^n (h+1)^m \varphi(r)|^2 < \infty, \quad n, m = 0, 1, 2, \ldots\} \,. \tag{4.2.82}$$

On $\mathbf{\Phi}$, we define the family of norms

$$\|\varphi\|_{n,m} := \sqrt{\int_0^\infty dr\, |(r+1)^n (h+1)^m \varphi(r)|^2} \,, \quad n, m = 0, 1, 2, \ldots \tag{4.2.83}$$

The quantities (4.2.83) fulfill the conditions to be a norm (cf. Proposition 1 of Appendix 4.4.4) and can be used to define a countably normed topology $\tau_{\mathbf{\Phi}}$ on $\mathbf{\Phi}$ (see [5]),

$$\varphi_\alpha \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \quad \text{iff} \quad \|\varphi_\alpha - \varphi\|_{n,m} \xrightarrow[\alpha\to\infty]{} 0 \,, \quad n, m = 0, 1, 2, \ldots \tag{4.2.84}$$

One can see that the space $\mathbf{\Phi}$ is stable under the action of H and that H is $\tau_{\mathbf{\Phi}}$-continuous (cf. Proposition 2 of Appendix 4.4.4).

Once we have constructed the space $\mathbf{\Phi}$, we can construct its topological dual $\mathbf{\Phi}^\times$ as the space of $\tau_{\mathbf{\Phi}}$-continuous antilinear functionals on $\mathbf{\Phi}$ (see [5]) and therewith the RHS of the square barrier potential (for $l = 0$)

$$\mathbf{\Phi} \subset L^2([0, \infty), dr) \subset \mathbf{\Phi}^\times \,. \tag{4.2.85}$$

The ket $|E\rangle$ in Eq. (4.2.79) is a well-defined antilinear functional on $\mathbf{\Phi}$, i.e., $|E\rangle$ belongs to $\mathbf{\Phi}^\times$ (cf. Proposition 3 of Appendix 4.4.4). The ket $|E\rangle$ is a generalized eigenvector of the Hamiltonian H (cf. Proposition 3 of Appendix 4.4.4),

$$H^\times |E\rangle = E|E\rangle \,, \tag{4.2.86}$$

i.e.,

$$\langle\varphi|H^\times|E\rangle = \langle H\varphi|E\rangle = E\langle\varphi|E\rangle \,, \quad \forall\varphi \in \mathbf{\Phi} \,. \tag{4.2.87}$$

On the space $\mathbf{\Phi}$, all the expectation values of the Hamiltonian and all the algebraic operations involving H are well-defined, and the generalized eigenvalue equation (4.2.87) holds. As we shall see in the next section, the functions φ of $\mathbf{\Phi}$ can be expanded by a Dirac basis vector expansion.

4.2.7 Dirac Basis Vector Expansion

We are now in a position to derive the Dirac basis vector expansion. This derivation consists of the restriction of the Weyl-Kodaira expansions (4.2.59) and (4.2.63) to the space $\mathbf{\Phi}$. If we denote $\langle r|\varphi\rangle \equiv \varphi(r)$ and $\langle E|r\rangle \equiv \overline{\sigma(r; E)}$, and if we define the action of the left ket $\langle E|$ on $\varphi \in \mathbf{\Phi}$ as $\langle E|\varphi\rangle := \widehat{\varphi}(E)$, then Eq. (4.2.59) becomes

$$\langle E|\varphi\rangle = \int_0^\infty dr\, \langle E|r\rangle \langle r|\varphi\rangle \,, \quad \varphi \in \mathbf{\Phi} \,. \tag{4.2.88}$$

If we denote $\langle r|E\rangle \equiv \sigma(r;E)$, then Eq. (4.2.63) becomes

$$\langle r|\varphi\rangle = \int_0^\infty dE\, \langle r|E\rangle\, \langle E|\varphi\rangle\,, \quad \varphi \in \mathbf{\Phi}\,. \tag{4.2.89}$$

This equation is the Dirac basis vector expansion of the square barrier potential. In fact, when we formally write (4.1.3) in the position representation, we get to (4.2.89).

In Eq. (4.2.89), the wave function $\langle r|\varphi\rangle$ is spanned in a "Fourier-type" expansion by the eigenfunctions $\langle r|E\rangle$. In this expansion, each eigenfunction $\langle r|E\rangle$ is weighted by $\langle E|\varphi\rangle = \widehat{\varphi}(E)$, which is the value of the wave function in the energy representation at the point E. Thus any function $\varphi(r) = \langle r|\varphi\rangle$ of $\mathbf{\Phi}$ can be written as a linear superposition of the monoenergetic eigenfunctions $\sigma(r;E) = \langle r|E\rangle$.

Although the Weyl-Kodaira expansions (4.2.59) and (4.2.63) are valid for every element of the Hilbert space, the Dirac basis vector expansions (4.2.88) and (4.2.89) are only valid for functions $\varphi \in \mathbf{\Phi}$ because only those functions fulfill both

$$\overline{\widehat{\varphi}(E)} = \langle \varphi|E\rangle \tag{4.2.90}$$

and

$$\langle \varphi|H^\times|E\rangle = \langle H\varphi|E\rangle = E\langle \varphi|E\rangle\,. \tag{4.2.91}$$

Another way to rephrase the Dirac basis vector expansion is the Nuclear Spectral (Gelfand-Maurin) Theorem. Instead of using the general statement of [5], we prove this theorem using the machinery of the Sturm-Liouville theory (see Proposition 4 of Appendix 4.4.5). The Nuclear Spectral Theorem allows us to write the scalar product of any two functions φ, ψ of $\mathbf{\Phi}$ in terms of the action of the kets $|E\rangle$ on φ, ψ:

$$(\varphi, \psi) = \int_0^\infty dE\, \langle \varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall \varphi, \psi \in \mathbf{\Phi}\,. \tag{4.2.92}$$

It also allows us to write the matrix elements of the Hamiltonian and all of its powers between two elements φ, ψ of $\mathbf{\Phi}$ in terms of the action of the kets $|E\rangle$ on φ, ψ:

$$(\varphi, H^n\psi) = \int_0^\infty dE\, E^n\langle \varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall \varphi, \psi \in \mathbf{\Phi}\,, n = 1, 2, \ldots \tag{4.2.93}$$

4.2.8 Energy Representation of the RHS

In this section, we construct the energy representation of the RHS. Since the unitary operator U transforms from the position representation into the energy representation, the action of U on the RHS provides the energy representation of the RHS.

We have already shown that in the energy representation the Hamiltonian H acts as the multiplication operator $\widehat{E}$. The energy representation of the space $\mathbf{\Phi}$ is defined as

$$\widehat{\mathbf{\Phi}} := U\mathbf{\Phi}\,. \tag{4.2.94}$$

It is very easy to see that $\widehat{\mathbf{\Phi}}$ is a linear subspace of $L^2([0,\infty), dE)$. In oder to endow $\widehat{\mathbf{\Phi}}$ with a topology $\tau_{\widehat{\mathbf{\Phi}}}$, we carry the topology on $\mathbf{\Phi}$ into $\widehat{\mathbf{\Phi}}$,

$$\tau_{\widehat{\mathbf{\Phi}}} := U\tau_{\mathbf{\Phi}} \,. \tag{4.2.95}$$

With this topology, the space $\widehat{\mathbf{\Phi}}$ is a linear topological space. If we denote the dual space of $\widehat{\mathbf{\Phi}}$ by $\widehat{\mathbf{\Phi}}^\times$, then we have

$$U^\times \mathbf{\Phi}^\times = (U\mathbf{\Phi})^\times = \widehat{\mathbf{\Phi}}^\times \,. \tag{4.2.96}$$

If we denote $|\widehat{E}\rangle \equiv U^\times |E\rangle$, then we can prove that $|\widehat{E}\rangle$ is the antilinear Schwartz delta functional, i.e., $|\widehat{E}\rangle$ is the antilinear functional that associates to each function $\widehat{\varphi}$ the complex conjugate of its value at the point E (see Proposition 5 of Appendix 4.4.6),

$$\begin{aligned} |\widehat{E}\rangle : \widehat{\mathbf{\Phi}} &\longmapsto \mathbb{C} \\ \widehat{\varphi} &\longmapsto \langle \widehat{\varphi} | \widehat{E}\rangle := \overline{\widehat{\varphi}(E)} \,. \end{aligned} \tag{4.2.97}$$

Therefore, the Schwartz delta functional appears in the (spectral) energy representation of the RHS associated to the Hamiltonian. If we write the action of the Schwartz delta functional as an integral operator, then the Dirac δ-function appears in the integrand of that integral operator.

It is very helpful to show the different realizations of the RHS through the following diagram:

$$\begin{array}{llcccccl} H; \quad \varphi(r) & \mathbf{\Phi} & \subset & L^2([0,\infty), dr) & \subset & \mathbf{\Phi}^\times & |E\rangle & \text{position repr.} \\ & \downarrow U & & \downarrow U & & \downarrow U^\times & & \\ \widehat{E}; \quad \widehat{\varphi}(E) & \widehat{\mathbf{\Phi}} & \subset & L^2([0,\infty), dE) & \subset & \widehat{\mathbf{\Phi}}^\times & |\widehat{E}\rangle & \text{energy repr.} \end{array} \tag{4.2.98}$$

On the top line of the diagram (4.2.98), we have the RHS, the Hamiltonian, the wave functions and the Dirac kets in the position representation. On the bottom line, we have their energy representation counterparts.

4.2.9 Meaning of the δ-normalization of the Eigenfunctions

In this section, we show that the δ-normalization of the eigenfunctions is related to the measure $d\mu(E)$ that is used to compute the scalar product of the wave functions in the energy representation,

$$(\varphi, \psi) = \int_0^\infty \overline{\varphi(E)} \psi(E) d\mu(E) \,. \tag{4.2.99}$$

We will see that if the measure in (4.2.99) is the Lebesgue measure dE, then the eigenfunctions are δ-normalized, and that if the measure is $\rho(E)dE$, then the eigenfunctions are ρ-normalized.

For the sake of simplicity, in this section we label the wave functions in the position and in the energy representation with the same symbol. With this notation, Eq. (4.2.89) leads to

$$\varphi(r) = \int_0^\infty dE\, \varphi(E)\sigma(r;E)\,, \tag{4.2.100a}$$

$$\psi(r) = \int_0^\infty dE\, \psi(E)\sigma(r;E)\,. \tag{4.2.100b}$$

Since $\varphi(r), \psi(r) \in L^2([0,\infty), dr)$, their scalar product is well-defined,

$$(\varphi,\psi) = \int_0^\infty dr\, \overline{\varphi(r)}\psi(r)\,. \tag{4.2.101}$$

Plugging (4.2.100) into (4.2.101), we obtain

$$(\varphi,\psi) = \int_0^\infty dE \int_0^\infty dE'\, \overline{\varphi(E)}\psi(E') \int_0^\infty dr\, \overline{\sigma(r;E)}\sigma(r;E')\,. \tag{4.2.102}$$

If we use the Lebesgue measure dE, then the scalar product (4.2.99) can be written as

$$(\varphi,\psi) = \int_0^\infty dE\, \overline{\varphi(E)}\psi(E)\,. \tag{4.2.103}$$

Comparison of (4.2.102) and (4.2.103) leads to

$$\int_0^\infty dr\, \overline{\sigma(r;E)}\sigma(r;E') = \delta(E-E')\,, \tag{4.2.104}$$

i.e., the eigenfunctions $\sigma(r;E)$ are δ-normalized.

We now consider the case in which the eigenfunctions are ρ-normalized. If we use the measure $d\mu(E) = \rho(E)dE$, then the scalar product of φ and ψ is given by

$$(\varphi,\psi) = \int_0^\infty \overline{\varphi_\rho(E)}\psi_\rho(E)\rho(E)\, dE\,, \tag{4.2.105}$$

where $\varphi_\rho(E) := \varphi(E)/\sqrt{\rho(E)}$ and $\psi_\rho(E) := \psi(E)/\sqrt{\rho(E)}$. If we define $\sigma_\rho(r;E) := \sigma(r;E)/\sqrt{\rho(E)}$, then Eq. (4.2.100) leads to

$$\varphi(r) = \int_0^\infty \varphi_\rho(E)\sigma_\rho(r;E)\rho(E)\, dE\,, \tag{4.2.106a}$$

$$\psi(r) = \int_0^\infty \psi_\rho(E)\sigma_\rho(r;E)\rho(E)\, dE\,. \tag{4.2.106b}$$

Plugging Eq. (4.2.106) into (4.2.101), we obtain

$$(\varphi,\psi) = \int_0^\infty dE \int_0^\infty dE'\, \overline{\varphi_\rho(E)}\psi_\rho(E')\rho(E)\rho(E') \int_0^\infty dr\, \overline{\sigma_\rho(r;E)}\sigma_\rho(r;E')\,. \tag{4.2.107}$$

Comparison of (4.2.107) and (4.2.105) leads to

$$\int_0^\infty dr\, \overline{\sigma_\rho(r;E)}\sigma_\rho(r;E') = \frac{1}{\rho(E)}\delta(E-E')\,, \tag{4.2.108}$$

i.e., the eigenfunctions $\sigma_\rho(r;E)$ are ρ-normalized.

4.3 Conclusion to Chapter 4

In this chapter, we have constructed the Rigged Hilbert Space of the square barrier Hamiltonian

$$\mathbf{\Phi} \subset L^2([0,\infty), dr) \subset \mathbf{\Phi}^\times \tag{4.3.1}$$

and its energy representation

$$\widehat{\mathbf{\Phi}} \subset L^2([0,\infty), dE) \subset \widehat{\mathbf{\Phi}}^\times . \tag{4.3.2}$$

The spectrum of the Hamiltonian H is the positive real semiaxis. For each value E of the spectrum of H, we have constructed a Dirac ket $|E\rangle$ that is a generalized eigenfunctional of H whose corresponding generalized eigenvalue is E. In the energy representation, $|E\rangle$ acts as the antilinear Schwartz delta functional. On the space $\mathbf{\Phi}$, all algebraic operations involving the Hamiltonian H are well-defined. In particular, the expectation values of the Hamiltonian in any element of $\mathbf{\Phi}$ are well-defined. Any element of $\mathbf{\Phi}$ can be expanded in terms of the eigenkets $|E\rangle$ by a Dirac basis vector expansion. The elements of $\mathbf{\Phi}$ are represented by well-behaved functions in contrast to the elements of the Hilbert space which are represented by sets of equivalent functions that can vary arbitrarily on any set of zero Lebesgue measure. Therefore, it seems natural to conclude that a physically acceptable wave function is not any element of the Hilbert space, but rather an element of the subspace $\mathbf{\Phi}$.

In our quest for the RHS of the square barrier potential, we have found a systematic method to construct the RHS of a large class of spherically symmetric potentials:

1. Expression of the formal differential operator.

2. Hilbert space $\mathcal{H}$ of square integrable functions on which the formal differential operator acts.

3. A domain $\mathcal{D}(H)$ of the Hilbert space on which the formal differential operator is self-adjoint.

4. Green functions (resolvent) of this self-adjoint operator.

5. Diagonalization of the self-adjoint operator, eigenfunction expansion of the elements of $\mathcal{H}$ in terms of the eigensolutions of the formal differential operator, and direct integral decomposition of $\mathcal{H}$ induced by the self-adjoint operator.

6. Subspace $\mathbf{\Phi}$ of $\mathcal{D}(H)$ on which all the expectation values of H are well-defined and on which the Dirac kets act as antilinear functionals.

7. Rigged Hilbert space $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$.

4.4 Appendices to Chapter 4

4.4.1 Appendix 1: Self-Adjoint Extension

In this appendix, we list the possible self-adjoint extensions associated to the differential operator h. We first need first some definitions (cf. [30]).

Definition 1 By $AC^2([0,\infty))$ we denote the space of all functions f which have a continuous derivative in $[0,\infty)$, and for which f' is not only continuous but also absolutely continuous over each compact subinterval of $[0,\infty)$. Thus $f^{(2)}$ exists almost everywhere, and is integrable over any compact subinterval of $[0,\infty)$. At 0 f' is continuous from the right.

The space $AC^2([0,\infty))$ is the largest space of functions on which the differential operator h can be defined. In the case of the square barrier potential (4.2.3), if $f(r)$ belongs to $AC^2([0,\infty))$, then $f(r)$ and $f'(r)$ are continuous at $r=a$ and at $r=b$.

Definition 2 We define the spaces

$$\mathcal{H}_h^2([0,\infty)) := \{f \in AC^2([0,\infty)) \mid f, hf \in L^2([0,\infty), dr)\} \tag{4.4.1}$$

$$\mathcal{H}^2([0,\infty)) := \{f \in AC^2([0,\infty) \mid f, f^{(2)} \in L^2([0,\infty), dr)\} \tag{4.4.2}$$

$$\mathcal{H}_0^2([0,\infty)) := \{f \in \mathcal{H}^2([0,\infty)) \mid f \text{ vanishes outside some compact subset of } (0,\infty)\}\,. \tag{4.4.3}$$

Using these spaces, we can define the necessary operators to calculate the self-adjoint extensions associated to h.

Definition 3 If h is the formal differential operator (4.2.5), we define the operators H_0 and H_1 on $L^2([0,\infty), dr)$ by the formulas

$$\mathcal{D}(H_0) = \mathcal{H}_0^2([0,\infty)), \quad H_0 f := hf, \quad f \in \mathcal{D}(H_0)\,. \tag{4.4.4}$$

$$\mathcal{D}(H_1) = \mathcal{H}_h^2([0,\infty)), \quad H_1 f := hf, \quad f \in \mathcal{D}(H_1)\,. \tag{4.4.5}$$

The operators H_0 and H_1 are sometimes called the *minimal* and the *maximal* operators associated to the differential operator h, respectively. The domain $\mathcal{D}(H_1)$ is the largest domain of the Hilbert space $L^2([0,\infty), dr)$ on which the action of the differential operator h can be defined and remains inside $L^2([0,\infty), dr)$. Further, $H_0^\dagger = H_1$.

The self-adjoint extensions of H_0 are given by the restrictions of the operator H_1 to domains determined by the conditions (see [30], page 1306)

$$f(0) + \alpha\, f'(0) = 0\,, \quad -\infty < \alpha \leq \infty\,. \tag{4.4.6}$$

These boundary conditions lead to the domains

$$\mathcal{D}_\alpha(H) = \{f \in \mathcal{D}(H_1) \mid f(0) + \alpha\, f'(0) = 0\}\,, \quad -\infty < \alpha \leq \infty\,. \tag{4.4.7}$$

On these domains, the formal differential operator h is self-adjoint. The boundary condition that fits spherically symmetric potentials is $f(0) = 0$, i.e., $\alpha = 0$. This condition selects our domain (4.2.13),

$$\mathcal{D}(H) = \mathcal{D}_{\alpha=0}(H) = \{f \in \mathcal{D}(H_1) \mid f(0) = 0\}\,. \tag{4.4.8}$$

4.4.2 Appendix 2: Resolvent and Green Function

The following theorem provides the procedure to compute the Green function of the Hamiltonian H (cf. Theorem XIII.3.16 of Ref. [30]):

Theorem 1 Let H be the self-adjoint operator (4.2.14) derived from the real formal differential operator (4.2.5) by the imposition of the boundary condition (4.2.11d). Let $\Im E \neq 0$. Then there is exactly one solution $\chi(r;E)$ of $(h-E)\sigma = 0$ square-integrable at 0 and satisfying the boundary condition (4.2.11d), and exactly one solution $\Theta(r;E)$ of $(h-E)\sigma = 0$ square-integrable at infinity. The resolvent $(E-H)^{-1}$ is an integral operator whose kernel $G(r,s;E)$ is given by

$$G(r,s;E) = \begin{cases} \frac{2m}{\hbar^2}\,\frac{\chi(r;E)\,\Theta(s;E)}{W(\chi,\Theta)} & r < s \\ \frac{2m}{\hbar^2}\,\frac{\chi(s;E)\,\Theta(r;E)}{W(\chi,\Theta)} & r > s\,, \end{cases} \tag{4.4.9}$$

where $W(\chi,\Theta)$ is the Wronskian of χ and Θ

$$W(\chi,\Theta) = \chi\Theta' - \chi'\Theta\,. \tag{4.4.10}$$

If we define

$$\widetilde{k} := \sqrt{-\frac{2m}{\hbar^2}\,E}\,, \tag{4.4.11a}$$

$$\widetilde{Q} := \sqrt{-\frac{2m}{\hbar^2}\,(E - V_0)}\,, \tag{4.4.11b}$$

then the functions $\widetilde{\mathcal{J}}(E)$ of Eq. (4.2.23) are given by

$$\widetilde{\mathcal{J}}_1(E) = \frac{1}{2}e^{-\widetilde{Q}a}\left[\left(1 + \frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}a} + \left(-1 + \frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}a}\right], \tag{4.4.12a}$$

$$\widetilde{\mathcal{J}}_2(E) = \frac{1}{2}e^{\widetilde{Q}a}\left[\left(1 - \frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}a} + \left(-1 - \frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}a}\right], \tag{4.4.12b}$$

$$\widetilde{\mathcal{J}}_3(E) = \frac{1}{2}e^{-\widetilde{k}b}\left[\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}b}\widetilde{\mathcal{J}}_1(E) + \left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}b}\widetilde{\mathcal{J}}_2(E)\right], \tag{4.4.12c}$$

$$\widetilde{\mathcal{J}}_4(E) = \frac{1}{2}e^{\widetilde{k}b}\left[\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}b}\widetilde{\mathcal{J}}_1(E) + \left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}b}\widetilde{\mathcal{J}}_2(E)\right], \tag{4.4.12d}$$

and the functions $\widetilde{\mathcal{A}}(E)$ of Eq. (4.2.26) by

$$\widetilde{\mathcal{A}}_3(E) = \frac{1}{2}e^{-\widetilde{Q}b}\left(1-\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}b}, \tag{4.4.13a}$$

$$\widetilde{\mathcal{A}}_4(E) = \frac{1}{2}e^{\widetilde{Q}b}\left(1+\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}b}, \tag{4.4.13b}$$

$$\widetilde{\mathcal{A}}_1(E) = \frac{1}{2}e^{-\widetilde{k}a}\left[\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{A}}_3(E) + \left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}a}\widetilde{\mathcal{A}}_4(E)\right], \tag{4.4.13c}$$

$$\widetilde{\mathcal{A}}_2(E) = \frac{1}{2}e^{\widetilde{k}a}\left[\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{A}}_3(E) + \left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\sqrt{-\widetilde{\lambda}}a}\widetilde{\mathcal{A}}_4(E)\right]. \tag{4.4.13d}$$

The expression for the Wronskian of $\widetilde{\chi}$ and $\widetilde{\Theta}_-$ is

$$W(\widetilde{\chi}, \widetilde{\Theta}_-) = -2\widetilde{k}\widetilde{\mathcal{J}}_3(E)\,. \tag{4.4.14}$$

If we define

$$k := \sqrt{\frac{2m}{\hbar^2}\,E}\,, \tag{4.4.15a}$$

$$Q := \sqrt{\frac{2m}{\hbar^2}\,(E-V_0)}\,, \tag{4.4.15b}$$

then the functions $\mathcal{J}(E)$ of Eq. (4.2.28) are given by

$$\mathcal{J}_1(E) = \frac{1}{2}e^{-iQa}\left(\sin(ka) + \frac{k}{iQ}\cos(ka)\right), \tag{4.4.16a}$$

$$\mathcal{J}_2(E) = \frac{1}{2}e^{iQa}\left(\sin(ka) - \frac{k}{iQ}\cos(ka)\right), \tag{4.4.16b}$$

$$\mathcal{J}_3(E) = \frac{1}{2}e^{-ikb}\left[\left(1+\frac{Q}{k}\right)e^{iQb}\mathcal{J}_1(E) + \left(1-\frac{Q}{k}\right)e^{-iQb}\mathcal{J}_2(E)\right], \tag{4.4.16c}$$

$$\mathcal{J}_4(E) = \frac{1}{2}e^{ikb}\left[\left(1-\frac{Q}{k}\right)e^{iQb}\mathcal{J}_1(E) + \left(1+\frac{Q}{k}\right)e^{-iQb}\mathcal{J}_2(E)\right], \tag{4.4.16d}$$

and the functions $\mathcal{A}^+(E)$ of Eq. (4.2.29) by

$$\mathcal{A}_3^+(E) = \frac{1}{2}e^{-iQb}\left(1+\frac{k}{Q}\right)e^{ikb}, \tag{4.4.17a}$$

$$\mathcal{A}_4^+(E) = \frac{1}{2}e^{iQb}\left(1-\frac{k}{Q}\right)e^{ikb}, \tag{4.4.17b}$$

$$\mathcal{A}_1^+(E) = \frac{1}{2}e^{-ika}\left[\left(1+\frac{Q}{k}\right)e^{iQa}\mathcal{A}_3^+(E) + \left(1-\frac{Q}{k}\right)e^{-iQa}\mathcal{A}_4^+(E)\right], \tag{4.4.17c}$$

$$\mathcal{A}_2^+(E) = \frac{1}{2}e^{ika}\left[\left(1-\frac{Q}{k}\right)e^{iQa}\mathcal{A}_3^+(E) + \left(1+\frac{Q}{k}\right)e^{-iQa}\mathcal{A}_4^+(E)\right]. \tag{4.4.17d}$$

The Wronskian of χ and Θ_+ is

$$W(\chi, \Theta_+) = 2ik\mathcal{J}_4(E)\,. \tag{4.4.18}$$

The functions $\mathcal{A}^-(E)$ of Eq. (4.2.31) are given by

$$\mathcal{A}_3^-(E) = \frac{1}{2}e^{-iQb}\left(1-\frac{k}{Q}\right)e^{-ikb}, \tag{4.4.19a}$$

$$\mathcal{A}_4^-(E) = \frac{1}{2}e^{iQb}\left(1+\frac{k}{Q}\right)e^{-ikb}, \tag{4.4.19b}$$

$$\mathcal{A}_1^-(E) = \frac{1}{2}e^{-ika}\left[\left(1+\frac{Q}{k}\right)e^{iQa}\mathcal{A}_3^-(E) + \left(1-\frac{Q}{k}\right)e^{-iQa}\mathcal{A}_4^-(E)\right], \tag{4.4.19c}$$

$$\mathcal{A}_2^-(E) = \frac{1}{2}e^{ika}\left[\left(1-\frac{Q}{k}\right)e^{iQa}\mathcal{A}_3^-(E) + \left(1+\frac{Q}{k}\right)e^{-iQa}\mathcal{A}_4^-(E)\right]. \tag{4.4.19d}$$

The Wronskian of χ and Θ_- is

$$W(\chi, \Theta_-) = -2ik\mathcal{J}_3(E)\,. \tag{4.4.20}$$

4.4.3 Appendix 3: Diagonalization and Eigenfunction Expansion

The theorem that provides the operator U that diagonalizes H is (cf. Theorem XIII.5.13 of Ref. [30])

Theorem 2 (Weyl-Kodaira) Let h be the formally self-adjoint differential operator (4.2.5) defined on the interval $[0,\infty)$. Let H be the self-adjoint operator (4.2.14). Let Λ be an open interval of the real axis, and suppose that there is given a set σ_1, σ_2 of functions, defined and continuous on $(0,\infty)\times\Lambda$, such that for each fixed E in Λ, $\sigma_1(\cdot;E)$, $\sigma_2(\cdot;E)$ forms a basis for the space of solutions of $h\sigma = E\sigma$. Then there exists a positive 2×2 matrix measure $\{\rho_{ij}\}$ defined on Λ, such that

1. the limit
$$[(Uf)_i(E) = \lim_{c\to 0}\lim_{d\to\infty}\left[\int_c^d f(r)\overline{\sigma_i(r;E)}dr\right] \tag{4.4.21}$$
exists in the topology of $L^2(\Lambda,\{\rho_{ij}\})$ for each f in $L^2([0,\infty),dr)$ and defines an isometric isomorphism U of $E(\Lambda)L^2([0,\infty),dr)$ onto $L^2(\Lambda,\{\rho_{ij}\})$;

2. for each Borel function G defined on the real line and vanishing outside Λ,

$$U\mathcal{D}(G(H)) = \{[f_i] \in L^2(\Lambda, \{\rho_{ij}\}) \mid [Gf_i] \in L^2(\Lambda, \{\rho_{ij}\})\} \tag{4.4.22}$$

and

$$(UG(H)f)_i(E) = G(E)(Uf)_i(E), \quad i = 1, 2,\ E \in \Lambda,\ f \in \mathcal{D}(G(H))\,. \tag{4.4.23}$$

The theorem that provides the inverse of the operator U is (cf. Theorem XIII.5.14 of Ref. [30])

Theorem 3 (Weyl-Kodaira) Let H, Λ, $\{\rho_{ij}\}$, etc., be as in Theorem 2. Let E_0 and E_1 be the end points of Λ. Then

1. the inverse of the isometric isomorphism U of $E(\Lambda)L^2([0,\infty), dr)$ onto $L^2(\Lambda, \{\rho_{ij}\})$ is given by the formula

$$(U^{-1}F)(r) = \lim_{\mu_0 \to E_0} \lim_{\mu_1 \to E_1} \int_{\mu_0}^{\mu_1} \left(\sum_{i,j=1}^{2} F_i(E)\sigma_j(r;E)\rho_{ij}(dE) \right) \tag{4.4.24}$$

   where $F = [F_1, F_2] \in L^2(\Lambda, \{\rho_{ij}\})$, the limit existing in the topology of $L^2([0,\infty), dr)$;

2. if G is a bounded Borel function vanishing outside a Borel set e whose closure is compact and contained in Λ, then $G(H)$ has the representation

$$(G(H)f)(r) = \int_0^\infty f(s)K(H,r,s)ds\,, \tag{4.4.25}$$

   where

$$K(H,r,s) = \sum_{i,j=1}^{2} \int_e G(E)\overline{\sigma_i(s;E)}\sigma_j(r;E)\rho_{ij}(dE)\,. \tag{4.4.26}$$

The spectral measures are provided by the following theorem (cf. Theorem XIII.5.18 of Ref. [30]):

Theorem 4 (Titchmarsh-Kodaira) Let Λ be an open interval of the real axis and O be an open set in the complex plane containing Λ. Let σ_1, σ_2 be a set of functions which form a basis for the solutions of the equation $h\sigma = E\sigma$, $E \in O$, and which are continuous on $(0,\infty) \times O$ and analytically dependent on E for E in O. Suppose that the kernel $G(r,s;E)$ for the resolvent $(E-H)^{-1}$ has a representation

$$G(r,s;E) = \begin{cases} \sum_{i,j=1}^{2} \theta_{ij}^{-}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} & r < s \\ \sum_{i,j=1}^{2} \theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} & r > s\,, \end{cases} \tag{4.4.27}$$

for all E in $\mathrm{Re}(H)\cap O$, and that $\{\rho_{ij}\}$ is a positive matrix measure on Λ associated with H as in Theorem 2. Then the functions $\theta_{ij}^{\pm}$ are analytic in $\mathrm{Re}(H)\cap O$, and given any bounded open interval $(E_1, E_2)\subset\Lambda$, we have for $1\le i,j\le 2$,

$$\begin{aligned}\rho_{ij}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\tfrac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{-}(E-i\epsilon)-\theta_{ij}^{-}(E+i\epsilon)]dE\\ &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\tfrac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{+}(E-i\epsilon)-\theta_{ij}^{+}(E+i\epsilon)]dE\,.\end{aligned} \tag{4.4.28}$$

The functions $\widetilde{\mathcal{B}}(E)$ of Eq. (4.2.32a) are given by

$$\widetilde{\mathcal{B}}_3(E)=\frac{1}{2}e^{-\widetilde{Q}b}\left(1+\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}b}, \tag{4.4.29a}$$

$$\widetilde{\mathcal{B}}_4(E)=\frac{1}{2}e^{\widetilde{Q}b}\left(1-\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}b}, \tag{4.4.29b}$$

$$\widetilde{\mathcal{B}}_1(E)=\frac{1}{2}e^{-\widetilde{k}a}\left[\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{B}}_3(E)+\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}a}\widetilde{\mathcal{B}}_4(E)\right], \tag{4.4.29c}$$

$$\widetilde{\mathcal{B}}_2(E)=\frac{1}{2}e^{\widetilde{k}a}\left[\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{B}}_3(E)+\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}a}\widetilde{\mathcal{B}}_4(E)\right]. \tag{4.4.29d}$$

The functions $\mathcal{C}(E)$ of Eq. (4.2.39b) are given by

$$\mathcal{C}_1(E)=\frac{1}{2}e^{-iQa}\left(\cos(ka)-\frac{k}{iQ}\sin(ka)\right), \tag{4.4.30a}$$

$$\mathcal{C}_2(E)=\frac{1}{2}e^{iQa}\left(\cos(ka)+\frac{k}{iQ}\sin(ka)\right), \tag{4.4.30b}$$

$$\mathcal{C}_3(E)=\frac{1}{2}e^{-ikb}\left[\left(1+\frac{Q}{k}\right)e^{iQb}\mathcal{C}_1(E)+\left(1-\frac{Q}{k}\right)e^{-iQb}\mathcal{C}_2(E)\right], \tag{4.4.30c}$$

$$\mathcal{C}_4(E)=\frac{1}{2}e^{ikb}\left[\left(1-\frac{Q}{k}\right)e^{iQb}\mathcal{C}_1(E)+\left(1+\frac{Q}{k}\right)e^{-iQb}\mathcal{C}_2(E)\right]. \tag{4.4.30d}$$

4.4.4 Appendix 4: Construction of the RHS

Proposition 1 The quantities

$$\|\varphi\|_{n,m}:=\sqrt{\int_0^\infty dr\;|(r+1)^n(h+1)^m\varphi(r)|^2},\quad n,m=0,1,2,\ldots,\ \varphi\in\mathbf{\Phi}\,, \tag{4.4.31}$$

are norms.

Proof It is very easy to show that the quantities (4.4.31) fulfill the conditions to be a norm,

$$\|\varphi+\psi\|_{n,m} \leq \|\varphi\|_{n,m} + \|\psi\|_{n,m}\,, \tag{4.4.32a}$$
$$\|\alpha\varphi\|_{n,m} = |\alpha|\,\|\varphi\|_{n,m}\,, \tag{4.4.32b}$$
$$\|\varphi\|_{n,m} \geq 0\,, \tag{4.4.32c}$$
$$\text{If } \|\varphi\|_{n,m} = 0, \text{ then } \varphi = 0\,. \tag{4.4.32d}$$

The only condition that is somewhat difficult to prove is (4.4.32d): if $\|\varphi\|_{n,m} = 0$, then

$$(1+r)^n(h+1)^m\varphi(r) = 0\,, \tag{4.4.33}$$

which yields

$$(h+1)^m\varphi(r) = 0\,. \tag{4.4.34}$$

If $m = 0$, then Eq. (4.4.34) implies $\varphi(r) = 0$. If $m = 1$, then Eq. (4.4.34) implies that -1 is an eigenvalue of H whose corresponding eigenvector is φ. Since -1 is not an eigenvalue of H, φ must be the zero vector. If $m > 1$, the proof is similar.

Proposition 2 The space $\mathbf{\Phi}$ is stable under the action of H, and H is $\tau_{\mathbf{\Phi}}$-continuous.

Proof In order to see that H is $\tau_{\mathbf{\Phi}}$-continuous, we just have to realize that

$$\begin{aligned} \|H\varphi\|_{n,m} &= \|(H+I)\varphi - \varphi\|_{n,m} \\ &\leq \|(H+I)\varphi\|_{n,m} + \|\varphi\|_{n,m} \\ &= \|\varphi\|_{n,m+1} + \|\varphi\|_{n,m}\,. \end{aligned} \tag{4.4.35}$$

We now prove that $\mathbf{\Phi}$ is stable under the action of H. Let $\varphi \in \mathbf{\Phi}$. To say that $\varphi \in \mathbf{\Phi}$ is equivalent to say that $\varphi \in \mathcal{D}$ and that the norms $\|\varphi\|_{n,m}$ are finite for every $n, m = 0, 1, 2, \ldots$ Since $H\varphi$ is also in $\mathcal{D}$, and since the norms $\|H\varphi\|_{n,m}$ are also finite (see Eq. (4.4.35)), the vector $H\varphi$ is also in $\mathbf{\Phi}$.

Proposition 3 The function

$$\begin{aligned} |E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r;E)dr = \overline{(U\varphi)(E)}\,. \end{aligned} \tag{4.4.36}$$

is an antilinear functional on $\mathbf{\Phi}$ that is a generalized eigenvector of (the restriction to $\mathbf{\Phi}$ of) H.

Proof From the definition (4.4.36), it is pretty easy to see that $|E\rangle$ is an antilinear functional. In order to show that $|E\rangle$ is continuous, we define

$$\mathcal{M}(E) := \sup_{r\in[0,\infty)} |\sigma(r;E)|\,. \tag{4.4.37}$$

Since

$$
\begin{aligned}
|\langle\varphi|E\rangle| &= |\overline{U\varphi(E)}| \\
&= \left|\int_0^\infty dr\, \overline{\varphi(r)}\sigma(r;E)\right| \\
&\leq \int_0^\infty dr\, |\overline{\varphi(r)}||\sigma(r;E)| \\
&\leq \mathcal{M}(E)\int_0^\infty dr\, |\varphi(r)| \\
&= \mathcal{M}(E)\int_0^\infty dr\, \frac{1}{1+r}(1+r)|\varphi(r)| \\
&\leq \mathcal{M}(E)\left(\int_0^\infty dr\, \frac{1}{(1+r)^2}\right)^{1/2}\left(\int_0^\infty dr\, |(1+r)\varphi(r)|^2\right)^{1/2} \\
&= \mathcal{M}(E)\left(\int_0^\infty dr\, \frac{1}{(1+r)^2}\right)^{1/2}\|\varphi\|_{1,0} \\
&= \mathcal{M}(E)\|\varphi\|_{1,0}\,, \qquad (4.4.38)
\end{aligned}
$$

the functional $|E\rangle$ is continuous when $\mathbf{\Phi}$ is endowed with the $\tau_{\mathbf{\Phi}}$ topology.

In order to prove that $|E\rangle$ is a generalized eigenvector of H, we make use of the conditions (4.2.78) and (4.2.81) satisfied the elements of $\mathbf{\Phi}$,

$$
\begin{aligned}
\langle\varphi|H^\times|E\rangle &= \langle H\varphi|E\rangle \\
&= \int_0^\infty dr\, \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)\overline{\varphi(r)}\sigma(r;E) \\
&= -\frac{\hbar^2}{2m}\left[\frac{d\overline{\varphi(r)}}{dr}\sigma(r;E)\right]_0^\infty + \frac{\hbar^2}{2m}\left[\overline{\varphi(r)}\frac{d\sigma(r;E)}{dr}\right]_0^\infty \\
&\quad + \int_0^\infty dr\, \overline{\varphi(r)}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)\sigma(r;E) \\
&= E\langle\varphi|E\rangle\,. \qquad (4.4.39)
\end{aligned}
$$

Similarly, one can also prove that

$$\langle\varphi|(H^\times)^n|E\rangle = E^n\langle\varphi|E\rangle\,. \qquad (4.4.40)$$

4.4.5 Appendix 5: Dirac Basis Vector Expansion

Proposition 4 (Nuclear Spectral Theorem) Let

$$\mathbf{\Phi} \subset L^2([0,\infty), dr) \subset \mathbf{\Phi}^\times \qquad (4.4.41)$$

be the RHS of the square barrier Hamiltonian H such that $\mathbf{\Phi}$ remains invariant under H and H is a $\tau_{\mathbf{\Phi}}$-continuous operator on $\mathbf{\Phi}$. Then, for each E in the spectrum of H there is a

generalized eigenvector $|E\rangle$ such that

$$H^{\times}|E\rangle = E|E\rangle \tag{4.4.42}$$

and such that

$$(\varphi, \psi) = \int_{\mathrm{Sp}(H)} dE\, \langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi, \psi \in \mathbf{\Phi}\,, \tag{4.4.43}$$

and

$$(\varphi, H^n\psi) = \int_{\mathrm{Sp}(H)} dE\, E^n \langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi, \psi \in \mathbf{\Phi}\,, n = 1, 2, \ldots \tag{4.4.44}$$

Proof Let φ and ψ be in $\mathbf{\Phi}$. Since U is unitary,

$$(\varphi, \psi) = (U\varphi, U\psi) = (\widehat{\varphi}, \widehat{\psi})\,. \tag{4.4.45}$$

The wave functions $\widehat{\varphi}$ and $\widehat{\psi}$ are in particular elements of $L^2([0, \infty), dE)$. Therefore their scalar product is well-defined,

$$(\widehat{\varphi}, \widehat{\psi}) = \int_{\mathrm{Sp}(H)} dE\, \overline{\widehat{\varphi}(E)}\widehat{\psi}(E)\,. \tag{4.4.46}$$

Since φ and ψ belong to $\mathbf{\Phi}$, the action of each eigenket $|E\rangle$ on them is well-defined,

$$\langle\varphi|E\rangle = \overline{\widehat{\varphi}(E)}\,, \tag{4.4.47a}$$

$$\langle E|\psi\rangle = \widehat{\psi}(E)\,. \tag{4.4.47b}$$

Plugging Eq. (4.4.47) into Eq. (4.4.46) and Eq. (4.4.46) into Eq. (4.4.45), we get to Eq. (4.4.43). The proof of (4.4.44) is similar:

$$\begin{aligned}
(\varphi, H^n\psi) &= (U\varphi, UH^nU^{-1}U\psi) \\
&= (\widehat{\phi}, \widehat{E}^n\widehat{\psi}) \\
&= \int_{\mathrm{Sp}(H)} dE\, \overline{\widehat{\varphi}(E)}(\widehat{E}^n\widehat{\psi})(E) \\
&= \int_{\mathrm{Sp}(H)} dE\, E^n\overline{\widehat{\varphi}(E)}\widehat{\psi}(E) \\
&= \int_{\mathrm{Sp}(H)} dE\, E^n\langle\varphi|E\rangle\langle E|\psi\rangle\,.
\end{aligned} \tag{4.4.48}$$

4.4.6 Appendix 6: Energy Representation of the RHS

Proposition 5 The energy representation $|\widehat{E}\rangle$ of the eigenket $|E\rangle$ is the antilinear Schwartz delta functional.

Proof Since

$$\begin{aligned}
\langle \widehat{\varphi} | U^{\times} | E \rangle &= \langle U^{-1} \widehat{\varphi} | E \rangle \\
&= \langle \varphi | E \rangle \\
&= \int_0^{\infty} \overline{\varphi(r)} \sigma(r; E) dr \\
&= \overline{\widehat{\varphi}(E)}\,, \qquad (4.4.49)
\end{aligned}$$

the functional $U^{\times}|E\rangle = |\widehat{E}\rangle$ is the antilinear Schwartz delta functional.

Chapter 5

Scattering off the Square Barrier Potential

In this chapter, we turn to the description of the Lippmann-Schwinger equation within the RHS formalism. The Lippmann-Schwinger eigenfunctions will be computed first. We shall define the Lippmann-Schwinger eigenkets in terms of these eigenfunctions and see that they act on different spaces of wave functions. The Møller operators and the S-matrix will be explicitly constructed.

It is so hard to be good!

Thales of Miletus

5.1 Introduction

In the previous chapter, we constructed a RHS of the square barrier potential. The RHS was meant to incorporate certain boundary conditions imposed upon the Schrödinger equation:

$$\boxed{\begin{array}{c}\text{Schrödinger equation}\\ + \\ \text{boundary conditions}\end{array}} \longrightarrow \mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times}.$$

The Hilbert space $\mathcal{H}$ was needed to incorporate the requirement that the wave functions be square integrable. The space $\mathbf{\Phi}^{\times}$ was needed to incorporate the Dirac kets associated to the eigenfunctions of the time independent Schrödinger equation subject to certain boundary conditions. The space $\mathbf{\Phi}$ was needed to incorporate the wave functions on which the Dirac kets act as continuous antilinear functionals. The space $\mathbf{\Phi}$ was identified with the space of physically preparable wave functions, because in $\mathbf{\Phi}$ all of the algebraic operations and all of the expectation values are well defined.

In this chapter, we consider the problem of scattering off the square barrier potential. Loosely speaking, we send a beam of prepared initial in-states φ^{in} towards the square barrier potential. After the collision takes place, the in-state φ^{in} becomes φ^{out}. We then measure the probability to find a final out-state ψ^{out}. The amplitude of this probability is given by the following scalar product:

$$(\psi^{out}, \varphi^{out}) = (\psi^{out}, S\varphi^{in}), \tag{5.1.1}$$

where S is the S-matrix. The canonical understanding is that the initial in-states φ^{in} and the final out-states ψ^{out} are asymptotic forms of the so-called in-state vector φ^{+} and out-state vector ψ^{-} in the remote past and in the distant future, respectively. In terms of these, the probability amplitude (5.1.1) can be written as

$$(\psi^{-}, \varphi^{+}). \tag{5.1.2}$$

The asymptotic states φ^{in} and ψ^{out} are related to the "exact" states φ^{+} and ψ^{-} by the so-called Møller operators:

$$\Omega_{+}\varphi^{in} = \varphi^{+}, \tag{5.1.3a}$$
$$\Omega_{-}\psi^{out} = \psi^{-}. \tag{5.1.3b}$$

Along with the (total) Hamiltonian H, it is customary to consider another "free" Hamiltonian H_0, which is assumed to differ from H by the (square barrier) potential V,

$$H = H_0 + V. \tag{5.1.4}$$

The potential V represents the interaction between the components of the initial prepared states, for instance, the interaction between the in-going beam and the target. The canonical

understanding is that the initial in-state φ^{in} and the final out-state ψ^{out} evolve under the influence of the free Hamiltonian H_0, whereas the in-state φ^+ and the out-state ψ^- evolve under the influence of the (total) Hamiltonian H.

The dynamics of a scattering system is therefore governed by the Schrödinger equation subject to certain boundary conditions. These boundary conditions specify what is "in" and what is "out."

The Lippmann-Schwinger equation for the in- and out-kets $|E^\pm\rangle$ has the scattering boundary conditions built into it. As we shall see, the Lippmann-Schwinger equation tells us what is "in" and what is "out" by specifying certain analytical properties of its solutions. The analytical properties satisfied by the in-ket $|E^+\rangle$ (or, equivalently, by the wave function $\langle\varphi^+|E^+\rangle$) are different to those satisfied by the out-ket $|E^-\rangle$ (or, equivalently, by the wave function $\langle\psi^-|E^-\rangle$). In incorporating these two different types of boundary conditions into a RHS framework, we will end up constructing two different RHSs:

$$\mathbf{\Phi}_\pm \subset \mathcal{H} \subset \mathbf{\Phi}_\pm^\times . \tag{5.1.5}$$

On our way, we will also construct the Møller operators and the S-matrix, and we will express the matrix element (5.1.2) in terms of the in- and out-Lippmann-Schwinger kets:

$$(\psi^-, \varphi^+) = \int_0^\infty dE\, \langle\psi^-|E^-\rangle S(E) \langle^+E|\varphi^+\rangle . \tag{5.1.6}$$

This expression will be used to derive the complex basis vector expansion in Chapter 6.

5.2 Lippmann-Schwinger Equation

5.2.1 Lippmann-Schwinger Kets

One of the fundamental equations of scattering theory is the Lippmann-Schwinger equation,[1]

$$|E^\pm\rangle = |E\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|E^\pm\rangle . \tag{5.2.1}$$

This equation is also written as

$$|E^\pm\rangle = |E\rangle + \frac{1}{E - H \pm i\epsilon} V|E\rangle . \tag{5.2.2}$$

In Eqs. (5.2.1) and (5.2.2), the kets $|E^\pm\rangle$ represent generalized eigenvector of the total Hamiltonian H,

$$H^\times|E^\pm\rangle = E|E^\pm\rangle , \tag{5.2.3}$$

whereas $|E\rangle$ represents a generalized eigenvector of the free Hamiltonian H_0,

$$H_0^\times|E\rangle = E|E\rangle . \tag{5.2.4}$$

[1] In this chapter, the symbol $|E\rangle$ will denote the generalized eigenket of the free Hamiltonian that appears in the Lippmann-Schwinger equation (5.2.1), and not an eigenket of the total Hamiltonian as in Chapter 4.

5.2.2 Radial Representation of the Lippmann-Schwinger Equation

Since our square barrier potential is spherically symmetric, we shall work in the radial representation. In this representation and for $l = 0$, H_0 acts as the formal differential operator h_0,

$$H_0 f(r) = h_0 f(r) = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} f(r)\,, \tag{5.2.5}$$

V acts as multiplication by the square barrier potential $V(r)$,

$$V(r) = \begin{cases} 0 & 0 < r < a \\ V_0 & a < r < b \\ 0 & b < r < \infty\,, \end{cases} \tag{5.2.6}$$

and H acts as the formal differential operator h,

$$Hf(r) = hf(r) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right) f(r)\,. \tag{5.2.7}$$

In the radial representation, Eqs. (5.2.1) and (5.2.2) become

$$\langle r|E^{\pm}\rangle = \langle r|E\rangle + \langle r|\frac{1}{E - H_0 \pm i\epsilon} V|E^{\pm}\rangle\,, \tag{5.2.8a}$$

$$\langle r|E^{\pm}\rangle = \langle r|E\rangle + \langle r|\frac{1}{E - H \pm i\epsilon} V|E\rangle\,. \tag{5.2.8b}$$

In Eq. (5.2.8), the quantities $\langle r|E\rangle$ are eigenfunctions of the formal differential operator h_0,

$$h_0\langle r|E\rangle = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\langle r|E\rangle = E\langle r|E\rangle\,, \tag{5.2.9}$$

whereas the quantities $\langle r|E^{\pm}\rangle$ are eigenfunctions of the formal differential operator h satisfying proper boundary conditions (that we will specify later),

$$h\langle r|E^{\pm}\rangle = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right)\langle r|E^{\pm}\rangle = E\langle r|E^{\pm}\rangle\,. \tag{5.2.10}$$

In the absence of potential, the Lippmann-Schwinger eigenfunctions tend to the free Hamiltonian eigenfunctions,

$$\lim_{V_0\to 0}\langle r|E^{\pm}\rangle = \langle r|E\rangle\,. \tag{5.2.11}$$

The generalized eigenvectors $|E\rangle$ of H_0 and the eigenfunctions $\langle r|E\rangle$ of h_0 are related by

$$\langle\varphi|E\rangle = \int_0^\infty dr\,\langle\varphi|r\rangle\langle r|E\rangle\,. \tag{5.2.12}$$

The generalized eigenvectors $|E^{\pm}\rangle$ of H and the eigenfunctions $\langle r|E^{\pm}\rangle$ of h are related by

$$\langle\varphi^+|E^+\rangle = \lim_{\epsilon\to 0}\int_0^\infty dr\,\langle\varphi^+|r\rangle\langle r|(E+i\epsilon)^+\rangle\,, \quad \varphi^+\in\mathbf{\Phi}_-\,, \tag{5.2.13a}$$

$$\langle\psi^-|E^-\rangle = \lim_{\epsilon\to 0}\int_0^\infty dr\,\langle\psi^-|r\rangle\langle r|(E-i\epsilon)^-\rangle\,, \quad \psi^-\in\mathbf{\Phi}_+\,. \tag{5.2.13b}$$

The wave functions φ^+ are usually called in-states, whereas the the wave functions ψ^- are called out-states. However, we shall call the ψ^- observables (or out-observables), because they are determined by the registration apparatus. In order to grasp the meaning of this terminology, let us consider the matrix element (ψ^-,φ^+). This scalar product is the amplitude of the probability to observe the out-state ψ^- in the in-state φ^+. Since ψ^- is determined by the property we want to measure, it stands to reason that we call it observable and denote it by a specific symbol.

The action of the Lippmann-Schwinger kets is defined as the limits in (5.2.13). We are now going to elaborate on that definition.

The difference between the in-states and the observables is reflected not only in the notation, but also in the fact that they belong to different subspaces of the Hilbert space. The reason for this is the following:[2] the boundary conditions built into the Lippmann-Schwinger equation for the in-ket $|E^+\rangle$ (or, equivalently, for the eigenfunction $\langle r|E^+\rangle$) are different to the boundary conditions for the ket $|E^-\rangle$ (or, equivalently, for the eigenfunction $\langle r|E^-\rangle$). Since the boundary conditions determine the space of test functions on which the kets act, the in-ket $|E^+\rangle$ acts on a space $\mathbf{\Phi}_-$, and the out-ket $|E^-\rangle$ acts on a space $\mathbf{\Phi}_+$, which is different to $\mathbf{\Phi}_-$.

The difference in the boundary conditions for the in- an out-kets is built into the $\pm i\epsilon$ of Eq. (5.2.1). The meaning of the $\pm i\epsilon$ is that we are approaching the cut (i.e., the spectrum of H) either from above $(+i\epsilon)$ or from below $(-i\epsilon)$. Therefore, the action of the Lippmann-Schwinger kets $|E^{\pm}\rangle$ should be viewed as the limit of the action of certain kets $|(E\pm i\epsilon)^{\pm}\rangle$ that have meaning when $\epsilon\neq 0$,

$$|(E\pm i\epsilon)^{\pm}\rangle \xrightarrow[\epsilon\to 0]{} |E^{\pm}\rangle\,. \tag{5.2.14}$$

If we want this limit process to be well-defined, the following integrals should be well-defined:

$$\langle\varphi^+|(E+i\epsilon)^+\rangle = \int_0^\infty dr\,\langle\varphi^+|r\rangle\langle r|(E+i\epsilon)^+\rangle\,, \quad \varphi^+\in\mathbf{\Phi}_-\,, \tag{5.2.15a}$$

$$\langle\psi^-|(E-i\epsilon)^-\rangle = \int_0^\infty dr\,\langle\psi^-|r\rangle\langle r|(E-i\epsilon)^-\rangle\,, \quad \psi^-\in\mathbf{\Phi}_+\,. \tag{5.2.15b}$$

Thus the action of the Lippmann-Schwinger kets, that has to be viewed as the limit of the action of the kets (5.2.15) when ϵ tends to zero, would be defined by

$$\langle\varphi^+|E^+\rangle = \lim_{\epsilon\to 0}\langle\varphi^+|(E+i\epsilon)^+\rangle\,, \quad \varphi^+\in\mathbf{\Phi}_-\,, \tag{5.2.16a}$$

$$\langle\psi^-|E^-\rangle = \lim_{\epsilon\to 0}\langle\psi^-|(E-i\epsilon)^-\rangle\,, \quad \psi^-\in\mathbf{\Phi}_+\,. \tag{5.2.16b}$$

[2]For a mathematical approach to this question in terms of RHSs of Hardy functions see Ref. [31].

In addition, we would like our spaces $\mathbf{\Phi}_\pm$ to be stable under the action of the Hamiltonian. This is why we should also impose the following conditions:

$$(E+i\epsilon)^n\langle\varphi^+|(E+i\epsilon)^+\rangle = \int_0^\infty dr\,\langle H^n\varphi^+|r\rangle\langle r|(E+i\epsilon)^+\rangle\,, \quad \varphi^+\in\mathbf{\Phi}_-\,, \tag{5.2.17a}$$

$$(E-i\epsilon)^n\langle\psi^-|(E-i\epsilon)^-\rangle = \int_0^\infty dr\,\langle H^n\psi^-|r\rangle\langle r|(E-i\epsilon)^-\rangle\,, \quad \psi^-\in\mathbf{\Phi}_+\,, \tag{5.2.17b}$$

for every $n=0,1,2,\ldots$ In the position representation, the conditions (5.2.17) should lead to restrictions in the asymptotic behavior of the wave functions $\varphi^+(r)$ and $\psi^-(r)$. In the energy representation, the conditions (5.2.17) should lead to analytical properties of the wave functions $\widehat{\varphi}^+(E)$ and $\widehat{\psi}^-(E)$.

The precise connection between the conditions satisfied by $\varphi^+(r)$ ($\psi^-(r)$) and those satisfied by $\widehat{\varphi}^+(E)$ ($\widehat{\psi}^-(E)$) is still an open problem. Our guess is that $\widehat{\varphi}^+(E)$ will be the limit value of a Hardy class function from below, and that $\widehat{\psi}^-(E)$ will be the limit value of a Hardy class function from above (cf. Appendix 5.5.2 for the definition and general properties of Hardy class functions).

5.2.3 Solution of the Radial Lippmann-Schwinger Equation

Instead of solving the integral equations (5.2.8), we solve the equivalent differential equations

$$h\langle r|E^\pm\rangle = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)\langle r|E^\pm\rangle = E\langle r|E^\pm\rangle \tag{5.2.18}$$

subject to the boundary conditions that are built into the integral equations (5.2.8). These boundary conditions are

$$\langle 0|E^\pm\rangle = 0\,, \tag{5.2.19a}$$

$$\langle r|E^\pm\rangle \text{ is continuous at } r=a \text{ and at } r=b\,, \tag{5.2.19b}$$

$$\frac{d}{dr}\langle r|E^\pm\rangle \text{ is continuous at } r=a \text{ and at } r=b\,, \tag{5.2.19c}$$

$$\lim_{V_0\to 0}\langle r|E^\pm\rangle = \langle r|E\rangle\,, \tag{5.2.19d}$$

$$\langle r|E^+\rangle \sim e^{-ikr} - S(E)e^{ikr} \text{ as } r\to\infty\,, \tag{5.2.19e}$$

$$\langle r|E^-\rangle \sim e^{ikr} - S^*(E)e^{-ikr} \text{ as } r\to\infty\,, \tag{5.2.19f}$$

where

$$k=\sqrt{\frac{2m}{\hbar^2}E} \tag{5.2.20}$$

and $S(E)$ is the S-matrix in the energy representation.

It is well-known (cf. [72, 73]) that the in- and out-eigenfunctions are given by

$$\chi^\pm(r;E) = \frac{\chi(r;E)}{\mathcal{J}_\pm(E)}\,, \tag{5.2.21}$$

where $\chi(r;E)$ is the eigenfunction (4.2.28),

$$\chi(r;E) = \begin{cases} \sin(\sqrt{\frac{2m}{\hbar^2}E}r) & 0 < r < a \\ \mathcal{J}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{J}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a < r < b \\ \mathcal{J}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{J}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b < r < \infty\,, \end{cases} \tag{5.2.22}$$

and $\mathcal{J}_\pm(E)$ are the Jost functions,

$$\mathcal{J}_+(E) = -2i\mathcal{J}_4(E)\,, \tag{5.2.23a}$$

$$\mathcal{J}_-(E) = 2i\mathcal{J}_3(E)\,. \tag{5.2.23b}$$

In terms of the Jost functions, the S-matrix is given by

$$S(E) = \frac{\mathcal{J}_-(E)}{\mathcal{J}_+(E)}\,. \tag{5.2.24}$$

From Eq. (5.2.21) it follows that the in- and out-eigenfunctions are proportional to each other,

$$\chi^+(r;E) = S(E)\chi^-(r;E)\,. \tag{5.2.25}$$

It is worthwhile noting that the boundary condition that singles out the in- and out-Lippmann-Schwinger eigenfunctions is their asymptotic behavior at infinity as functions of r (see Eqs. (5.2.19e) and (5.2.19f)). That asymptotic behavior is transfered into the energy representation as a certain analytical property of the eigenfunction $\chi^\pm(r;E)$ as a function of E. Since the boundary conditions satisfied by the elements of the space of test functions are related to the boundary conditions satisfied by the eigenfunctions of the Schrödinger equation, it seems reasonable to expect that the boundary conditions that single out the $\varphi^+(r)$ and the $\psi^-(r)$ are related to their asymptotic behavior, and that this asymptotic behavior is transfered into the energy representation as a condition on the analytical properties of the wave functions $\widehat{\varphi}^+(E)$ and $\widehat{\psi}^-(E)$.

5.2.4 Direct Integral Decomposition Associated to the In-States

Once we have obtained the in-Lippmann-Schwinger eigenfunction, we can construct the direct integral decomposition induced by it. In order to do so, we follow the procedure of Section 4.2.4.

The domain $\mathcal{D}(H)$ on which the formal differential operator h is self-adjoint was obtained in Section 4.2.2,

$$\mathcal{D}(H) = \{f(r) \mid f(r), hf(r) \in L^2([0,\infty), dr),\ f(r) \in AC^2[0,\infty),\ f(0) = 0\}\,. \tag{5.2.26}$$

As we saw in Section 4.2.2, this domain induces a self-adjoint operator H,

$$(Hf)(r) := hf(r) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right)f(r)\,, \quad f(r) \in \mathcal{D}(H)\,. \tag{5.2.27}$$

The spectrum of H is $[0,\infty)$ (cf. Section 4.2.4).

It is worthwhile noting that the space $\mathbf{\Phi}_-$ associated to the in-Lippmann-Schwinger eigenfunction $\chi^+(r;E)$ will be a subspace of $\mathcal{D}(H)$. In fact, it will be a subspace of the maximal invariant subspace of H. However, the space $\mathbf{\Phi}_-$ will be different to the space $\mathbf{\Phi}$ of Chapter 4, because the boundary conditions fulfilled by the elements of $\mathbf{\Phi}_-$ are different to the boundary conditions fulfilled by the elements of $\mathbf{\Phi}$.

The Green function of H was computed in Section 4.2.3 for different regions of the complex plane. Since we want to expand the wave functions in terms of the eigenfunction $\chi^+(r;E)$, we write the Green function in terms of $\chi^+(r;E)$. From Eqs.(4.2.27) and (5.2.21), we can see that

$$G(r,s;E)=\begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\chi^+(r;E)\,\Theta_+(s;E) & r<s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\chi^+(s;E)\,\Theta_+(r;E) & r>s \end{cases} \qquad \Re(E)>0,\ \Im(E)>0\,. \tag{5.2.28}$$

From Eqs. (4.2.30) and (5.2.21), we can see that

$$G(r,s;E)=\begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\chi^-(r;E)\,\Theta_-(s;E) & r<s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\chi^-(s;E)\,\Theta_-(r;E) & r>s \end{cases} \qquad \Re(E)>0,\ \Im(E)<0\,. \tag{5.2.29}$$

We are now in a position to compute the generalized Fourier transform U_+ induced by the Lippmann-Schwinger eigenfunction $\chi^+(r;E)$. In order to be able to apply Theorem 4 of Section 4.4.3, we choose the following basis for the space of solutions of $h\sigma=E\sigma$ that is continuous on $(0,\infty)\times\Lambda$ and analytically dependent on E:

$$\sigma_1(r;E)=\chi^+(r;E)\,, \tag{5.2.30a}$$

$$\sigma_2(r;E)=\begin{cases} \cos(\sqrt{\frac{2m}{\hbar^2}E}r) & 0<r<a \\ \mathcal{C}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r}+\mathcal{C}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \mathcal{C}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r}+\mathcal{C}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{5.2.30b}$$

The functions $\mathcal{C}_1-\mathcal{C}_4$ are given by Eq. (4.4.30) of Appendix 4.4.3.

Eqs. (4.2.29), (4.2.31) and (5.2.30) lead to

$$\Theta_+(r;E)=\frac{2i\mathcal{J}_4(E)\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E)+\frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E) \tag{5.2.31}$$

and to

$$\Theta_-(r;E)=-\frac{2i\mathcal{J}_4(E)\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E)-\frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\,, \tag{5.2.32}$$

where

$$W(E)=\mathcal{J}_4(E)\mathcal{C}_3(E)-\mathcal{J}_3(E)\mathcal{C}_4(E)\,. \tag{5.2.33}$$

By substituting Eq. (5.2.31) into Eq. (5.2.28) we get to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\left[\frac{2i\mathcal{J}_4(E)\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)>0\,,\; r>s\,. \qquad (5.2.34)$$

By substituting Eq. (5.2.32) into Eq. (5.2.29) we get to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{\mathcal{J}_4(E)}{\mathcal{J}_3(E)}\left[-\frac{2i\mathcal{J}_4(E)\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)<0\,,\; r>s\,, \qquad (5.2.35)$$

where we have used the fact that

$$\chi^-(r;E) = -\frac{\mathcal{J}_4(E)}{\mathcal{J}_3(E)}\chi^+(r;E)\,. \qquad (5.2.36)$$

Since

$$\overline{\sigma_1(s;\overline{E})} = -\frac{\mathcal{J}_4(E)}{\mathcal{J}_3(E)}\sigma_1(s;E)\,, \qquad (5.2.37)$$

Eq. (5.2.34) leads to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{W(E)}\left[2i\mathcal{J}_3(E)\mathcal{C}_4(E)\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} + \mathcal{J}_3(E)\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)>0\,,\; r>s\,, \qquad (5.2.38)$$

and Eq. (5.2.35) leads to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{W(E)}\left[2i\mathcal{J}_4(E)\mathcal{C}_3(E)\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} + \mathcal{J}_3(E)\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)<0\,,\; r>s\,. \qquad (5.2.39)$$

The expression of the resolvent in terms of the basis σ_1, σ_2 can be written as (see Theorem 4 in Appendix 4.4.3)

$$G(r,s;E) = \sum_{i,j=1}^{2}\theta_{ij}^+(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, \qquad r>s\,. \qquad (5.2.40)$$

By comparing (5.2.40) to (5.2.38) we get to

$$\theta_{ij}^+(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{2i\mathcal{J}_3(E)\mathcal{C}_4(E)}{W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{\mathcal{J}_3(E)}{W(E)} & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\; \Im(E)>0\,. \qquad (5.2.41)$$

By comparing (5.2.40) to (5.2.39) we get to

$$\theta^+_{ij}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{2i\mathcal{J}_4(E)\mathcal{C}_3(E)}{W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{\mathcal{J}_3(E)}{W(E)} & 0 \end{pmatrix}, \quad \Re(E) > 0\,,\ \Im(E) < 0\,. \tag{5.2.42}$$

From Eqs. (5.2.41) and (5.2.42) we can see that the measures ρ_{12}, ρ_{21} and ρ_{22} in Theorem 4 of Appendix 4.4.3 are zero and that the measure ρ_{11} is given by

$$\begin{aligned} \rho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}\left[\theta^+_{11}(E-i\epsilon)-\theta^+_{11}(E+i\epsilon)\right]dE \\ &= \int_{E_1}^{E_2}\frac{1}{\pi}\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,dE\,, \end{aligned} \tag{5.2.43}$$

which leads to

$$\rho^+(E) \equiv \rho_{11}(E) = \frac{1}{\pi}\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,, \quad E\in(0,\infty)\,. \tag{5.2.44}$$

By Theorem 2 of Appendix 4.4.3, there is a unitary map $\widetilde{U}_+$ defined by

$$\begin{aligned} \widetilde{U}_+ : L^2([0,\infty),dr) &\longmapsto L^2((0,\infty),\rho^+(E)dE) \\ f(r) &\longmapsto \widetilde{f}(E) = (\widetilde{U}_+f)(E) = \int_0^\infty dr\,f(r)\overline{\chi^+(r;E)}\,, \end{aligned} \tag{5.2.45}$$

that brings $\mathcal{D}(H)$ onto the space

$$\mathcal{D}(\widetilde{E}) = \{\widetilde{f}(E)\in L^2((0,\infty),\rho^+(E)dE)\,|\,\int_0^\infty dE\,E^2|\widetilde{f}(E)|^2\rho^+(E)<\infty\}\,. \tag{5.2.46}$$

Eqs. (5.2.45) and (5.2.46) provide a ρ^+-diagonalization of H. If we seek a δ-diagonalization, then the measure $\rho^+(E)$ must be absorbed by the eigenfunctions

$$\sigma^+(r;E) := \sqrt{\rho^+(E)}\,\chi^+(r;E)\,, \tag{5.2.47}$$

and by the wave functions

$$\widehat{f}(E) := \sqrt{\rho^+(E)}\widetilde{f}(E)\,, \quad \widetilde{f}(E)\in L^2((0,\infty),\rho^+(E)dE)\,. \tag{5.2.48}$$

The function $\sigma^+(r;E)$ is the eigensolution of the Lippmann-Schwinger equation (5.2.8) that is δ-normalized. Using Eq. (5.2.48) we can construct the unitary operator

$$\begin{aligned} \widehat{U}_+ : L^2((0,\infty)),\rho^+(E)dE) &\longmapsto L^2((0,\infty),dE) \\ \widetilde{f} &\longmapsto \widehat{f}(E) = (\widehat{U}_+\widetilde{f})(E) := \sqrt{\rho^+(E)}\widetilde{f}(E)\,. \end{aligned} \tag{5.2.49}$$

The operator that δ-diagonalizes our Hamiltonian is $U_+ := \widehat{U}_+\widetilde{U}_+$,

$$\begin{aligned} U_+ : L^2([0,\infty)),dr) &\longmapsto L^2((0,\infty),dE) \\ f &\longmapsto U_+f := \widehat{f}\,. \end{aligned} \tag{5.2.50}$$

The action of U_+ can be written as an integral operator,

$$\widehat{f}(E) = (U_+ f)(E) = \int_0^\infty dr\, f(r)\overline{\sigma^+(r;E)}\,, \quad f(r) \in L^2([0,\infty), dr)\,. \tag{5.2.51}$$

The image of $\mathcal{D}(H)$ under the action of U_+ is

$$\mathcal{D}(\widehat{E}) := U_+\mathcal{D}(H) = \{\widehat{f}(E) \in L^2((0,\infty), dE) \mid \int_0^\infty E^2|\widehat{f}(E)|^2 dE < \infty\}\,. \tag{5.2.52}$$

Therefore, we have constructed a unitary operator

$$\begin{aligned} U_+ : \mathcal{D}(H) \subset L^2([0,\infty), dr) &\longmapsto \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) \\ f &\longmapsto \widehat{f} = U_+ f \end{aligned} \tag{5.2.53}$$

that transforms from the position representation into the energy representation. The operator U_+ diagonalizes H, i.e., $\widehat{E} \equiv U_+ H U_+^{-1}$ is the multiplication operator,

$$\begin{aligned} \widehat{E} : \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) &\longmapsto L^2((0,\infty), dE) \\ \widehat{f} &\longmapsto \widehat{E}\widehat{f}(E) := E\widehat{f}(E)\,. \end{aligned} \tag{5.2.54}$$

The inverse operator of U_+ is given by (see Theorem 3 of Appendix 4.4.3)

$$f(r) = U_+^{-1}\widehat{f}(r) = \int_0^\infty dE\, \widehat{f}(E)\sigma^+(r,E)\,, \quad \widehat{f}(E) \in L^2((0,\infty), dE)\,. \tag{5.2.55}$$

The operator U_+^{-1} transforms from the energy representation into the position representation.

The expressions (5.2.51) and (5.2.55) provide the eigenfunction expansion of any wave function in terms of the δ-normalized eigensolutions $\sigma^+(r;E)$ of the Lippmann-Schwinger equation.

The unitary operator U_+ can be also looked at as a sort of generalized Fourier transform that connects the position and the energy representations. The eigenfunctions $\sigma^+(r;E)$ can be viewed as "transition elements" between the r- and the E-representations.

Thus we have constructed the direct integral decomposition of the Hilbert space associated to the eigenfunction $\chi^+(r;E)$ of the Lippmann-Schwinger equation,

$$\begin{aligned} \mathcal{H} &\longmapsto U_+\mathcal{H} \equiv \widehat{\mathcal{H}} = \oplus \int_{\mathrm{Sp}(H)} \mathcal{H}(E)dE \\ f &\longmapsto U_+ f \equiv \{\widehat{f}(E)\}, \quad f \in \mathcal{D}(H)\,,\ \widehat{f}(E) \in \mathcal{H}(E)\,. \end{aligned} \tag{5.2.56}$$

In Eq. (5.2.56), the Hilbert spaces $\mathcal{H}$, $\widehat{\mathcal{H}}$ and $\mathcal{H}(E)$ are the same as in Eq. (4.2.64).

5.2.5 Direct Integral Decomposition Associated to the Observables

In this section, we compute the unitary operator U_- induced by the Lippmann-Schwinger eigenfunction $\chi^-(r;E)$. Since the computations are very similar to the computations performed in Section 5.2.4 for the in-states, we will restrict the explanations to the minimum and just write down the results.

The functions

$$\sigma_1(r;E) = \chi^-(r;E)\,, \tag{5.2.57a}$$

$$\sigma_2(r;E) = \begin{cases} \cos(\sqrt{\frac{2m}{\hbar^2}E}r) & 0<r<a \\ \mathcal{C}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{C}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \mathcal{C}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{C}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{5.2.57b}$$

form a basis for the space of solutions of $h\sigma = E\sigma$ that is continuous on $(0,\infty)\times\Lambda$ and analytically dependent on E. Therefore, we are allowed to apply Theorem 4 of Appendix 4.4.3.

Eqs. (4.2.29), (4.2.31) and (5.2.57) lead to

$$\Theta_+(r;E) = -\frac{2i\mathcal{J}_3(E)\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E) \tag{5.2.58}$$

and to

$$\Theta_-(r;E) = \frac{2i\mathcal{J}_3(E)\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\,, \tag{5.2.59}$$

where

$$W(E) = \mathcal{J}_4(E)\mathcal{C}_3(E) - \mathcal{J}_3(E)\mathcal{C}_4(E)\,. \tag{5.2.60}$$

By substituting Eq. (5.2.58) into Eq. (5.2.28) we get to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\mathcal{J}_3(E)}{\mathcal{J}_4(E)}\left[-\frac{2i\mathcal{J}_3(E)\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)>0\,,\ r>s\,. \tag{5.2.61}$$

By substituting Eq. (5.2.59) into Eq. (5.2.29) we get to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\left[\frac{2i\mathcal{J}_3(E)\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)<0\,,\ r>s\,. \tag{5.2.62}$$

Since

$$\overline{\sigma_1(s;\overline{E})} = -\frac{\mathcal{J}_3(E)}{\mathcal{J}_4(E)}\sigma_1(s;E)\,, \tag{5.2.63}$$

Eq. (5.2.61) leads to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{W(E)}\left[2i\mathcal{J}_3(E)\mathcal{C}_4(E)\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} - \mathcal{J}_4(E)\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)>0\,,\; r>s\,, \qquad (5.2.64)$$

and Eq. (5.2.62) leads to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{W(E)}\left[2i\mathcal{J}_4(E)\mathcal{C}_3(E)\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} - \mathcal{J}_4(E)\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)<0\,,\; r>s\,. \qquad (5.2.65)$$

The expression of the resolvent in terms of the basis σ_1, σ_2 can be written as (see Theorem 4 in Appendix 4.4.3)

$$G(r,s;E) = \sum_{i,j=1}^{2} \theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, \qquad r>s\,. \qquad (5.2.66)$$

By comparing (5.2.66) to (5.2.64) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{2i\mathcal{J}_3(E)\mathcal{C}_4(E)}{W(E)} & 0 \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{\mathcal{J}_4(E)}{W(E)} & 0 \end{pmatrix}, \quad \Re(E)>0\,,\; \Im(E)>0\,. \qquad (5.2.67)$$

By comparing (5.2.66) to (5.2.65) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{2i\mathcal{J}_4(E)\mathcal{C}_3(E)}{W(E)} & 0 \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{\mathcal{J}_4(E)}{W(E)} & 0 \end{pmatrix}, \quad \Re(E)>0\,,\; \Im(E)<0\,. \qquad (5.2.68)$$

From Eqs. (5.2.67) and (5.2.68) we can see that the measures ρ_{12}, ρ_{21} and ρ_{22} in Theorem 4 of Appendix 4.4.3 are zero and that the measure ρ_{11} is given by

$$\begin{aligned} \rho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}\left[\theta_{11}^{+}(E-i\epsilon)-\theta_{11}^{+}(E+i\epsilon)\right]dE \\ &= \int_{E_1}^{E_2}\frac{1}{\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,dE\,, \end{aligned} \qquad (5.2.69)$$

which leads to

$$\rho^{-}(E) \equiv \rho_{11}(E) = \frac{1}{\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,, \quad E\in(0,\infty)\,. \qquad (5.2.70)$$

In order to δ-normalize, we define

$$\sigma^{-}(r;E) := \sqrt{\rho^{-}(E)}\,\chi^{-}(r;E)\,, \qquad (5.2.71)$$

which is the eigensolution of the Lippmann-Schwinger equation (5.2.8) that is δ-normalized, and

$$\widehat{f}(E) := \sqrt{\rho^-(E)}\widetilde{f}(E)\,, \quad \widetilde{f}(E) \in L^2((0,\infty),\rho(E)dE)\,. \tag{5.2.72}$$

The unitary operator that δ-diagonalizes the Hamiltonian is,

$$\widehat{f}(E) = (U_- f)(E) = \int_0^\infty dr f(r)\overline{\sigma^-(r;E)}\,, \quad f(r) \in L^2([0,\infty),dr)\,. \tag{5.2.73}$$

The inverse operator of U_- is given by (see Theorem 3 of Appendix 4.4.3)

$$f(r) = (U_-^{-1}\widehat{f})(r) = \int_0^\infty dE\,\widehat{f}(E)\sigma^-(r,E)\,, \quad \widehat{f}(E) \in L^2((0,\infty),dE)\,. \tag{5.2.74}$$

Therefore, we have constructed a unitary operator

$$\begin{aligned} U_- : \mathcal{D}(H) \subset L^2([0,\infty),dr) &\longmapsto \mathcal{D}(\widehat{E}) \subset L^2((0,\infty),dE) \\ f &\longmapsto \widehat{f} = U_- f \end{aligned} \tag{5.2.75}$$

that transforms from the position representation into the energy representation. The operator U_- diagonalizes H. The operator U_-^{-1} transforms from the energy representation into the position representation.

The expressions (5.2.73) and (5.2.74) provide the eigenfunction expansion of any wave function in terms of the δ-normalized eigensolutions $\sigma^-(r;E)$ and the direct integral decomposition of $\mathcal{H}$ associated to the observables.

5.3 Construction of the Lippmann-Schwinger Kets and Dirac Basis Vector Expansion

In this section, we sketch the construction of the spaces $\mathbf{\Phi}_\pm$ on which the Lippmann-Schwinger kets act as antilinear functionals.

In order to associate a ket $|E^+\rangle$ to the eigenfunction $\langle r|E^+\rangle$, we define

$$\begin{aligned} |E^+\rangle : \mathbf{\Phi}_- &\longmapsto \mathbb{C} \\ \varphi^+ &\longmapsto \langle\varphi^+|E^+\rangle := \lim_{\epsilon\to 0}\int_0^\infty dr\,\langle\varphi^+|r\rangle\langle r|(E+i\epsilon)^+\rangle\,. \end{aligned} \tag{5.3.1}$$

As mentioned above, the action of the Lippmann-Schwinger ket $|E^+\rangle$ should be viewed as the limit of the action of some ket $|(E+i\epsilon)^+\rangle$ when ϵ tends to zero. This is why we define the action of $|E^+\rangle$ on φ^+ as the limit of the integral in Eq. (5.3.1), and not just as

$$\int_0^\infty dr\,\langle\varphi^+|r\rangle\langle r|E^+\rangle\,. \tag{5.3.2}$$

The functions $\varphi^+ \in \mathbf{\Phi}_-$ on which the action of the in-ket of Eq. (5.3.1) is well defined satisfy (at least) the following conditions:

i.) They belong to the maximal invariant subspace of H.
ii.) They are such that the limit in Eq. (5.3.1) makes sense.
iii.) They satisfy (5.2.17a) for every $n = 0, 1, 2, \ldots$

By means of the unitary operator U_+, which was constructed in Section 5.2.4, we can obtain the energy representation of the space $\mathbf{\Phi}_-$,

$$U_+\mathbf{\Phi}_- = \widehat{\mathbf{\Phi}}_-|_{\mathbb{R}^+} \,. \tag{5.3.3}$$

We have denoted the energy representation of the space $\mathbf{\Phi}_-$ by $\widehat{\mathbf{\Phi}}_-|_{\mathbb{R}^+}$ (rather than by $\widehat{\mathbf{\Phi}}_-$), because its elements are boundary values on the positive real line of functions that have meaning for complex energies. As we said above, those functions $\widehat{\varphi}^+(E)$ seem to be realized by analytic functions from below. For the sake of definiteness, we shall assume that

$$\widehat{\mathbf{\Phi}}_-|_{\mathbb{R}^+} = \mathcal{S} \cap \mathcal{H}^2_-|_{\mathbb{R}^+} \,, \tag{5.3.4}$$

where $\mathcal{S}$ is the Schwartz space and $\mathcal{H}^2_-$ is the space of Hardy functions from below (cf. Appendix 5.5.2).

Under the assumptions made on the elements of the space $\mathbf{\Phi}_-$, one can prove that $|E^+\rangle$ is a well defined antilinear functional and that $|E^+\rangle$ is a generalized eigenvector of the Hamiltonian H (the proof is almost identical to the proof of Proposition 3 of Appendix 4.4.4),

$$H^\times|E^+\rangle = E|E^+\rangle \,, \tag{5.3.5}$$

i.e.,

$$\langle\varphi^+|H^\times|E^+\rangle = \langle H\varphi^+|E^+\rangle = E\langle\varphi^+|E^+\rangle \,, \quad \forall\varphi^+ \in \mathbf{\Phi}_- \,. \tag{5.3.6}$$

The in-ket $|E^+\rangle$ can be used to expand the in-states $\varphi^+ \in \mathbf{\Phi}_-$ in a Dirac basis vector expansion. This expansion is the restriction of the eigenfunction expansions (5.2.51) and (5.2.55) to the space $\mathbf{\Phi}_-$,

$$\langle{}^+E|\varphi^+\rangle = \int_0^\infty dr\, \langle{}^+E|r\rangle\langle r|\varphi^+\rangle \,, \quad \varphi^+ \in \mathbf{\Phi}_- \,, \tag{5.3.7a}$$

$$\langle r|\varphi^+\rangle = \int_0^\infty dE\, \langle r|E^+\rangle\langle{}^+E|\varphi^+\rangle \,, \quad \varphi^+ \in \mathbf{\Phi}_- \,. \tag{5.3.7b}$$

Similarly, the out-ket $|E^-\rangle$ associated to the eigenfunction $\langle r|E^-\rangle$ is defined by

$$\begin{aligned} |E^-\rangle : \mathbf{\Phi}_+ &\longmapsto \mathbb{C} \\ \psi^- &\longmapsto \langle\psi^-|E^-\rangle := \lim_{\epsilon\to 0}\int_0^\infty dr\, \langle\psi^-|r\rangle\langle r|(E-i\epsilon)^-\rangle \,. \end{aligned} \tag{5.3.8}$$

The functions $\psi^- \in \mathbf{\Phi}_+$ satisfy (at least) the following conditions:

i.) They belong to the maximal invariant subspace of H.

ii.) They are such that the limit in Eq. (5.3.8) makes sense.
iii.) They satisfy (5.2.17b) for every $n = 0, 1, 2, \ldots$

By means of the unitary operator U_-, which was constructed in Section 5.2.5, we can obtain the energy representation of the space $\mathbf{\Phi}_+$,

$$U_- \mathbf{\Phi}_+ = \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+} \,. \tag{5.3.9}$$

For the sake of definiteness, we shall assume that

$$\widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+} = \mathcal{S} \cap \mathcal{H}^2_+|_{\mathbb{R}^+} \,, \tag{5.3.10}$$

where $\mathcal{H}^2_+$ is the space of Hardy functions from above (cf. Appendix 5.5.2).

The out-ket is also a generalized eigenvector of H,

$$\langle \psi^- | H^\times | E^- \rangle = \langle H\psi^- | E^- \rangle = E \langle \psi^- | E^- \rangle \,, \quad \forall \psi^- \in \mathbf{\Phi}_+ \,. \tag{5.3.11}$$

The Dirac basis vector expansion induced by the out-ket reads

$$\langle {}^-E | \psi^- \rangle = \int_0^\infty dr \, \langle {}^-E | r \rangle \langle r | \psi^- \rangle \,, \quad \psi^- \in \mathbf{\Phi}_+ \,, \tag{5.3.12a}$$

$$\langle r | \psi^- \rangle = \int_0^\infty dE \, \langle r | E^- \rangle \langle {}^-E | \psi^- \rangle \,, \quad \psi^- \in \mathbf{\Phi}_+ \,. \tag{5.3.12b}$$

The Møller operators $\Omega_\pm$ can be expressed in terms of the operators $U_\pm$ (cf. Sections 5.2.4 and 5.2.5) and U_0 (cf. Appendix 5.5.1) as (cf. [75])

$$\Omega_\pm = U_\pm^\dagger U_0 \,. \tag{5.3.13}$$

Obviously, $\Omega_\pm$ are unitary operators in the Hilbert space $L^2([0,\infty), dr)$. The Møller operators can be used to construct the space $\mathbf{\Phi}_{in}$ of asymptotic in-states φ^{in} and the space $\mathbf{\Phi}_{out}$ of asymptotic out-observables ψ^{out},

$$\mathbf{\Phi}_{\substack{in \\ out}} = \Omega_\pm^\dagger \mathbf{\Phi}_\mp \,. \tag{5.3.14}$$

A vector φ^{in} belongs to $\mathbf{\Phi}_{in}$ if

$$\langle {}^+E | \varphi^+ \rangle = \langle E | \varphi^{in} \rangle \,, \tag{5.3.15}$$

where $\varphi^+ = \Omega_+ \varphi^{in}$. A vector ψ^{out} belongs to $\mathbf{\Phi}_{out}$ if

$$\langle {}^-E | \psi^- \rangle = \langle E | \psi^{out} \rangle \,, \tag{5.3.16}$$

where $\psi^- = \Omega_- \psi^{out}$. From the last two equations it follows that

$$\Omega_\pm^\times | E \rangle = | E^\pm \rangle \,. \tag{5.3.17}$$

The following diagram summarizes the results concerning the states:

$$\begin{array}{llllllll}
H_0; & \varphi^{in}(r) & \mathbf{\Phi}_{in} & \subset & L^2([0,\infty),dr) & \subset & \mathbf{\Phi}_{in}^{\times} & |E\rangle & \text{position repr.} \\
 & & \downarrow \Omega_+ & & \downarrow \Omega_+ & & \downarrow \Omega_+^{\times} & & \\
H; & \varphi^{+}(r) & \mathbf{\Phi}_{-} & \subset & L^2([0,\infty),dr) & \subset & \mathbf{\Phi}_{-}^{\times} & |E^+\rangle & \text{position repr.} \\
 & & \downarrow U_+ & & \downarrow U_+ & & \downarrow U_+^{\times} & & \\
\widehat{E}; & \widehat{\varphi}^{+}(E) & \widehat{\mathbf{\Phi}}_{-}|_{\mathbb{R}^+} & \subset & L^2([0,\infty),dE) & \subset & (\widehat{\mathbf{\Phi}}_{-}|_{\mathbb{R}^+})^{\times} & |\widehat{E}^+\rangle & \text{energy repr.}
\end{array} \tag{5.3.18}$$

The results concerning the observables are summarized by the following diagram:

$$\begin{array}{llllllll}
H_0; & \psi^{out}(r) & \mathbf{\Phi}_{out} & \subset & L^2([0,\infty),dr) & \subset & \mathbf{\Phi}_{out}^{\times} & |E\rangle & \text{position repr.} \\
 & & \downarrow \Omega_- & & \downarrow \Omega_- & & \downarrow \Omega_-^{\times} & & \\
H; & \psi^{-}(r) & \mathbf{\Phi}_{+} & \subset & L^2([0,\infty),dr) & \subset & \mathbf{\Phi}_{+}^{\times} & |E^-\rangle & \text{position repr.} \\
 & & \downarrow U_- & & \downarrow U_- & & \downarrow U_-^{\times} & & \\
\widehat{E}; & \widehat{\psi}^{-}(E) & \widehat{\mathbf{\Phi}}_{+}|_{\mathbb{R}^+} & \subset & L^2([0,\infty),dE) & \subset & (\widehat{\mathbf{\Phi}}_{+}|_{\mathbb{R}^+})^{\times} & |\widehat{E}^-\rangle & \text{energy repr.}
\end{array} \tag{5.3.19}$$

5.4 S-matrix and Møller Operators

Our next goal is to construct the S-matrix and to compute the expression of the S-matrix element in terms of the Lippmann-Schwinger kets (see Eq. (5.4.11) below).

As we said in Section 5.1, the S-matrix element

$$(\psi^{out}, \varphi^{out}) = (\psi^{out}, S\varphi^{in}) = (\psi^{-}, \varphi^{+}) \tag{5.4.1}$$

is to represent the probability to detect the property described by ψ^{out} (or, equivalently, by ψ^-) in the prepared ingoing beam characterized by φ^{in} (or, equivalently, by φ^+). The expression of the S-matrix operator in terms of the Møller operators read

$$S = \Omega_-^{\dagger}\Omega_+ \,. \tag{5.4.2}$$

The operator S is a unitary operator in the Hilbert space $L^2([0,\infty),dr)$. In the energy representation, the operator (5.4.2) acts as the operator multiplication by the function $S(E) = \mathcal{J}_-(E)/\mathcal{J}_+(E)$. To be more precise, if we define the operator $\widehat{S}$ as

$$\begin{aligned}
\widehat{S} : L^2([0,\infty),dE) &\longmapsto L^2([0,\infty),dE) \\
\widehat{f} &\longmapsto (\widehat{S}\widehat{f})(E) = S(E)\,\widehat{f}(E)\,,
\end{aligned} \tag{5.4.3}$$

then it can proved that

$$\widehat{S} = U_0 S U_0^{-1} \,. \tag{5.4.4}$$

In order to prove Eq. (5.4.4), we first prove that

$$(U_-g)(E) = S(E)(U_+g)(E)\,, \quad \forall g \in L^2([0,\infty), dr)\,. \tag{5.4.5}$$

Since

$$\sigma^+(r;E) = S(E)\sigma^-(r;E)\,, \tag{5.4.6}$$

and since

$$\overline{S(E)} = \frac{1}{S(E)}\,, \quad E > 0\,, \tag{5.4.7}$$

we conclude that

$$\sigma^-(r;E) = \overline{S(E)}\sigma^+(r;E)\,. \tag{5.4.8}$$

By substituting Eq. (5.4.8) into the integral expression (5.2.73) of the operator U_- we get to

$$(U_-g)(E) = \int_0^\infty dr\, g(r)S(E)\overline{\sigma^+(r;E)}\,. \tag{5.4.9}$$

Comparison of (5.4.9) to the integral expression (5.2.51) of U_+ leads to (5.4.5).

Now,

$$\begin{aligned}(U_0SU_0^{-1})\widehat{f} &= (U_0\Omega_-^\dagger\Omega_+U_0^{-1})\widehat{f}\\ &= (U_0U_0^{-1}U_-U_+^\dagger U_0U_0^{-1})\widehat{f}\\ &= (U_-U_+^\dagger)\widehat{f}\\ &= \widehat{S}\widehat{f}\,,\end{aligned} \tag{5.4.10}$$

where we have applied Eq. (5.4.5) to $g = U_+^\dagger\widehat{f}$ in the next to the last step.

As we said in Section 5.1, the S-matrix element can be written in terms of the Lippmann-Schwinger eigenkets as

$$(\psi^-, \varphi^+) = \int_0^\infty dE\, \langle\psi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle\,. \tag{5.4.11}$$

The proof of Eq. (5.4.11) is as follows: Let $\psi^- \in \mathbf{\Phi}_+$ and $\varphi^+ \in \mathbf{\Phi}_-$. Since ψ^- and φ^+ belong, in particular, to the Hilbert space $L^2([0,\infty), dr)$, we can let the unitary operator U_- act on both of them,

$$(\psi^-, \varphi^+) = (U_-\psi^-, U_-\varphi^+)\,. \tag{5.4.12}$$

The vectors $U_-\psi^-$ and $U_-\varphi^+$ belong to $L^2([0,\infty), dE)$. Therefore,

$$(U_-\psi^-, U_-\varphi^+) = \int_0^\infty dE\, \overline{(U_-\psi^-)(E)}(U_-\varphi^+)(E)\,. \tag{5.4.13}$$

From Eq. (5.4.5) it follows that

$$(U_-\varphi^+)(E) = S(E)(U_+\varphi^+)(E)\,. \tag{5.4.14}$$

Thus,

$$(U_-\psi^-, U_-\varphi^+) = \int_0^\infty dE\, \overline{(U_-\psi^-)(E)} S(E)(U_+\varphi^+)(E)\,. \tag{5.4.15}$$

Since $\psi^- \in \mathbf{\Phi}_+$, we are allowed to write

$$\overline{(U_-\psi^-)(E)} = \langle \psi^- | E^- \rangle\,. \tag{5.4.16}$$

Since $\varphi^+ \in \mathbf{\Phi}_-$, we are allowed to write

$$(U_+\varphi^+)(E) = \langle {}^+E | \varphi^+ \rangle\,. \tag{5.4.17}$$

Substitution of (5.4.16) and (5.4.17) into (5.4.15) leads to (5.4.11).

A similar argument to that used to prove Eq. (5.4.11) can be used to prove that

$$(\psi^{out}, S\varphi^{in}) = \int_0^\infty dE\, \langle \psi^{out} | E \rangle S(E) \langle E | \varphi^{in} \rangle\,. \tag{5.4.18}$$

Many formal identities follow from Eqs. (5.4.11) and (5.4.18). For instance,

$$\langle E | S | E' \rangle = \langle {}^-E | E'^+ \rangle = S(E)\delta(E - E')\,, \tag{5.4.19}$$

$$\int_0^\infty dr\, \langle E | r \rangle \langle r | E' \rangle = \int_0^\infty dr\, \langle {}^\pm E | r \rangle \langle r | E'^\pm \rangle = \delta(E - E')\,, \tag{5.4.20}$$

and

$$\int_0^\infty dr\, \langle {}^-E | r \rangle \langle r | E'^+ \rangle = S(E)\delta(E - E')\,. \tag{5.4.21}$$

The "proof" of these identities follows the pattern of Section 4.2.9.

5.5 Appendices to Chapter 5

5.5.1 Appendix 7: Free Hamiltonian

In this appendix, we compute the RHS associated to the free Hamiltonian. We will follow the method used in Chapter 4 for the total Hamiltonian.

Self-Adjoint Extension

The first step is to define a linear operator on a Hilbert space corresponding to the formal differential operator

$$h_0 \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\,. \tag{5.5.1}$$

The Hilbert space that is in the RHS of the free Hamiltonian is realized by the space $L^2([0,\infty), dr)$ of square integrable functions $f(r)$ defined on the interval $[0,\infty)$. The same

procedure that was used to find the domain of the total Hamiltonian can be applied to the free Hamiltonian,

$$\mathcal{D}(H_0) = \{f(r) \mid f(r), h_0 f(r) \in L^2([0,\infty), dr),\ f(r) \in AC^2[0,\infty),\ f(0) = 0\}\,. \tag{5.5.2}$$

On $\mathcal{D}(H_0)$ the formal differential operator h_0 is self-adjoint. In choosing (5.5.2) as the domain of our formal differential operator h_0, we define a linear operator H_0 by

$$H_0 f(r) := h_0 f(r) = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} f(r)\,, \quad f(r) \in \mathcal{D}(H_0)\,. \tag{5.5.3}$$

Resolvent and Green Functions

The expression of the free Green function $G^0(r,s;E)$ is be given in terms of eigenfunctions of the differential operator h_0 subject to certain boundary conditions (cf. Theorem 1 in Section 4.4.2).

Region $\Re(E) < 0$, $\Im(E) \neq 0$

For $\Re(E) < 0$, $\Im(E) \neq 0$, the free Green function (see Theorem 1 in Section 4.4.2) is given by

$$G^0(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\,\frac{\widetilde{\chi}^0(r;E)\,\widetilde{\Theta}^0(s;E)}{2} & r < s \\ -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\,\frac{\widetilde{\chi}^0(s;E)\,\widetilde{\Theta}^0(r;E)}{2} & r > s \end{cases} \qquad \Re(E) < 0\,,\ \Im(E) \neq 0\,. \tag{5.5.4}$$

The eigenfunction $\widetilde{\chi}^0(r;E)$ satisfies the equation

$$h_0 \widetilde{\chi}^0(r;E) = E\widetilde{\chi}^0(r;E) \tag{5.5.5}$$

and the boundary conditions (4.2.21),

$$\widetilde{\chi}^0(r;E) = e^{\sqrt{-\frac{2m}{\hbar^2}E}\,r} - e^{-\sqrt{-\frac{2m}{\hbar^2}E}\,r}\,, \quad 0 < r < \infty\,. \tag{5.5.6}$$

The eigenfunction $\widetilde{\Theta}^0(r;E)$ satisfies the equation (5.5.5) and the boundary conditions (4.2.24),

$$\widetilde{\Theta}^0(r;E) = e^{-\sqrt{-\frac{2m}{\hbar^2}E}\,r}\,, \quad 0 < r < \infty\,. \tag{5.5.7}$$

Region $\Re(E) > 0$, $\Im(E) > 0$

When $\Re(E) > 0$, $\Im(E) > 0$, the expression of the free Green function is

$$G^0(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\,\chi^0(r;E)\,\Theta^0_+(s;E) & r < s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\,\chi^0(s;E)\,\Theta^0_+(r;E) & r > s \end{cases} \qquad \Re(E) > 0,\ \Im(E) > 0\,. \tag{5.5.8}$$

The eigenfunction $\chi^0(r;E)$ satisfies the Schrödinger equation (5.5.5) and the boundary conditions (4.2.21),

$$\chi^0(r;E) = \sin(\sqrt{\frac{2m}{\hbar^2}E}r)\,, \quad 0 < r < \infty\,. \tag{5.5.9}$$

The eigenfunction $\Theta^0_+(r;E)$ satisfies the equation (5.5.5) subject to the boundary conditions (4.2.24),

$$\Theta^0_+(r;E) = e^{i\sqrt{\frac{2m}{\hbar^2}E}r}\,, \quad 0 < r < \infty\,. \tag{5.5.10}$$

Region $\Re(E) > 0$, $\Im(E) < 0$

In the region $\Re(E) > 0$, $\Im(E) < 0$, the free Green function reads

$$G^0(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\chi^0(r;E)\,\Theta^0_-(s;E) & r < s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\chi^0(s;E)\,\Theta^0_-(r;E) & r > s \end{cases} \qquad \Re(E) > 0,\ \Im(E) < 0\,. \tag{5.5.11}$$

The eigenfunction $\chi^0(r;E)$ is given by (5.5.9). The eigenfunction $\Theta^0_-(r;E)$ satisfies the equation (5.5.5) and the boundary conditions (4.2.24),

$$\Theta^0_-(r;E) = e^{-i\sqrt{\frac{2m}{\hbar^2}E}r}\,, \quad 0 < r < \infty\,. \tag{5.5.12}$$

Spectrum of H_0

We compute the spectrum $\mathrm{Sp}(H_0)$ of the operator H_0 by applying the method used in Section 4.2.4 to compute the spectrum of H.

Subset $\Lambda = (-\infty, 0)$

We first take Λ from Theorem 4 of Section 4.4.3 to be $(-\infty, 0)$. We choose a basis for the space of solutions of the equation $h_0\sigma = E\sigma$ as

$$\widetilde{\sigma}_1(r;E) = e^{\sqrt{-\frac{2m}{\hbar^2}E}r}\,, \tag{5.5.13a}$$

$$\widetilde{\sigma}_2(r;E) = \widetilde{\Theta}^0(r;E)\,. \tag{5.5.13b}$$

Obviously,

$$\widetilde{\chi}^0(r;E) = \widetilde{\sigma}_1(r;E) - \widetilde{\sigma}_2(r;E)\,, \tag{5.5.14}$$

which along with Eq. (5.5.4) leads to

$$G^0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{1}{2}\,[\widetilde{\sigma}_1(r;E) - \widetilde{\sigma}_2(r;E)]\,\widetilde{\sigma}_2(s;E)\,,\ r < s\,,\ \Re(E) < 0\,, \Im(E) \neq 0\,. \tag{5.5.15}$$

Since

$$\overline{\widetilde{\sigma}_2(s;\overline{E})} = \widetilde{\sigma}_2(s;E)\,, \tag{5.5.16}$$

we can write Eq. (5.5.15) as

$$G^0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{1}{2}\,\left[\widetilde{\sigma}_1(r;E)\overline{\widetilde{\sigma}_2(s;\overline{E})} - \widetilde{\sigma}_2(r;E)\overline{\widetilde{\sigma}_2(s;\overline{E})}\right],$$
$$r<s\,,\ \Re(E)<0\,,\Im(E)\neq 0\,. \tag{5.5.17}$$

On the other hand, by Theorem 4 in Section 4.4.3 we have

$$G^0(r,s;E) = \sum_{i,j=1}^{2}\theta^-_{ij}(E)\widetilde{\sigma}_i(r;E)\overline{\widetilde{\sigma}_j(s;\overline{E})} \qquad r<s\,. \tag{5.5.18}$$

By comparing Eqs. (5.5.17) and (5.5.18) we see that

$$\theta^-_{ij}(E) = \begin{pmatrix} 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2} \\ 0 & \frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2} \end{pmatrix}, \quad \Re(E)<0\,,\ \Im(E)\neq 0\,. \tag{5.5.19}$$

The functions $\theta^-_{ij}(E)$ are analytic in a neighborhood of $\Lambda=(-\infty,0)$. Therefore, the interval $(-\infty,0)$ is in the resolvent set $\mathrm{Re}(H_0)$ of the operator H_0.

Subset $\Lambda=(0,\infty)$

In this case, we choose the following basis for the space of solutions of $h_0\sigma = E\sigma$:

$$\sigma_1(r;E) = \chi^0(r;E)\,, \tag{5.5.20a}$$

$$\sigma_2(r;E) = \cos(\sqrt{\frac{2m}{\hbar^2}E}r)\,. \tag{5.5.20b}$$

Eqs. (5.5.10), (5.5.12) and (5.5.20) lead to

$$\Theta^0_+(r;E) = i\sigma_1(r;E) + \sigma_2(r;E) \tag{5.5.21}$$

and to

$$\Theta^0_-(r;E) = -i\sigma_1(r;E) + \sigma_2(r;E)\,. \tag{5.5.22}$$

By substituting Eq. (5.5.21) into Eq. (5.5.8) we get to

$$G^0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\sigma_1(s;E)\left[i\sigma_1(r;E)+\sigma_2(r;E)\right]\,,\ r>s\,,\ \Re(E)>0,\Im(E)>0\,. \tag{5.5.23}$$

By substituting Eq. (5.5.22) into Eq. (5.5.11) we get to

$$G^0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\sigma_1(s;E)\left[-i\sigma_1(r;E)+\sigma_2(r;E)\right]\,, r>s\,,\ \Re(E)>0, \Im(E)<0\,. \tag{5.5.24}$$

Since

$$\overline{\sigma_1(s;\overline{E})} = \sigma_1(s;E)\,, \tag{5.5.25}$$

Eq. (5.5.23) leads to

$$G^0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\left[i\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})}+\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]\,,$$
$$\Re(E)>0, \Im(E)>0\,,\ r>s\,, \tag{5.5.26}$$

and Eq. (5.5.24) leads to

$$G^0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\left[-i\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})}+\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)<0\,,\ r>s\,. \tag{5.5.27}$$

The expression of the resolvent in terms of the basis σ_1, σ_2 can be written as (see Theorem 4 in Section 4.4.3)

$$G^0(r,s;E) = \sum_{i,j=1}^{2}\theta^+_{ij}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, \qquad r>s\,. \tag{5.5.28}$$

By comparing (5.5.28) to (5.5.26) we get to

$$\theta^+_{ij}(E) = \begin{pmatrix} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}i & -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}} \\ 0 & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\ \Im(E)>0\,. \tag{5.5.29}$$

By comparing (5.5.28) to (5.5.27) we get to

$$\theta^+_{ij}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}i & -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}} \\ 0 & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\ \Im(E)<0\,. \tag{5.5.30}$$

From Eqs. (5.5.29) and (5.5.30) we can see that the measures ρ_{12}, ρ_{21} and ρ_{22} in Theorem 4 of Section 4.4.3 are zero and that the measure ρ_{11} is given by

$$\begin{aligned}\rho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}\left[\theta^+_{11}(E-i\epsilon)-\theta^+_{11}(E+i\epsilon)\right]dE \\ &= \int_{E_1}^{E_2}\frac{1}{\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,dE\,,\end{aligned} \tag{5.5.31}$$

which leads to

$$\rho^0(E) \equiv \rho_{11}(E) = \frac{1}{\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,, \quad E\in(0,\infty)\,. \tag{5.5.32}$$

The function $\theta^+_{11}(E)$ has a branch cut along $(0,\infty)$, and therefore $(0,\infty)$ is included in $\mathrm{Sp}(H_0)$. Since $\mathrm{Sp}(H_0)$ is a closed set, $\mathrm{Sp}(H_0)=[0,\infty)$.

Diagonalization and Eigenfunction Expansion

In the present section, we diagonalize our Hamiltonian H_0 and construct the expansion of the wave functions in terms of the eigenfunctions of the differential operator h_0.

By Theorem 2 of Section 4.4.3, there is a unitary map $\widetilde{U}_0$ defined by

$$\begin{aligned} \widetilde{U}_0 : L^2([0,\infty), dr) &\longmapsto L^2((0,\infty), \rho^0(E)dE) \\ f(r) &\longmapsto \widetilde{f}(E) = \widetilde{U}_0 f(E) = \int_0^\infty dr f(r)\overline{\chi^0(r;E)}\,, \end{aligned} \tag{5.5.33}$$

that brings $\mathcal{D}(H_0)$ onto the space

$$\mathcal{D}(\widetilde{E}) = \{\widetilde{f}(E) \in L^2((0,\infty), \rho^0(E)dE) \mid \int_0^\infty dE\, E^2 |\widetilde{f}(E)|^2 \rho^0(E) < \infty\}\,. \tag{5.5.34}$$

In order to δ-normalize, we define

$$\sigma^0(r;E) := \sqrt{\rho^0(E)}\,\chi^0(r;E)\,, \tag{5.5.35}$$

which is the eigensolution of the differential operator h_0 that is δ-normalized, and

$$\widehat{f}(E) := \sqrt{\rho^0(E)}\widetilde{f}(E)\,, \quad \widetilde{f}(E) \in L^2((0,\infty), \rho^0(E)dE)\,, \tag{5.5.36}$$

and construct the unitary operator

$$\begin{aligned} \widehat{U}_0 : L^2((0,\infty)), \rho^0(E)dE) &\longmapsto L^2((0,\infty), dE) \\ \widetilde{f} &\longmapsto \widehat{f}(E) = \widehat{U}_0 \widetilde{f}(E) := \sqrt{\rho^0(E)}\widetilde{f}(E)\,. \end{aligned} \tag{5.5.37}$$

The operator that δ-diagonalizes our Hamiltonian is $U_0 := \widehat{U}_0\widetilde{U}_0$,

$$\begin{aligned} U_0 : L^2([0,\infty)), dr) &\longmapsto L^2((0,\infty), dE) \\ f &\longmapsto U_0 f := \widehat{f}\,. \end{aligned} \tag{5.5.38}$$

The action of U_0 can be written as an integral operator,

$$\widehat{f}(E) = U_0 f(E) = \int_0^\infty dr f(r)\overline{\sigma^0(r;E)}\,, \quad f(r) \in L^2([0,\infty), dr)\,. \tag{5.5.39}$$

The image of $\mathcal{D}(H_0)$ under the action of U_0 is

$$\mathcal{D}(\widehat{E}) := U\mathcal{D}(H_0) = \{\widehat{f}(E) \in L^2((0,\infty), dE) \mid \int_0^\infty E^2 |\widehat{f}(E)|^2 dE < \infty\}\,. \tag{5.5.40}$$

Therefore, we have constructed a unitary operator

$$\begin{aligned} U_0 : \mathcal{D}(H) \subset L^2([0,\infty), dr) &\longmapsto \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) \\ f &\longmapsto \widehat{f} = U_0 f \end{aligned} \tag{5.5.41}$$

that transforms from the position representation into the energy representation. The operator U_0 diagonalizes the free Hamiltonian in the sense that $\widehat{E} \equiv U_0 H_0 U_0^{-1}$ is the multiplication operator. The inverse operator of U_0 is given by (see Theorem 3 of Section 4.4.3)

$$f(r) = U_0^{-1}\widehat{f}(r) = \int_0^\infty dE\, \widehat{f}(E)\sigma^0(r,E)\,, \quad \widehat{f}(E) \in L^2((0,\infty), dE)\,. \tag{5.5.42}$$

The operator U_0^{-1} transforms from the energy representation into the position representation.

The expressions (5.5.39) and (5.5.42) provide the eigenfunction expansion of any square integrable function in terms of the eigensolutions $\sigma^0(r;E)$ of h_0. One can easily see that

$$\lim_{V_0 \to 0} U_\pm = U_0\,. \tag{5.5.43}$$

Construction of the RHS of the Free Hamiltonian

The Sturm-Liouville theory only provides a domain $\mathcal{D}(H_0)$ on which the Hamiltonian H_0 is self-adjoint and a unitary operator U_0 that diagonalizes H_0. This unitary operator induces a direct integral decomposition of the Hilbert space (see [4, 5]),

$$\begin{aligned} \mathcal{H} &\longmapsto U_0\mathcal{H} \equiv \widehat{\mathcal{H}} = \oplus \int_{\mathrm{Sp}(H_0)} \mathcal{H}(E)dE \\ f &\longmapsto U_0 f \equiv \{\widehat{f}(E)\}, \quad \widehat{f}(E) \in \mathcal{H}(E)\,. \end{aligned} \tag{5.5.44}$$

As we saw in Chapter 4, the direct integral decomposition does not provide us with a dense invariant domain $\mathbf{\Phi}_0$ on which all the powers of H_0 and all the expectation values of H_0 are well-defined, and on which the Dirac kets act as antilinear functionals. In order to construct $\mathbf{\Phi}_0$, we first construct the maximal invariant subspace $\mathcal{D}_0$ of H_0,

$$\mathcal{D}_0 := \bigcap_{n=0}^{\infty} \mathcal{D}(H_0^n)\,. \tag{5.5.45}$$

It is easy to check that

$$\begin{aligned} \mathcal{D}_0 = \{\varphi \in L^2([0,\infty), dr) \mid\ & h_0^n\varphi(r) \in L^2([0,\infty), dr),\ h_0^n\varphi(0) = 0, n = 0,1,2,\ldots, \\ & \varphi(r) \in C^\infty([0,\infty))\}\,. \end{aligned} \tag{5.5.46}$$

The second step is to find a subspace $\mathbf{\Phi}_0$ on which the eigenkets $|E\rangle$ of H_0 are well-defined as antilinear functionals. That subspace is given by

$$\mathbf{\Phi}_0 = \{\varphi \in \mathcal{D}_0 \mid \int_0^\infty dr\ |(r+1)^n(h_0+1)^m\varphi(r)|^2 < \infty, \quad n,m = 0,1,2,\ldots\}\,. \tag{5.5.47}$$

On $\mathbf{\Phi}_0$, we define the family of norms

$$\|\varphi\|_{n,m}^0 := \sqrt{\int_0^\infty dr\ |(r+1)^n(h_0+1)^m\varphi(r)|^2}\,, \quad n,m = 0,1,2,\ldots \tag{5.5.48}$$

The quantities (5.5.48) fulfill the conditions to be a norm (the proof is almost identical to the proof of Proposition 1 of Section 4.4.4) and can be used to define a countably normed topology $\tau_{\mathbf{\Phi}_0}$ on $\mathbf{\Phi}_0$ (see [5]),

$$\varphi_\alpha \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}_0}} \varphi \quad \text{iff} \quad \|\varphi_\alpha - \varphi\|^0_{n,m} \xrightarrow[\alpha\to\infty]{} 0\,, \quad n,m = 0,1,2,\ldots \tag{5.5.49}$$

One can see that the space $\mathbf{\Phi}_0$ is stable under the action of H_0 and that H_0 is $\tau_{\mathbf{\Phi}_0}$-continuous (the proof is almost identical to the proof of Proposition 2 of Section 4.4.4).

Once we have constructed the space $\mathbf{\Phi}_0$, we can construct its topological dual $\mathbf{\Phi}_0^\times$ as the space of $\tau_{\mathbf{\Phi}_0}$-continuous antilinear functionals on $\mathbf{\Phi}_0$ (see [5]) and therewith the RHS of the free Hamiltonian

$$\mathbf{\Phi}_0 \subset L^2([0,\infty), dr) \subset \mathbf{\Phi}_0^\times\,. \tag{5.5.50}$$

For each $E \in \mathrm{Sp}(H_0)$, we associate a ket $|E\rangle$ to the generalized eigenfunction $\sigma^0(r;E)$ through

$$\begin{aligned} |E\rangle : \mathbf{\Phi}_0 &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma^0(r;E)dr = \overline{(U_0\varphi)(E)}\,. \end{aligned} \tag{5.5.51}$$

The ket $|E\rangle$ in Eq. (5.5.51) is a well-defined antilinear functional on $\mathbf{\Phi}_0$, i.e., $|E\rangle$ belongs to $\mathbf{\Phi}_0^\times$ (the proof is almost identical to the proof of Proposition 3 of Section 4.4.4). The ket $|E\rangle$ is a generalized eigenvector of the free Hamiltonian H_0 (the proof is almost identical to the proof of Proposition 3 of Section 4.4.4),

$$H_0^\times|E\rangle = E|E\rangle\,, \tag{5.5.52}$$

i.e.,

$$\langle\varphi|H_0^\times|E\rangle = \langle H_0\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi \in \mathbf{\Phi}_0\,. \tag{5.5.53}$$

Dirac Basis Vector Expansion for H_0

We are now in a position to derive the Dirac basis vector expansion for the free Hamiltonian. This derivation consists of the restriction of the Weyl-Kodaira expansions (5.5.39) and (5.5.42) to the space $\mathbf{\Phi}_0$. If we denote $\langle r|\varphi\rangle \equiv \varphi(r)$ and $\langle E|r\rangle \equiv \overline{\sigma^0(r;E)}$, and if we define the action of the left ket $\langle E|$ on $\varphi \in \mathbf{\Phi}_0$ as $\langle E|\varphi\rangle := \widehat{\varphi}(E)$, then Eq. (5.5.39) becomes

$$\langle E|\varphi\rangle = \int_0^\infty dr\,\langle E|r\rangle\langle r|\varphi\rangle\,, \quad \varphi \in \mathbf{\Phi}_0\,. \tag{5.5.54}$$

If we denote $\langle r|E\rangle \equiv \sigma^0(r;E)$, then Eq. (5.5.42) becomes

$$\langle r|\varphi\rangle = \int_0^\infty dE\,\langle r|E\rangle\langle E|\varphi\rangle\,, \quad \varphi \in \mathbf{\Phi}_0\,. \tag{5.5.55}$$

This equation is the Dirac basis vector expansion of the wave function φ in terms of the free eigenkets $|E\rangle$. We can also prove the Nuclear Spectral Theorem for the free Hamiltonian (the proof is almost identical to the proof of Proposition 4 of Section 4.4.5),

$$(\varphi, H_0^n\psi) = \int_0^\infty dE\,E^n\langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi,\psi \in \mathbf{\Phi}_0\,, n = 1,2,\ldots \tag{5.5.56}$$

Energy Representation of the RHS of H_0

We have already shown that in the energy representation the Hamiltonian H_0 acts as the multiplication operator $\widehat{E}$. The energy representation of the space $\mathbf{\Phi}_0$ is defined as

$$\widehat{\mathbf{\Phi}}_0 := U_0 \mathbf{\Phi}_0 \,. \tag{5.5.57}$$

Obviously $\widehat{\mathbf{\Phi}}_0$ is a linear subspace of $L^2([0,\infty), dE)$. In oder to endow $\widehat{\mathbf{\Phi}}_0$ with a topology $\tau_{\widehat{\mathbf{\Phi}}_0}$, we carry the topology on $\mathbf{\Phi}_0$ into $\widehat{\mathbf{\Phi}}_0$,

$$\tau_{\widehat{\mathbf{\Phi}}_0} := U_0 \tau_{\mathbf{\Phi}_0} \,. \tag{5.5.58}$$

With this topology, the space $\widehat{\mathbf{\Phi}}_0$ is a linear topological space. If we denote the dual space of $\widehat{\mathbf{\Phi}}_0$ by $\widehat{\mathbf{\Phi}}_0^\times$, then we have

$$U_0^\times \mathbf{\Phi}_0^\times = (U_0 \mathbf{\Phi}_0)^\times = \widehat{\mathbf{\Phi}}_0^\times \,. \tag{5.5.59}$$

If we denote $|\widehat{E}\rangle \equiv U_0^\times |E\rangle$, then we can prove that $|\widehat{E}\rangle$ is the antilinear Schwartz delta functional, (the proof is almost identical to the proof of Proposition 5 of Section 4.4.6),

$$\begin{aligned} |\widehat{E}\rangle : \widehat{\mathbf{\Phi}} &\longmapsto \mathbb{C} \\ \widehat{\varphi} &\longmapsto \langle \widehat{\varphi} | \widehat{E} \rangle := \overline{\widehat{\varphi}(E)} \,. \end{aligned} \tag{5.5.60}$$

It is very helpful to show the different realizations of the RHS through the following diagram:

$$\begin{array}{llllllll} H_0; & \varphi(r) & \mathbf{\Phi}_0 & \subset & L^2([0,\infty), dr) & \subset & \mathbf{\Phi}_0^\times & |E\rangle & \text{position repr.} \\ & & \downarrow U_0 & & \downarrow U_0 & & \downarrow U_0^\times & & \\ \widehat{E}; & \widehat{\varphi}(E) & \widehat{\mathbf{\Phi}}_0 & \subset & L^2([0,\infty), dE) & \subset & \widehat{\mathbf{\Phi}}_0^\times & |\widehat{E}\rangle & \text{energy repr.} \end{array} \tag{5.5.61}$$

We should stress that the space $\mathbf{\Phi}_0$ is neither $\mathbf{\Phi}_{in}$ nor $\mathbf{\Phi}_{out}$—the boundary conditions satisfied by the elements of the spaces $\mathbf{\Phi}_{in,out}$ are different to the boundary conditions satisfied by the elements of $\mathbf{\Phi}_0$.

5.5.2 Appendix 8: Spaces of Hardy Functions

In this Appendix, we list the definition and main properties of functions of Hardy class and review the Bohm-Gadella construction of RHS of Hardy functions.

General Properties of Hardy Functions

A Hardy function $f(z)$ on the upper half of the complex plane $\mathbb{C}^+$ is a function satisfying the following conditions [76, 77, 78, 79]:

i.) It is an analytic function on the open upper half plane, i.e., on the set of complex numbers with positive imaginary part.

ii.) For any value of $y > 0$, the integral

$$\int_{-\infty}^{\infty} |f(x+iy)|^2 \, dx \tag{5.5.62}$$

converges.

iii.) For all $y > 0$, these integrals are bounded by the *same* constant K,

$$\sup_{y>0} \int_{-\infty}^{+\infty} |f(x+iy)|^2 \, dx < K \, . \tag{5.5.63}$$

The set of Hardy functions on the upper half plane, often referred to as Hardy functions from above, is a vector space that we denote by $\mathcal{H}^2_+$.

Similarly, Hardy functions on the lower half plane $\mathbb{C}^-$ are analytic on the open lower half plane, and for these functions the conditions (ii) and (iii) hold with $y < 0$. We denote the vector space of Hardy functions from below by $\mathcal{H}^2_-$.

Boundary values for Hardy functions are defined at almost all (with respect to the Lebesgue measure) points of the real axis. For any Hardy function, these boundary values yield a square integrable function $f(x)$, which is uniquely defined on the real line, save for a set of zero Lebesgue measure,

$$\lim_{y\to 0} f(x \pm iy) = f(x) \, , \quad f \in \mathcal{H}^2_\pm \, . \tag{5.5.64}$$

The square norm of $f(x)$ is also bounded by K. Thus, a function in $\mathcal{H}^2_\pm$ uniquely determines (almost everywhere) a square integrable function on $\mathbb{R}$.

An important theorem, due to Titchmarsh [80], states that Hardy functions can be recovered by their boundary values on the real line. If $f(x)$ is the function representing the boundary values of a Hardy function $f(z)$ on $\mathbb{C}^\pm$, then

$$f(z) = \pm \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{f(x)}{x-z} \, dx \, , \tag{5.5.65}$$

where the signs $(+)$ and $(-)$ correspond to Hardy functions on the upper and lower half plane, respectively.

Another important theorem on Hardy functions is that by Paley and Wiener [81, 76, 77, 78, 79], which determines whether a square integrable function is also a Hardy function. The theorem asserts that the Fourier transform $\mathcal{F}$ is bijection between $\mathcal{H}^2_-$, the space of Hardy functions from below, and $L^2(\mathbb{R}^+)$ the space of square integrable functions defined on the positive real axis. The conclusion holds also for $\mathcal{H}^2_+$ and $L^2(\mathbb{R}^-)$. That is,

$$\mathcal{F} L^2(\mathbb{R}^-) = \mathcal{H}^2_+ \, , \tag{5.5.66a}$$

$$\mathcal{F} L^2(\mathbb{R}^+) = \mathcal{H}^2_- \, . \tag{5.5.66b}$$

There is another version of the same result that can be summarized as follows:

$$\mathcal{F} \mathcal{H}^2_+ = L^2(\mathbb{R}^+) \, , \tag{5.5.67a}$$

$$\mathcal{F} \mathcal{H}^2_- = L^2(\mathbb{R}^-) \, . \tag{5.5.67b}$$

Since the Fourier transform is an isometry on $L^2(\mathbb{R})$, we conclude that $\mathcal{H}^2_+$ and $\mathcal{H}^2_-$ are closed subspaces of $L^2(\mathbb{R})$, and hence Hilbert spaces. Since $L^2(\mathbb{R}) = L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^-)$, where $\oplus$ stands for orthogonal direct sum, we have

$$L^2(\mathbb{R}) = \mathcal{H}^2_+ \oplus \mathcal{H}^2_- \,. \tag{5.5.68}$$

A theorem due to van Winter [53] establishes that a Hardy function can be recovered by its boundary values on the semi-axis $\mathbb{R}^+$. Whether the recovered function is an element of $\mathcal{H}^2_+$ or $\mathcal{H}^2_-$ is to be determined by means of the Mellin transform. Thus, if we call $\mathcal{H}^2_{++}$ the space of boundary values on $\mathbb{R}^+$ of the functions in $\mathcal{H}^2_+$ and $\mathcal{H}^2_{-+}$ the space of boundary values on $\mathbb{R}^+$ of the functions in $\mathcal{H}^2_-$, we have the following bijection:

$$\theta\mathcal{H}^2_+ = \mathcal{H}^2_{++} \,, \tag{5.5.69a}$$
$$\theta\mathcal{H}^2_- = \mathcal{H}^2_{-+} \,, \tag{5.5.69b}$$

where the image of any $f_\pm(x) \in \mathcal{H}^2_\pm$ by θ is a function which is equal to $f_\pm(x)$ for $x \in \mathbb{R}^+$ and is not defined for negative values of x.

The following are among the other interesting properties of Hardy functions [80]:

i.) Let us define the Hilbert transform for an $L^2(\mathbb{R})$ function f as

$$\mathfrak{H}f(x) = \frac{1}{\pi}\,\mathcal{P}\int_{-\infty}^{\infty} \frac{f(t)}{t-x}\,dt \,, \tag{5.5.70}$$

where $\mathcal{P}$ denotes the Cauchy principal value. The Hilbert transform is linear and its image also lies in $L^2(\mathbb{R})$. A square integrable complex function $f(x)$, with real part $u(x)$ and imaginary part $v(x)$, belongs to $\mathcal{H}^2_\pm$ if and only if

$$\mathfrak{H}u = \pm v \quad \text{and} \quad \mathfrak{H}v = \mp u \,. \tag{5.5.71}$$

In particular, a Hardy function cannot be either real or purely imaginary on the whole real line.

ii.) From i.), we immediately see that $f(x) \in \mathcal{H}^2_\pm$ if and only if its complex conjugate $f^*(x) \in \mathcal{H}^2_\mp$.

iii.) Hardy functions vanish at infinity. More precisely, they behave for large values of $|z|$ as $1/\sqrt{z}$ (cf. [79]).

iv.) Some Hardy functions on $\mathbb{C}^\pm$ admit analytic continuation beyond the real axis to $\mathbb{C}^\mp$. We may consider the functions $f(x) \in L^2(\mathbb{R}^\pm)$ such that there is a positive number α with the property that $e^{\alpha|x|}f(x) \in L^2(\mathbb{R}^\pm)$. Then, the Fourier transforms of these functions are Hardy functions on $\mathbb{C}^\mp$, and they admit an analytic continuation beyond the real axis to a strip of width α. This means that if $e^{\alpha|x|}f(x) \in L^2(\mathbb{R}^-)$, its Fourier transform is analytic on $\{z \in \mathbb{C}\ ;\ -\alpha < \operatorname{Im} z < \infty\}$ and if $e^{\alpha|x|}f(x) \in L^2(\mathbb{R}^+)$, its Fourier transform is analytic on $\{z \in \mathbb{C}\ ;\ -\infty < \operatorname{Im} z < \alpha\}$ (cf. [82]).

v.) A function which is simultaneously Hardy on both the upper and lower half planes would be obviously entire, and, as a consequence of above condition iii), is also bounded.

Hence, Liouville theorem asserts that such a function is constant. A constant function cannot be square integrable unless it is zero almost everywhere. However, there exist entire functions that are also Hardy either on the upper or the lower half plane.

vi.) It is now clear that the spaces $\mathcal{H}^2_+$ and $\mathcal{H}^2_-$ have a trivial intersection. However, the spaces of functions which are restrictions of Hardy functions to the positive semiaxis $\mathbb{R}^+$ have a nontrivial intersection. Moreover, the intersection $\mathcal{H}^2_{++} \cap \mathcal{H}^2_{-+}$ is dense in $L^2(\mathbb{R}^+)$ [83].

Rigged Hilbert Spaces of Hardy Functions

We now summarize the Bohm-Gadella construction to describe resonances. This construction is based on RHS of Hardy functions.

All functions fulfilling the following conditions yield two rigged Hilbert spaces [20]:

i.) They belong to the Schwartz space $\mathcal{S}$.

ii.) Their supports are in $\mathbb{R}^\pm$.

We call these spaces $\mathcal{S}^\pm$, respectively. Take their Fourier transforms. Since the Fourier transform of a Schwartz function is again a Schwartz function, the Fourier transforms of the functions in $\mathcal{S}^\pm$ have the following properties:

a.) They belong to the Schwartz space.

b.) They belong to $\mathcal{H}^2_\mp$.

c.) The space of all these Fourier transforms $\mathcal{F}\mathcal{S}^\pm$ coincide with the intersection of $\mathcal{S}$ and $\mathcal{H}^2_\mp$, i.e., $\mathcal{F}\mathcal{S}^\pm = \mathcal{S} \cap \mathcal{H}^2_\mp$.

d.) Since $\mathcal{S}^\pm$ is dense in $L^2(\mathbb{R}^\pm)$, $\mathcal{S} \cap \mathcal{H}^2_\mp$ is dense in $\mathcal{H}^2_\mp$ with respect to the Hilbert space topology inherited from $L^2(\mathbb{R})$.

e.) Note however that the direct sum of spaces $\mathcal{S} \cap \mathcal{H}^2_+ \oplus \mathcal{S} \cap \mathcal{H}^2_-$ does not coincide with $\mathcal{S}$, since the Fourier transform of any of its functions vanish at zero.

f.) Since $\mathcal{S} \cap \mathcal{H}^2_\pm$ are subspaces of $\mathcal{S}$, they inherit the topology of $\mathcal{S}$. They have good enough properties so that

$$\mathcal{S} \cap \mathcal{H}^2_\pm \subset \mathcal{H}^2_\pm \subset (\mathcal{S} \cap \mathcal{H}^2_\pm)^\times \tag{5.5.72}$$

are well defined rigged Hilbert spaces.

We mentioned earlier in this Appendix that Hardy functions are determined by their values on the positive semiaxis plus a specification which says if they are Hardy on the upper or the lower half planes. Thus, we have defined the spaces $\theta\mathcal{H}^2_+ = \mathcal{H}^2_{++}$ and $\theta\mathcal{H}^2_- = \mathcal{H}^2_{-+}$. Now consider:

$$\mathcal{S} \cap \mathcal{H}^2_+\big|_{\mathbb{R}^+} = \theta_+(\mathcal{S} \cap \mathcal{H}^2_+)\,, \tag{5.5.73a}$$

$$\mathcal{S} \cap \mathcal{H}^2_-\big|_{\mathbb{R}^+} = \theta_-(\mathcal{S} \cap \mathcal{H}^2_-)\,. \tag{5.5.73b}$$

The spaces $\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+}$ are dense in $L^2(\mathbb{R}^+)$. Since θ is a bijection, we can transport the topology from $\mathcal{S} \cap \mathcal{H}^2_\pm$ to $\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+}$ by means of θ. The transported topologies have the same properties as the original ones and they are finer than the Hilbert topology on $L^2(\mathbb{R}^+)$. In particular, $\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+}$ are metrizable topological vector spaces and

$$\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+} \subset L^2(\mathbb{R}^+) \subset (\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+})^\times \tag{5.5.74}$$

are RHS. The spaces $\mathcal{S} \cap \mathcal{H}^2_+\big|_{\mathbb{R}^+}$ and $\mathcal{S} \cap \mathcal{H}^2_-\big|_{\mathbb{R}^+}$ have a nontrivial intersection [84].

We can define the dual of the mapping θ using the following formula:

$$\langle \theta f_\pm(x) | \theta^\times F_\pm \rangle = \langle f_\pm(x) | F_\pm \rangle \,, \quad \forall f_\pm(x) \in \mathcal{S} \cap \mathcal{H}^2_\pm \,, \; \forall \, F_\pm \in (\mathcal{S} \cap \mathcal{H}^2_\pm)^\times \,. \tag{5.5.75}$$

The mapping $\theta^\times$ is a bijection. Moreover, the following property is fulfilled algebraically and topologically:

$$\theta^\times (\mathcal{S} \cap \mathcal{H}^2_\pm)^\times \equiv (\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+})^\times = (\theta(\mathcal{S} \cap \mathcal{H}^2_\pm))^\times \,, \tag{5.5.76}$$

i.e., the topology on $(\mathcal{S} \cap \mathcal{H}^2_\pm\big|_{\mathbb{R}^+})^\times$ is transported from $(\mathcal{S} \cap \mathcal{H}^2_\pm)^\times$ by $\theta^\times$.

It is important, however, that the mapping $\theta^\times$ does not extend θ. The cause lies in the non unitarity of the latter.

Chapter 6

The Gamow Vectors of the Square Barrier Potential Resonances

In this chapter, we study the resonances of the square barrier potential. We first compute the resonance energies as poles of the S-matrix. The integral equation of A. Mondragón *et al.* for the Gamow vectors will be translated into the RHS language. Next, we compute the Gamow eigenfunctions in the position representation as the solutions of the time independent Schrödinger equation subject to the purely outgoing boundary condition. The $[0, \infty)$-energy representation of the Gamow eigenfunction will be related to the complex delta function, and the $(-\infty, \infty)$-energy representation of the Gamow eigenfunction will be related to the Breit-Wigner amplitude. The semigroup time evolution of the Gamow vectors will also be computed. The Gamow vectors will be used as basis vectors. We shall see that the Gamow vectors do not form a complete basis—an additional set of kets needs to be added in order to obtain a complete basis. The time asymmetry of the purely outgoing boundary condition will be disclosed. To finish this chapter, we shall discuss the exponential decay law of the Gamow vectors.

It don't bring you

Well I know it ain't been roses lately
Baby it's just been thorns
And no matter what we do
Nothing seems to change
Love has always been my shelter
For you it's been a storm
But for awhile I thought
We'd almost beat the rain

Now there's a hole here in my pocket
Where all my dreams have gone
Falling out like so many nickels
        and dimes
And last of all you
You'd always been my good luck charm
I should've known that luck
Is a waste of time

Cause it don't bring you love if you don't love
And it don't bring you time if you ain't got time
And it don't bring you strength baby if you ain't strong
And it don't bring you kindness if you ain't kind

Now there's a whole lot in life to be unsure of
But there's one thing I can safely say I know
That of all the things that finally desert us
Pride is always the last thing to go

But it won't bring you love if you don't love
And it won't bring you time if you ain't got time
And it won't bring you strength baby if you ain't strong
And it won't bring you kindness if you ain't kind

And now I wish you only the roses without the thorns
And I hope your dreams are always within reach
And I wish you shelter baby from all your storms
They scared you but they never seemed to teach

That I can't bring you love if you don't love
And I can't bring you time if you ain't got time
And I can't bring you strength baby if you ain't strong
And I can't bring you kindness if you ain't kind
And I can't bring you kindness if you ain't kind

Mary Chapin Carpenter, *State of the Heart*

6.1 Introduction

Most elementary particles are only quasistable states decaying through various interactions and thus have finite lifetimes of various orders of magnitude [36]. Several theoretical schemes have been proposed to describe quasistable particles. The S-matrix and the Gamow vectors are two of the most widely used schemes.

Experimentally, resonances often appear as peaks in the cross section that resemble the well-known Breit-Wigner distribution [50]. The Breit-Wigner distribution has two characteristic parameters: the energy E_R at which the peak reaches its maximum, and its width Γ_R at half-maximum. The inverse of Γ_R is the lifetime of the decaying state [33]. The peak of the Breit-Wigner is related to a first-order pole of the S-matrix in the energy representation $S(E)$ at the complex number $z_R = E_R - i\Gamma_R/2$. The shape of the theoretical expression of the cross section in terms of $S(E)$ fits the shape of the experimental cross section in the neighborhood of E_R. This is why the first-order pole of the S-matrix is often taken as the theoretical definition of a resonance.

Although a resonance has a finite lifetime, it is otherwise assigned all the properties that are also attributed to stable particles, such as angular momentum, charge, spin, parity and other particle labels. For example, a radioactive nucleus has a finite lifetime, but otherwise it possesses all the properties of stable nuclei. In fact, radioactive nuclei are included in the periodic table of the elements together with the stable nuclei. Therefore, it seems natural to seek a theoretical description that provides "particle status" to the quasistable states. The Gamow vectors provide this particle status. The description of resonances by Gamow vectors allows us to interpret resonances as autonomous experimentally decaying physical systems. This description, impossible in the Hilbert space, can be accomplished within the Rigged Hilbert Space.

The original energy eigenfunction with complex eigenvalue $E_R - i\Gamma_R/2$ was introduced by Gamow [38]. The quantities E_R and Γ_R are interpreted as the resonance energy and the resonance width of the decaying state, respectively. However, Gamow's heuristic approach cannot be made rigorous in the Hilbert space framework, because self-adjoint operators on a Hilbert space can only have real eigenvalues. An extended framework is therefore needed. As we shall see, the Rigged Hilbert Space is the most natural framework to describe Gamow vectors.

In this chapter, Gamow eigenkets will be obtained as solutions of a homogeneous integral equation of the Lippmann-Schwinger type. In the radial position representation, this integral equation is equivalent to the time-independent Schrödinger equation subject to a purely outgoing boundary condition. The resonance spectrum is therefore singled out by the purely outgoing boundary condition. As we shall see, this is the same resonance spectrum as that defined by the poles of the S-matrix. The Gamow eigenfunctions will be associated to certain eigenfunctionals, that we call Gamow kets. These Gamow kets are generalized eigenvectors of the square barrier potential Hamiltonian with complex eigenvalue $E_R - i\Gamma_R/2$.

The energy representation of the Gamow vectors will be obtained. We shall see that in the $[0, \infty)$-energy representation (i.e., in the representation associated to the physical spectrum), the Gamow vector is represented by the complex delta function, whereas in the

$(-\infty, \infty)$-energy representation (i.e., in the representation associated to the support of the Breit-Wigner amplitude), the Gamow vector is represented by the Breit-Wigner amplitude. We shall also obtain the time evolution of the Gamow vectors, which is given by a semigroup.

Therefore, the Gamow vectors have all of the properties that are demanded from a resonance state:

1. They are eigenvectors of the Hamiltonian with complex eigenvalues.
2. They correspond to the Breit-Wigner amplitude in the energy representation.
3. Their time evolution is given by a semigroup, and obeys the exponential decay law.

The organization of this chapter is as follows. In Section 6.2, we compute the resonance energies as poles of the S-matrix. In Section 6.3, we introduce the integral equation that is satisfied by the Gamow vectors. Next, we compute the Gamow eigenfunctions in the position representation as the solutions of the time independent Schrödinger equation with complex eigenvalues subject to a purely outgoing boundary condition. These eigensolutions will be associated to certain eigenfunctionals (Gamow kets). The $[0, \infty)$-energy representation of the Gamow eigenfunction will be related to the complex delta function, and the $(-\infty, \infty)$-energy representation of the Gamow eigenfunction will be related to the Breit-Wigner amplitude. In Section 6.4, the Gamow vectors will be used as basis vectors. We shall see that the Gamow vectors do not form a complete basis—an additional set of kets needs to be added in order to obtain a complete basis. The time evolution of the Gamow vectors is computed in Section 6.5. Section 6.6 deals with the time asymmetry behind the purely outgoing boundary condition. Section 6.7 studies the exponential decay law of the Gamow vectors.

6.2 S-matrix Resonances

The S-matrix in the energy representation is given by (see Section 5.4)

$$S(E) = \frac{\mathcal{J}_-(E)}{\mathcal{J}_+(E)}\,, \quad E > 0\,. \tag{6.2.1}$$

As it stands, this expression is valid only for positive energies. As we said in Section 6.1, the S-matrix resonances are associated to the poles of the analytic continuation of $S(E)$ into the whole complex plane. Since $S(E)$ is not a single-valued function, it is convenient to write the S-matrix as a function of the momentum k before we perform the analytic continuation,

$$S(k) = \frac{\mathcal{J}_-(k)}{\mathcal{J}_+(k)}\,, \quad k > 0\,. \tag{6.2.2}$$

Here the momentum k is given by

$$k = \sqrt{\frac{2m}{\hbar^2}E}\,. \tag{6.2.3}$$

Eq. (6.2.3) provides a Riemann surface in a natural way. The analytic continuation of the numerator and the denominator of $S(k)$ yield two analytic functions $\mathcal{J}_{\pm}(k)$. Therefore, the continuation of $S(k)$ is analytic except at its poles. These are precisely the zeros of the denominator of $S(k)$ (see [85]),

$$\mathcal{J}_{+}(k) = 0\,, \tag{6.2.4}$$

where now k is complex. From Eqs. (4.4.16d) and (5.2.23a) it follows that the equality (6.2.4) is equivalent to the following:

$$(1-\frac{Q}{k})e^{iQ(b-a)}\left(\sin(ka)+\frac{k}{iQ}\cos(ka)\right)+(1+\frac{Q}{k})e^{-iQ(b-a)}\left(\sin(ka)-\frac{k}{iQ}\cos(ka)\right)=0\,. \tag{6.2.5}$$

The solutions of (6.2.5) are the (S-matrix) resonances of the square barrier potential. Equation (6.2.5) has a denumerable infinite number of complex resonance energy solutions. These solutions come in pairs $E_R \pm i\Gamma_R/2$ (see Figure 6.2 of Appendix 6.9). The pole $E_R - i\Gamma_R/2$ is associated with the decaying part of the resonance, and it is located on the lower half-plane of the second sheet of the two-sheeted Riemann surface corresponding to the square root mapping (see Figure 6.2a of Appendix 6.9). The pole $E_R + i\Gamma_R/2$ is associated with the growing or formation part of the resonance, and it is located on the upper half-plane of the second sheet of the Riemann surface (see Figure 6.2b of Appendix 6.9). In the momentum plane, this pair of energy poles corresponds to a pair of poles $\pm\mathrm{Re}(k) - i\mathrm{Im}(k)$ in the lower half of the k-plane that are mirror images of one another with respect to the imaginary axis (see Figure 6.1 of Appendix 6.9).

The width of the resonances increases as the energy increases, and therefore their lifetime $\tau_R = \hbar/\Gamma_R$ decreases. The resonances whose energies are below the top of the barrier $E = V_0$ are close to the real axis. As E keeps increasing the resonances move away from the real axis towards infinity. The square barrier potential poles never correspond to a bound or a virtual state, i.e., they do not lie in the imaginary axis of the momentum plane. The square barrier potential poles are always simple (cf. [86] for an example of a barrier with double poles).

In order to distinguish each of the denumerable infinite number of resonance poles, the decaying resonance energies of the square barrier potential will be denoted by

$$z_n = E_n - i\frac{\Gamma_n}{2}\,, \quad n = 1, 2, \ldots, \tag{6.2.6}$$

whereas the growing resonance energies will be denoted by

$$z_n^* = E_n + i\frac{\Gamma_n}{2}\,, \quad n = 1, 2, \ldots \tag{6.2.7}$$

The corresponding momentum poles will be denoted respectively by

$$k_n = \mathrm{Re}(k_n) - i\,\mathrm{Im}(k_n) = \sqrt{z_n}\,, \quad n = 1, 2, \ldots, \tag{6.2.8}$$

and by

$$-k_n^* = -\mathrm{Re}(k_n) - i\,\mathrm{Im}(k_n) = \sqrt{z_n^*}\,, \quad n = 1, 2, \ldots \tag{6.2.9}$$

6.3 The Gamow Vectors

Gamow vectors are usually defined as eigensolutions of the Schrödinger equation subject to a purely outgoing boundary condition (see Section 6.3.2 below). Although we could start the study of Gamow vectors with that definition, we will follow instead the procedure used for the Lippmann-Schwinger kets. We will define a Gamow vector as the solution of an integral equation. This integral equation has that purely outgoing boundary condition built into it. Needless to say, the solutions of that integral equation will be found by solving the time independent Schrödinger equation subject to the purely outgoing boundary condition.

6.3.1 Lippmann-Schwinger Equation of the Gamow Vectors

The Gamow vectors are solutions of an integral equation of the Lippmann-Schwinger type. If $z_R = E_R - i\Gamma_R/2$ denotes the complex energy associated to a resonance of energy E_R and width Γ_R, then the decaying Gamow vector $|z_R^-\rangle$ fulfills

$$|z_R^-\rangle = \frac{1}{z_R - H_0 + i0} V|z_R^-\rangle \,. \tag{6.3.1}$$

This equation was introduced (with a different notation) by A. Mondragón *et al.* in Ref. [40]. The $+i0$ in Eq. (6.3.1) means that we are working with the retarded free Green function, which has a purely outgoing boundary condition built into it. The retarded free Green function is analytically continued across the cut into the lower half plane (of the second sheet of the Riemann surface), where the complex number z_R is located. Therefore, as A. Mondragón has pointed out, Eq. (6.3.1) should be written as

$$|z_R^-\rangle = \lim_{E \to z_R} \frac{1}{E - H_0 + i0} V|E\rangle \,. \tag{6.3.2}$$

The notation in this equation expresses better the fact that we first have to compute the retarded free Green function $(E - H_0 + i0)^{-1}$ and then continue it across the cut into the lower half plane.[1] The minus sign in $|z_R^-\rangle$ means that the decaying Gamow vector will be defined as an antilinear functional over the $\psi^- \in \mathbf{\Phi}_+$.

As we said above, the integral equation (6.3.1) has a purely outgoing boundary condition built into it. To be more precise, Eq. (6.3.1) in the position representation is equivalent to the time independent Schrödinger equation subject to the condition that far away from the potential region the solution behave as a purely outgoing wave.

As we saw in Section 6.2, to each decaying pole $z_R = E_R - i\Gamma_R/2$ of the S-matrix there corresponds a growing pole $z_R^* = E_R + i\Gamma_R/2$. We now associate a growing Gamow vector

[1] This also shows that a consistent notation will always have flipping of signs like $\varphi^+ \in \mathbf{\Phi}_-$, $\psi^- \in \mathbf{\Phi}_+$, etc. This flipping of signs comes from the fact that we perform analytic continuations from the upper (lower) rim of the cut, which is labeled by $+i0$ ($-i0$), into the lower (upper) half plane, which is labeled by $\mathbb{C}^-$ ($\mathbb{C}^+$).

$|z_R^{*+}\rangle$ to the pole of the S-matrix at z_R^*. The integral equation satisfied by $|z_R^{*+}\rangle$ should read

$$|z_R^{*+}\rangle = \frac{1}{z_R^* - H_0 - i0} V|z_R^{*+}\rangle = \lim_{E\to z_R^*} \frac{1}{E - H_0 - i0} V|E\rangle \,. \tag{6.3.3}$$

In contrast to Eq. (6.3.1), Eq. (6.3.3) has a purely *incoming* boundary condition built into it. That is, Eq. (6.3.3) in the position representation is equivalent to the time independent Schrödinger equation subject to the condition that far away from the potential region the solution behave as a purely incoming wave.

6.3.2 The Gamow Vectors in Position Representation

In this section, we obtain the solutions of the integral equations (6.3.1) and (6.3.3). In oder to do so, we will work in the radial position representation. In this representation we will solve the Schrödinger equation under purely outgoing boundary conditions. We will see that there is a one-to-one correspondence between the complex poles of the analytically continued S-matrix and the complex generalized eigenvalues obtained under purely outgoing boundary conditions.

In the radial representation, Eqs. (6.3.1) and (6.3.3) read

$$\langle r|z_R^-\rangle = \langle r|\frac{1}{z_R - H_0 + i0} V|z_R^-\rangle = \lim_{E\to z_R} \langle r|\frac{1}{E - H_0 + i0} V|E\rangle \,, \tag{6.3.4a}$$

$$\langle r|z_R^{*+}\rangle = \langle r|\frac{1}{z_R^* - H_0 - i0} V|z_R^{*+}\rangle = \lim_{E\to z_R^*} \langle r|\frac{1}{E - H_0 - i0} V|E\rangle \,. \tag{6.3.4b}$$

Instead of solving these integral equations, we solve the equivalent Schrödinger differential equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right)\langle r|z_R\rangle = z_R\langle r|z_R\rangle \,, \tag{6.3.5}$$

subject to the boundary conditions built into them,

$$\langle 0|z_R\rangle = 0 \tag{6.3.6a}$$

$$\langle r|z_R\rangle \text{ is continuous at } r = a \text{ and at } r = b \tag{6.3.6b}$$

$$\frac{d}{dr}\langle r|z_R\rangle \text{ is continuous at } r = a \text{ and at } r = b \tag{6.3.6c}$$

$$\langle r|z_R\rangle \sim e^{ik_R r} \text{ as } r \to \infty \,, \tag{6.3.6d}$$

where

$$k_R = \sqrt{\frac{2m}{\hbar^2} z_R} \,. \tag{6.3.7}$$

In Eqs. (6.3.5) and (6.3.6), we have used the same symbol $\langle r|z_R\rangle$ to denote both $\langle r|z_R^-\rangle$ and $\langle r|z_R^{*+}\rangle$. This will create no confusion, because whenever $z_R = E_R - i\Gamma_R/2$, then $\langle r|z_R\rangle$ will mean $\langle r|z_R^-\rangle$, and whenever $z_R = E_R + i\Gamma_R/2$, then $\langle r|z_R\rangle$ will mean $\langle r|z_R^{*+}\rangle$. Condition (6.3.6d) is the purely outgoing boundary condition. At first glance, it may look

like we have imposed also a purely outgoing boundary condition upon the growing Gamow eigenfunctions $\langle r|z_R^{*+}\rangle$. However, since k_R is complex, the function $e^{ik_R r}$ is not always an outgoing wave. In fact, it is an outgoing wave only when $\mathrm{Re}(k_R)$ is positive, i.e., when we are working with the decaying Gamow vector $\langle r|z_R^-\rangle$, and it is an incoming wave only when $\mathrm{Re}(k_R)$ is negative, i.e., when we are working with the growing Gamow vector $\langle r|z_R^{*+}\rangle$. This means that working with the momentum k_R rather than with z_R will allow us to obtain the decaying and the growing Gamow vectors at the same time.

The purely outgoing boundary condition (6.3.6d) is often written as

$$\lim_{r\to\infty} \frac{du(r;z_R)}{dr} - ik_R u(r;z_R) = 0\,, \tag{6.3.8}$$

where

$$u(r;z_R) = \langle r|z_R\rangle\,. \tag{6.3.9}$$

One can easily check that (6.3.8) is equivalent to (6.3.6d).

If we impose the conditions (6.3.6a)-(6.3.6c) upon the general solution of Eq. (6.3.5), we obtain that, up to a normalization factor, the solution has the form

$$\chi(r;z_R) \equiv \chi(r;k_R) = \begin{cases} \sin(k_R r) & 0<r<a \\ \mathcal{J}_1(k_R)e^{iQ_R r} + \mathcal{J}_2(k_R)e^{-iQ_R r} & a<r<b \\ \mathcal{J}_3(k_R)e^{ik_R r} + \mathcal{J}_4(k_R)e^{-ik_R r} & b<r<\infty\,, \end{cases} \tag{6.3.10}$$

where

$$Q_R = \sqrt{k_R^2 - \frac{2m}{\hbar^2}V_0} = \sqrt{\frac{2m}{\hbar^2}(z_R - V_0)}\,. \tag{6.3.11}$$

The eigensolution (6.3.10), which does not satisfy the purely outgoing boundary condition yet, is equal to the analytic continuation of the regular solution $\chi(r;E)$ of Eq. (5.2.22). In Eq. (6.3.10), there is no restriction on the values that z_R can take, i.e., before imposing the purely outgoing boundary condition z_R can be any complex number. If we now impose (6.3.6d) upon the eigensolution (6.3.10), then the coefficient $\mathcal{J}_4(k_R) = i/2\,\mathcal{J}_+(k_R)$ must be zero. Since this condition is the same as the condition (6.2.4) for the complex poles of the S-matrix, the set of generalized complex eigenvalues z_R must include the set of S-matrix resonance poles. We now show that these two sets of solutions are the same.

The boundary conditions (6.3.6) can be written in terms of the coefficients of (6.3.10) as

$$\mathcal{J}_1 e^{iQ_R a} + \mathcal{J}_2 e^{-iQ_R a} = \sin(k_R a) \tag{6.3.12a}$$

$$iQ_R(\mathcal{J}_1 e^{iQ_R a} - \mathcal{J}_2 e^{-iQ_R a}) = k_R\cos(k_R a) \tag{6.3.12b}$$

$$\mathcal{J}_3 e^{ik_R b} = \mathcal{J}_1 e^{iQ_R b} + \mathcal{J}_2 e^{-iQ_R b} \tag{6.3.12c}$$

$$ik_R\mathcal{J}_3 e^{ik_R b} = iQ_R(\mathcal{J}_1 e^{iQ_R b} - \mathcal{J}_2 e^{-iQ_R b})\,. \tag{6.3.12d}$$

Writing this set of linear equations as a matrix equation we obtain

$$\begin{pmatrix} \sin(k_R a) & 0 & -e^{iQ_R a} & -e^{-iQ_R a} \\ k_R\cos(k_R a) & 0 & -iQ_R e^{iQ_R a} & iQ_R e^{-iQ_R a} \\ 0 & e^{ik_R b} & -e^{iQ_R b} & -e^{-iQ_R b} \\ 0 & ik_R e^{ik_R b} & -iQ_R e^{iQ_R b} & iQ_R e^{-iQ_R b} \end{pmatrix} \begin{pmatrix} 1 \\ \mathcal{J}_3 \\ \mathcal{J}_1 \\ \mathcal{J}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}\,. \tag{6.3.13}$$

This is a homogeneous system of four equations with four unknowns. The system has a non-trivial solution iff the determinant of the coefficients is equal to zero,

$$\begin{vmatrix} \sin(k_R a) & 0 & -e^{iQ_R a} & -e^{-iQ_R a} \\ k_R\cos(k_R a) & 0 & -iQ_R e^{iQ_R a} & iQ_R e^{-iQ_R a} \\ 0 & e^{ik_R b} & -e^{iQ_R b} & -e^{-iQ_R b} \\ 0 & ik_R e^{ik_R b} & -iQ_R e^{iQ_R b} & iQ_R e^{-iQ_R b} \end{vmatrix} = 0\,. \tag{6.3.14}$$

Straightforward computations show that the condition (6.3.14) is the same as the condition (6.2.5). Thus the set of generalized eigenvalues of the time independent Schrödinger equation subject to purely outgoing boundary conditions is the same as the set of S-matrix poles.

As we mentioned earlier, the solutions of (6.2.5) come in pairs of a growing and a decaying pole. We have denoted those poles by z_n and z_n^* and their corresponding momenta by k_n and $-k_n^*$. The eigenfunction associated to $z_n = E_n - i\Gamma_n/2$ is the decaying Gamow vector in the position representation, whose radial part, up to a normalization factor, is

$$u_n(r;z_n) \equiv u_n(r;k_n) = \begin{cases} \frac{1}{\mathcal{J}_3(k_n)}\sin(k_n r) & 0<r<a \\ \frac{\mathcal{J}_1(k_n)}{\mathcal{J}_3(k_n)}e^{iQ_n r} + \frac{\mathcal{J}_2(k_n)}{\mathcal{J}_3(k_n)}e^{-iQ_n r} & a<r<b \\ e^{ik_n r} & b<r<\infty\,. \end{cases} \tag{6.3.15}$$

The eigenfunction associated to $z_n^* = E_n + i\Gamma_n/2$ is the growing Gamow vector in the position representation, whose radial part, up to a normalization factor, is

$$u_n(r;z_n^*) \equiv u_n(r;-k_n^*) = \begin{cases} \frac{1}{\mathcal{J}_3(-k_n^*)}\sin(-k_n^* r) & 0<r<a \\ \frac{\mathcal{J}_1(-k_n^*)}{\mathcal{J}_3(-k_n^*)}e^{-iQ_n^* r} + \frac{\mathcal{J}_2(-k_n^*)}{\mathcal{J}_3(-k_n^*)}e^{iQ_n^* r} & a<r<b \\ e^{-ik_n^* r} & b<r<\infty\,. \end{cases} \tag{6.3.16}$$

Form equations (6.3.10), (6.3.15) and (6.3.16) it follows that the Gamow eigenfunctions are proportional to the analytic continuation of the regular solution,

$$u_n(r;k_n) = \frac{2i}{\mathcal{J}_-(k_n)}\chi(r;k_n)\,, \tag{6.3.17a}$$

$$u_n(r;-k_n^*) = \frac{2i}{\mathcal{J}_-(-k_n^*)}\chi(r;-k_n^*)\,. \tag{6.3.17b}$$

The Gamow vector (6.3.15) is defined up to a normalization factor. By normalization we mean the function N_n of z_n by which we can multiply the Gamow eigenfunction $u_n(r;z_n)$ to obtain another eigenfunction $N_n u_n(r;z_n)$ with the same eigenvalue z_n and satisfying the same boundary conditions (6.3.6). If no confusion arises, we denote the normalized Gamow vector also by $u_n(r;z_n)$,

$$u_n(r;z_n) \equiv u_n(r;k_n) = \begin{cases} \frac{N_n}{\mathcal{J}_3(k_n)}\sin(k_n r) & 0<r<a \\ \frac{N_n\mathcal{J}_1(k_n)}{\mathcal{J}_3(k_n)}e^{iQ_n r} + \frac{N_n\mathcal{J}_2(k_n)}{\mathcal{J}_3(k_n)}e^{-iQ_n r} & a<r<b \\ N_n e^{ik_n r} & b<r<\infty\,. \end{cases} \tag{6.3.18}$$

After this normalization Eq. (6.3.17a) becomes

$$u_n(r;z_n) \equiv u_n(r;k_n) = \frac{2iN_n}{\mathcal{J}_-(k_n)}\chi(r;k_n) \tag{6.3.19}$$

There is an extensive literature on the normalization of Gamow vectors (cf. [40] and references therein). We shall not treat this problem here, although we would like to mention that the normalization proposed by A. Mondragón *et al.* [40] seems to be the most suitable.

The eigenfunctions $u_n(r;z_n)$ of the differential operator h are obviously not square integrable, i.e., they do not belong to the Hilbert space $L^2([0,\infty),dr)$. In order to construct an eigenket $|z_n^-\rangle$ of the Hamiltonian H associated to the eigenfunction $u_n(r;z_n)$, we follow the pattern of Section 5.3. The Gamow ket $|z_n^-\rangle$ associated to the eigenfunction $u_n(r;z_n)$ is defined by

$$\begin{aligned} |z_n^-\rangle : \mathbf{\Phi}_+ &\longmapsto \mathbb{C} \\ \psi^- &\longmapsto \langle\psi^-|z_n^-\rangle := \int_0^\infty dr\, \overline{\psi^-(r)}u(r;z_n)\,. \end{aligned} \tag{6.3.20}$$

Under the assumptions made upon the elements ψ^- of $\mathbf{\Phi}_+$, the function $|z_n^-\rangle$ is a well-defined antilinear functional. It is easy to show that the function $|z_n^-\rangle$ is a generalized eigenvector of H with complex eigenvalue z_n,

$$H^\times|z_n^-\rangle = z_n|z_n^-\rangle\,, \tag{6.3.21}$$

or more precisely,

$$\langle\psi^-|H^\times|z_n^-\rangle = z_n\langle\psi^-|z_n^-\rangle\,, \quad \forall\psi^- \in \mathbf{\Phi}_+\,. \tag{6.3.22}$$

In a similar vein, we can define a ket $|z_n^{*+}\rangle$ associated to the eigenfunction $u_n(r;z_n^*)$,

$$\begin{aligned} |z_n^{*+}\rangle : \mathbf{\Phi}_- &\longmapsto \mathbb{C} \\ \varphi^+ &\longmapsto \langle\varphi^+|z_n^{*+}\rangle := \int_0^\infty dr\, \overline{\varphi^+(r)}u(r;z_n^*)\,, \end{aligned} \tag{6.3.23}$$

and prove that this is a well defined antilinear eigenfunctional of the Hamiltonian H with complex eigenvalue z_n^*,

$$\langle\varphi^+|H^\times|z_n^{*+}\rangle = z_n^*\langle\varphi^+|z_n^{*+}\rangle\,, \quad \forall\varphi^+ \in \mathbf{\Phi}_-\,. \tag{6.3.24}$$

6.3.3 The Gamow Vectors in Energy Representation

Once we have constructed the Gamow vector $|z_n^-\rangle$ in the position representation, it is straightforward to compute its energy representation. We shall obtain the Gamow vector in two different energy representations. One of them is the standard energy representation associated to the physical spectrum, which is $[0,\infty)$ in our example. The other one is associated to the $(-\infty,\infty)$ spectrum. These two representations are related by the function θ of

Appendix 5.5.2. We shall show that in the $[0,\infty)$-energy representation the Gamow vector acts as the antilinear complex delta functional[2] multiplied by a normalization factor. In the $(-\infty,\infty)$-energy representation, the Gamow vector can be associated to the Breit-Wigner amplitude multiplied by a normalization factor.

First, we define the antilinear complex delta functional $|\widehat{z_n^-}\rangle$,

$$\begin{aligned} |\widehat{z_n^-}\rangle : \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+} &\longmapsto \mathbb{C} \\ \widehat{\psi}^- &\longmapsto \langle\widehat{\psi}^-|\widehat{z_n^-}\rangle := \widetilde{\psi}^-(z_n)\,, \end{aligned} \tag{6.3.25}$$

where the function $\widetilde{\psi}^-(z)$ is defined by

$$\widetilde{\psi}^-(z) := \overline{\widehat{\psi}^-(\overline{z})}\,. \tag{6.3.26}$$

The function $|\widehat{z_n^-}\rangle$ is a well defined antilinear functional over the space $\widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}$, since the elements $\widehat{\psi}^-$ of $\widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}$ were taken to be in $\mathcal{H}^2_+$.

It can be shown that the $[0,\infty)$-energy representation of $|z_n^-\rangle$ is the antilinear complex delta functional $|\widehat{z_n^-}\rangle$ save for a normalization factor A_n,

$$U_-^\times|z_n^-\rangle = A_n|\widehat{z_n^-}\rangle\,. \tag{6.3.27}$$

The proof of Eq. (6.3.27) is as follows: from Eqs. (5.2.21) and (6.3.19) we conclude that the Gamow eigenfunction $u(r;k_n)$ is proportional to the analytic continuation of the Lippmann-Schwinger eigenfunction $\chi^-(r;k)$,

$$u_n(r;k_n) = 2iN_n\chi^-(r;k_n)\,. \tag{6.3.28}$$

Then the Gamow eigenfunction is proportional to the analytic continuation of the eigenfunction $\sigma^-(r;E)$,

$$u_n(r;z_n) = A_n\sigma^-(r;z_n)\,. \tag{6.3.29}$$

From Eq. (6.3.29) and from the (assumed) properties of the elements $\psi^- \in \mathbf{\Phi}_+$ (see Section 5.3) it follows that

$$\begin{aligned} \langle\widehat{\psi}^-|U_-^\times|z_n^-\rangle &= \langle\psi^-|z_n^-\rangle \\ &= \int_0^\infty dr\,\overline{\psi^-(r)}u_n(r;z_n) \\ &= A_n\int_0^\infty dr\,\overline{\psi^-(r)}\sigma^-(r;z_n) \\ &= A_n\,\overline{\widehat{\psi}^-(\overline{z_n})} \\ &= A_n\langle\widehat{\psi}^-|\widehat{z_n^-}\rangle\,, \quad \forall\widehat{\psi}^- \in \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}\,, \end{aligned} \tag{6.3.30}$$

where in the last step we have used the definition (6.3.25). This proves Eq. (6.3.27).

[2]For a great deal of information about the antilinear complex delta functional and its representations, the reader is referred to [87].

If we write the action of $|\widehat{z_n^-}\rangle$ as an integral operator, the kernel of integration is the complex delta function,

$$\langle\widehat{\psi}^-|\widehat{z_n^-}\rangle = \int_0^\infty dE\, A_n \delta(E - z_n)\overline{\widehat{\psi}^-(E)}\,. \tag{6.3.31}$$

We are now going to study the relation between the complex delta function and the Breit-Wigner amplitude. We shall show that

$$\theta^\times|\frac{1}{E - z_n}{}^-\rangle = A_n|\widehat{z_n^-}\rangle\,, \tag{6.3.32}$$

where $\theta^\times$ is the dual extension of the function θ, and θ is the function that takes any function of $\widehat{\mathbf{\Phi}}_+$ into its restriction to the positive real line (cf. Appendix 5.5.2). The functional $|\frac{1}{E-z_n}{}^-\rangle$ of Eq. (6.3.32) is associated to the Breit-Wigner amplitude by

$$\begin{aligned} |\frac{1}{E - z_n}{}^-\rangle : \widehat{\mathbf{\Phi}}_+ &\longmapsto \mathbb{C} \\ \theta^{-1}\widehat{\psi}^- &\longmapsto \langle\theta^{-1}\widehat{\psi}^-|\frac{1}{E - z_n}{}^-\rangle := \int_{-\infty}^\infty dE\, \left(-\frac{1}{2\pi i}\frac{A_n}{E - z_n}\right)\overline{\theta^{-1}\widehat{\psi}^-(E)}\,, \end{aligned} \tag{6.3.33}$$

where A_n is the normalization factor of Eq. (6.3.27). We shall call the functional defined by Eq. (6.3.33) the Breit-Wigner functional. By Titchmarsh theorem [80], the Breit-Wigner functional is a well defined antilinear functional.

The key property that will be used to prove (6.3.32) is that the functions $\widehat{\psi}^-$ of $\widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}$ are boundary values of Hardy functions from above. In order to build the ground of that proof, we first show the relation between the $[0,\infty)$-energy representation and the $(-\infty,\infty)$-energy representation:

$$\begin{array}{ccccccc} \widehat{\psi}^-\,, & \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+} & \subset & L^2([0,\infty), dE) & \subset & (\widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+})^\times & [0,\infty)-\text{energy repr.} \\ & \uparrow\theta & & & & \uparrow\theta^\times & \\ \theta^{-1}\widehat{\psi}^-\,, & \widehat{\mathbf{\Phi}}_+ & \subset & \mathcal{H}_+^2 & \subset & \widehat{\mathbf{\Phi}}_+^\times & (-\infty,\infty)-\text{energy repr.} \end{array} \tag{6.3.34}$$

where $\mathcal{H}_+^2$ is the space of Hardy functions from above. It is worthwhile noting that although we have denoted the functions $\theta^{-1}\widehat{\psi}^-$ and $\widehat{\psi}^-$ by a different symbol, they are indeed the *same* function. More precisely, they are different "pieces" of the same function. In particular, the value of their analytic continuation at a complex number z is the same,

$$\theta^{-1}\widehat{\psi}^-(z) = \widehat{\psi}^-(z)\,. \tag{6.3.35}$$

Obviously, the functions $\widetilde{\psi}^-$ and $\theta^{-1}\widetilde{\psi}^-$ enjoy an analogous property,

$$\theta^{-1}\widetilde{\psi}^-(z) = \widetilde{\psi}^-(z)\,. \tag{6.3.36}$$

The reason why we use a different symbol for different "pieces" of the same function is that the the proof on the connection between the Breit-Wigner amplitude and the complex delta function becomes more apparent:

Let $\theta^{-1}\widehat{\psi}^- \in \widehat{\mathbf{\Phi}}_+^\times$. Then $\theta^{-1}\widetilde{\psi}^- = \overline{\theta^{-1}\widehat{\psi}^-} \in \mathcal{H}_-^2$. By Titchmarsh theorem [80],

$$\theta^{-1}\widetilde{\psi}^-(z_n) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE\, \frac{1}{E-z_n}\, \theta^{-1}\widetilde{\psi}^-(E)\,. \tag{6.3.37}$$

Multiplying this equation by A_n we obtain

$$A_n\theta^{-1}\widetilde{\psi}^-(z_n) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE\, \frac{A_n}{E-z_R}\, \theta^{-1}\widetilde{\psi}^-(E)\,. \tag{6.3.38}$$

From Eqs. (6.3.33) and (6.3.38) it follows that

$$A_n\theta^{-1}\widetilde{\psi}^-(z_n) = \langle \theta^{-1}\widehat{\psi}^- | \frac{1}{E-z_n}{}^- \rangle\,. \tag{6.3.39}$$

We now define the action of $\theta^\times$ on $|\frac{1}{E-z_n}{}^-\rangle$ by

$$\langle \widehat{\psi}^- | \theta^\times | \frac{1}{E-z_n}{}^- \rangle := \langle \theta^{-1}\widehat{\psi}^- | \frac{1}{E-z_n}{}^- \rangle\,. \tag{6.3.40}$$

Eqs. (6.3.39) and (6.3.40) lead to

$$\langle \widehat{\psi}^- | \theta^\times | \frac{1}{E-z_n}{}^- \rangle = A_n\, \theta^{-1}\widetilde{\psi}^-(z_n)\,. \tag{6.3.41}$$

Taking advantage of Eq. (6.3.36) we can write (6.3.41) as

$$\langle \widehat{\psi}^- | \theta^\times | \frac{1}{E-z_n}{}^- \rangle = A_n\, \widetilde{\psi}^-(z_n)\,, \quad \forall \widehat{\psi}^- \in \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}\,. \tag{6.3.42}$$

The right hand side of this equation equals the action of the complex delta function at $\widehat{\psi}^-$ multiplied by A_n,

$$\langle \widehat{\psi}^- | \theta^\times | \frac{1}{E-z_n}{}^- \rangle = A_n\, \langle \widehat{\psi}^- | \widehat{z_n^-} \rangle\,, \quad \forall \widehat{\psi}^- \in \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}\,, \tag{6.3.43}$$

which proves (6.3.36).

Therefore, the Gamow eigenfunction $u_n(r;z_n)$, the complex delta function (multiplied by a normalization factor) $A_n\delta(E-z_n)$ and the Breit-Wigner amplitude (multiplied by a normalization factor) $iA_n/2\pi(E-z_n)$ correspond to the same object in different representations,

$$\begin{array}{ccccc} u_n(r;z_n) & \longleftrightarrow & A_n\delta(E-z_n)\,,\ E\in[0,\infty) & \longleftrightarrow & -\frac{1}{2\pi i}\,\frac{A_n}{E-z_n}\,,\ E\in(-\infty,\infty) \\ \text{posit. repr.} & & [0,\infty)\text{-energy repr.} & & -(\infty,\infty)\text{-energy repr.} \end{array} \tag{6.3.44}$$

We summarize the results of this section in the following diagram:

$$
\begin{array}{llcccl}
H; \quad \psi^-(r) & \mathbf{\Phi}_+ & \subset & L^2([0,\infty), dr) & \subset & \mathbf{\Phi}_+^\times \qquad \langle r|z_n^-\rangle \equiv u_n(r;z_n) \\
 & \downarrow U_- & & \downarrow U_- & & \downarrow U_-^\times \\
\widehat{E}; \quad \widehat{\psi}^-(E) & \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+} & \subset & L^2([0,\infty), dE) & \subset & (\widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+})^\times \qquad \langle {}^-E|z_n^-\rangle \equiv A_n\delta(E-z_n) \\
 & \uparrow \theta & & & & \uparrow \theta^\times \\
\widehat{E}; \quad \widehat{\psi}^-(E) & \widehat{\mathbf{\Phi}}_+ & \subset & \mathcal{H}_+^2 & \subset & \widehat{\mathbf{\Phi}}_+^\times \qquad \langle {}^-E|z_n^-\rangle \equiv -\frac{1}{2\pi i}\frac{A_n}{E-z_n}
\end{array}
\tag{6.3.45}
$$

In this diagram, we have denoted both $\widehat{\psi}^-(E) \in \widehat{\mathbf{\Phi}}_+|_{\mathbb{R}^+}$ and $\theta^{-1}\widehat{\psi}^-(E) \in \widehat{\mathbf{\Phi}}_+$ by the same symbol $\widehat{\psi}^-(E)$, since no distinction is necessary any more. We stress that in the second line of (6.3.45) the energy is allowed to run over the physical spectrum $[0,\infty)$, whereas in the bottom line the energy is allowed to run over $(-\infty,\infty)$.

6.4 Complex Basis Vector Expansion

The Lippmann-Schwinger kets are basis vectors that were used to expand a normalizable smooth function φ^+ as in (5.3.7). The Gamow vectors are also basis vectors. The expansion generated by the Gamow vectors is called the complex basis vector expansion. However, the Gamow vectors do not form a complete basis system. The complex basis vector expansion needs an additional set of Dirac kets corresponding to the energies that lie in the negative real axis of the second sheet of the Riemann surface. This has been realized also by other authors [40, 43, 42], who have used the Green function to construct the complex basis vector expansion.

In this section, we expand a normalizable wave function in terms of the Gamow vectors and a continuous set of Dirac kets. The Gamow vectors contain the resonance contribution, whereas the contribution of the additional set of Dirac kets is interpreted as a background. The complex basis vector expansion is not valid for every normalizable wave function, i.e., for every element of the Hilbert space, but only for functions $\varphi^+ \in \mathbf{\Phi}_-$. The technicalities of that expansion can be found in [88].

In a scattering experiment, we measure the transition probability from a state (in-state) φ^+ into an observable (out-state) ψ^-. In Section 5.4, we wrote the amplitude of this probability as

$$
\big(\psi^-, \varphi^+\big) = \int_0^\infty \langle \psi^-|E^-\rangle S(E) \langle E^+|\varphi^+\rangle dE\,. \tag{6.4.1}
$$

The function $S(E)$ is the energy representation of the S-matrix. This function can be analytically continued into a two-sheeted Riemann surface, and the quantity $S(E)$ in (6.4.1) represents the boundary value of this analytic function on the upper lip of the cut in the Riemann surface. We now extract the resonance contribution out of (6.4.1). This resonance contribution is carried by the Gamow vectors. In order to do so, we deform the contour of

integration into the lower half-plane of the second sheet of the Riemann surface, where the decaying resonance poles are located (see Figure 6.3a of Appendix 6.9). Using the results that appear in [88], we can write (6.4.1) as

$$\left(\psi^-, \varphi^+\right) = \int_0^{-\infty} \langle \psi^- | E^- \rangle S(E) \langle E^+ | \varphi^+ \rangle dE - 2\pi i \sum_{n=0}^{\infty} r_n \langle \psi^- | z_n^- \rangle \langle {}^+ z_n | \varphi^+ \rangle \,, \tag{6.4.2}$$

where r_n denotes the residue of the S-matrix at z_n. The integral in Eq. (6.4.2) is done on the negative real semiaxis of the second sheet of the Riemann surface. The series in (6.4.2) can be shown to be convergent [88]. Omitting ψ^- in (6.4.2), we get the complex basis vector expansion for the states,

$$\varphi^+ = \int_0^{-\infty} |E^-\rangle S(E) \langle {}^+ E | \varphi^+ \rangle dE - 2\pi i \sum_{n=0}^{\infty} r_n |z_n^-\rangle \langle {}^+ z_n | \varphi^+ \rangle \,. \tag{6.4.3}$$

In Eq. (6.4.3), the infinite sum contains the resonances contribution, while the integral is interpreted as the background contribution. Needless to say, the Gamow vectors in Eq. (6.4.3) are defined up to a normalization factor.

Similarly, we obtain the complex basis vector expansion for the observable ψ^- [88], but now we deform the contour of integration into the upper half-plane of the second sheet of the Riemann surface, where the growing resonance poles are located (see Figure 6.3b)

$$\psi^- = \int_0^{-\infty} |E^+\rangle \overline{S(E)} \langle E^- | \psi^- \rangle dE + 2\pi i \sum_{n=0}^{\infty} r_n^* |z_n^{*+}\rangle \langle {}^- z_n^* | \psi^- \rangle \,. \tag{6.4.4}$$

In this equation, r_n^* denotes the residue of S-matrix at z_n^*. The integration in (6.4.4) is performed on the negative real semiaxis of the second sheet of the Riemann surface. The series in (6.4.4) has been shown to be convergent [88].

6.5 Semigroup Time Evolution of the Gamow Vectors

Now, we want to study the time evolution of the Gamow vectors. In order to do it, we need to consider the operator $\mathcal{U}(t) = e^{-iHt/\hbar}$, which governs the time evolution of the vector states in Hilbert space. The operator conjugate to $\mathcal{U}(t)$ is defined by

$$\langle \phi | \mathcal{U}^\times(t) | F \rangle = \langle \mathcal{U}^\dagger(t) \phi | F \rangle \,, \tag{6.5.1}$$

where ϕ denotes $\varphi^+ \in \mathbf{\Phi}_-$ or $\psi^- \in \mathbf{\Phi}_+$ and F belongs to $\mathbf{\Phi}_-^\times$ or $\mathbf{\Phi}_+^\times$, respectively. Eq. (6.5.1) will also be denoted as

$$\langle \phi | e^{-iH^\times t/\hbar} | F \rangle = \langle e^{iHt/\hbar} \phi | F \rangle \,. \tag{6.5.2}$$

The conjugate operator $\mathcal{U}^\times(t)$ determines the time evolution of the elements in $\mathbf{\Phi}_\pm^\times$, whenever it can be defined.

We have assumed that $\widehat{\mathbf{\Phi}}_\pm = \mathcal{S} \cap \mathcal{H}^2_\pm$. Under this assumption, the following statements can be proved [20, 91]:

i.) For any $t \geq 0$, $e^{iHt/\hbar}\mathbf{\Phi}_+ \subset \mathbf{\Phi}_+$ and $e^{iHt/\hbar}$ is continuous on $\mathbf{\Phi}_+$. For any $t < 0$, there is a $\psi^- \in \mathbf{\Phi}_+$ such that $e^{iHt/\hbar}\psi^- \notin \mathbf{\Phi}_+$.

ii.) For any $t \leq 0$, $e^{iHt/\hbar}\mathbf{\Phi}_- \subset \mathbf{\Phi}_-$ and $e^{iHt/\hbar}$ is continuous on $\mathbf{\Phi}_-$. For any $t > 0$, there is a $\varphi^+ \in \mathbf{\Phi}_-$ such that $e^{iHt/\hbar}\varphi^+ \notin \mathbf{\Phi}_-$.

This leads to the following consequences:

i.) For any $t \geq 0$, one can define the conjugate of $\mathcal{U}(t) = e^{-iHt/\hbar}$, which extends the evolution operator $\mathcal{U}(t) = e^{-iHt/\hbar}$ to a continuous operator and defines the time evolution on $\mathbf{\Phi}^\times_+$. This cannot be done for any $t < 0$. We denote this extension as $\mathcal{U}^\times_+(t) = e^{-iH^\times t/\hbar}_+$.

ii.) For any $t \leq 0$, one can define the conjugate of $\mathcal{U}(t) = e^{-iHt/\hbar}$, which extends the evolution operator $\mathcal{U}(t) = e^{-iHt/\hbar}$ to a continuous operator and defines the time evolution on $\mathbf{\Phi}^\times_-$. This cannot be done for any $t > 0$. We denote this extension as $\mathcal{U}^\times_-(t) = e^{-iH^\times t/\hbar}_-$.

It seems natural to consider these extensions as the operators that determine the time evolution of the objects in the dual spaces. We observe that this time evolution is *not* defined for all values of t. This has important consequences for the time evolution of the Gamow vectors.

Consider the decaying Gamow vector $|z_n^-\rangle$. From the above comments, it is not difficult to see [20] that the evolution operator $\mathcal{U}^\times_+(t)$ acts on $|z_n^-\rangle$ if and only if $t \geq 0$,

$$\mathcal{U}^\times_+(t)|z_n^-\rangle = e^{-iE_nt/\hbar}\, e^{-\Gamma_n t/(2\hbar)}|z_n^-\rangle\,, \quad \text{only for } t \geq 0\,, \tag{6.5.3}$$

or more precisely,

$$\langle\psi^-|\mathcal{U}^\times_+(t)|z_n^-\rangle = e^{-iE_nt/\hbar}\, e^{-\Gamma_n t/(2\hbar)}\langle\psi^-|z_n^-\rangle\,, \quad \forall\psi^- \in \mathbf{\Phi}_+\,,\ t \geq 0 \text{ only}\,. \tag{6.5.4}$$

We see that the Gamow vector decays exponentially. Thus it fulfills the properties that are demanded from the decaying resonance states. Much more significant is the property that the time evolution of the decaying Gamow vectors occurs for $t > 0$ only—the time evolution of Gamow vectors is time asymmetric.

Consider now the Gamow vector $|z_n^{*+}\rangle$. The evolution operator $\mathcal{U}^\times_-(t)$ acts on $|z_n^{*+}\rangle$ if and only if $t \leq 0$,

$$\mathcal{U}^\times_-(t)|z_n^{*+}\rangle = e^{-iE_nt/\hbar}\, e^{\Gamma_n t/(2\hbar)}|z_n^{*+}\rangle\,, \quad \text{only for } t \leq 0\,, \tag{6.5.5}$$

or more precisely,

$$\langle\varphi^+|\mathcal{U}^\times_-(t)|z_n^{*+}\rangle = e^{-iE_nt/\hbar}\, e^{\Gamma_n t/(2\hbar)}\langle\varphi^+|z_n^{*+}\rangle\,, \quad \forall\varphi^+ \in \mathbf{\Phi}_-\,,\ t \leq 0 \text{ only}\,. \tag{6.5.6}$$

Therefore, the symmetric group evolution of the Hilbert space splits up into two semigroups, expressing time asymmetry on a microscopic level.[3]

[3]For more on the description of time asymmetry in Quantum Mechanics in terms of the propagators, the reader is referred to [32].

6.6 Time Asymmetry of the Purely Outgoing Boundary Condition

The semigroup time evolution of the Gamow vectors expresses the time asymmetry built into them. We will show here that the purely outgoing boundary condition that singles out the resonance energies has also a time asymmetry built into it. To be more precise, we will show that the purely outgoing boundary condition should read as *purely outgoing* only for the decaying part of a resonance and as *purely incoming* for the growing part of the resonance. Because the purely incoming condition is the time reversed of the purely outgoing one, the growing Gamow vector can be viewed as the time reversed of the decaying Gamow vector [60] (see also next chapter).

6.6.1 Outgoing Boundary Condition in Phase

First, we study the meaning of the purely outgoing boundary condition when it is imposed on the decaying part of the resonance. The complex energy associated to the decaying part of a resonance is $z_n = E_n - i\Gamma_n/2$ $(E_n, \Gamma_n > 0)$ which lies in the fourth quarter of the second sheet of the Riemann surface (see Figure 6.2a). Its corresponding momentum $k_n = \mathrm{Re}(k_n) - i\mathrm{Im}(k_n)$ $(\mathrm{Re}(k_n), \mathrm{Im}(k_n) > 0)$ lies in the fourth quadrant of the momentum plane (see Figure 6.1). The decaying Gamow vector $u_n(r; z_n)$ of Eq. (6.3.15) was obtained after imposing the purely outgoing boundary condition (6.3.6d) upon (6.3.10). If we had not imposed this condition, we would had obtained a solution of the form (6.3.10), and every complex number would had been a generalized eigenvalue of the Hamiltonian. In the region $r > b$, this solution would had been the sum of two linearly independent solutions

$$\begin{aligned} u^{decaying}_{incoming}(r; z_n; t) &= \mathcal{J}_4 e^{-ik_n r} e^{-iz_n t/\hbar} \\ &= \left(\mathcal{J}_4 e^{-\mathrm{Im}(k_n)r - \Gamma_n t/(2\hbar)}\right) e^{-i\mathrm{Re}(k_n)r - iE_n t/\hbar}, \quad r > b, \end{aligned} \tag{6.6.1}$$

which we call incoming decaying Gamow vector, and

$$\begin{aligned} u^{decaying}_{outgoing}(r; z_n; t) &= \mathcal{J}_3 e^{ik_n r} e^{-iz_n t/\hbar} \\ &= \left(\mathcal{J}_3 e^{\mathrm{Im}(k_n)r - \Gamma_n t/(2\hbar)}\right) e^{i\mathrm{Re}(k_n)r - iE_n t/\hbar}, \quad r > b, \end{aligned} \tag{6.6.2}$$

which we call outgoing decaying Gamow vector. These names come from the standard interpretation (see, for instance, [92]) of plane waves with a complex exponent: the exponential with purely imaginary exponent—the term that carries the phase—is interpreted as the term that governs the propagation of the wave, and the exponential with real exponent is interpreted as the term that just changes the amplitude of the wave on the surfaces of equal phase [92]. We are going to interpret (6.6.1) and (6.6.2) in the same fashion. The terms between brackets in (6.6.1) and (6.6.2) determine the amplitude of the waves. The propagation of $u^{decaying}_{outgoing}$ is governed by $e^{i\mathrm{Re}(k_n)r} e^{-iE_n t/\hbar}$, and therefore $u^{decaying}_{outgoing}$ is an outgoing wave (in phase). Analogously, the propagation of $u^{decaying}_{incoming}$ is governed by $e^{-i\mathrm{Re}(k_n)r} e^{-iE_n t/\hbar}$, and thus $u^{decaying}_{incoming}$ is an incoming wave (in phase). Imposing the purely outgoing boundary

condition $\mathcal{J}_4 = 0$ is tantamount to forbidding $u^{decaying}_{incoming}$. Thus for the decaying part of the resonance the purely outgoing boundary condition allows only purely outgoing waves (in phase).

The meaning of the purely outgoing boundary condition applied to the growing part of the resonance is the opposite. The growing energy eigenvalue $z_n^* = E_n + i\Gamma_n/2$ lies in the first quadrant of the second sheet of the Riemann surface (see Figure 6.2b), and its momentum $-k_n^* = -\mathrm{Re}(k_n) - i\mathrm{Im}(k_n)$ lies in the third quadrant of the momentum plane (see Figure 6.1). The growing Gamow vector $u_n(r; z_n^*)$ of Eq. (6.3.16) was obtained after imposing the condition $\mathcal{J}_4 = 0$ on (6.3.10). If we had not imposed this condition, in the region $r > b$ the solution would had been the sum of two linearly independent solutions

$$\begin{aligned} u^{growing}_{incoming}(r; z_n^*; t) &= \mathcal{J}_3 e^{-ik_n^* r} e^{-iz_n^* t/\hbar} \\ &= \left(\mathcal{J}_3 e^{\mathrm{Im}(k_n)r + \Gamma_n t/(2\hbar)}\right) e^{-i\mathrm{Re}(k_n)r - iE_n t/\hbar}, \quad r > b, \end{aligned} \tag{6.6.3}$$

that we call incoming growing Gamow vector, and

$$\begin{aligned} u^{growing}_{outgoing}(r; z_n^*; t) &= \mathcal{J}_4 e^{ik_n^* r} e^{-iz_n^* t/\hbar} \\ &= \left(\mathcal{J}_4 e^{-\mathrm{Im}(k_n)r + \Gamma_n t/(2\hbar)}\right) e^{i\mathrm{Re}(k_n)r - iE_n t/\hbar}, \quad r > b, \end{aligned} \tag{6.6.4}$$

that we call outgoing growing Gamow vector. The names come also after the standard interpretation [92] of plane waves with a complex exponent. Therefore, the purely outgoing boundary condition $\mathcal{J}_4 = 0$, when applied to the growing part of a resonance, bans $u^{growing}_{outgoing}$ and allows only purely incoming waves (in phase).

6.6.2 Outgoing Boundary Condition in Probability Density

In the previous section, we showed how the time asymmetry built into the purely outgoing boundary condition affected the phase of the Gamow vectors. In this section, we show the same time asymmetry but now considering the probability density of the Gamow vectors.

For the decaying part of the resonance, the probability densities (before imposing the purely outgoing boundary condition) are obtained by taking the absolute value square of (6.6.1)

$$\begin{aligned} \rho^{decaying}_{incoming}(r; z_n; t) = |u^{decaying}_{incoming}(r; z_n; t)|^2 &= |\mathcal{J}_4|^2 e^{-2\mathrm{Im}(k_n)r - \Gamma_n t/\hbar} \\ &= |\mathcal{J}_4|^2 e^{-\Gamma_n/\hbar(t + r/v_n)}, \quad r > b, \end{aligned} \tag{6.6.5}$$

that we call incoming decaying probability density, and of (6.6.2)

$$\begin{aligned} \rho^{decaying}_{outgoing}(r; z_n; t) = |u^{decaying}_{outgoing}(r; z_n; t)|^2 &= |\mathcal{J}_3|^2 e^{2\mathrm{Im}(k_n)r - \Gamma_n t/\hbar} \\ &= |\mathcal{J}_3|^2 e^{-\Gamma_n/\hbar(t - r/v_n)}, \quad r > b, \end{aligned} \tag{6.6.6}$$

that we call outgoing decaying probability density ($v_n = \Gamma_n/(2\hbar\mathrm{Im}(k_n))$). By imposing the purely outgoing boundary condition $\mathcal{J}_4 = 0$, we only allow (6.6.6) and forbid (6.6.5), which

we interpret by saying that we have a purely outgoing probability density condition for the decaying part of the resonance.

For the growing part of the resonance, the probability densities (before imposing $\mathcal{J}_4 = 0$) are the absolute value square of (6.6.3)

$$\begin{aligned} \rho^{growing}_{incoming}(r; z_n^*; t) = |u^{growing}_{incoming}(r; z_n^*; t)|^2 &= |\mathcal{J}_3|^2 e^{2\mathrm{Im}(k_n)r + \Gamma_n t/\hbar} \\ &= |\mathcal{J}_3|^2 e^{\Gamma_n/\hbar(t + r/v_n)}\,, \quad r > b\,, \end{aligned} \tag{6.6.7}$$

that we call the incoming growing probability density, and of (6.6.4)

$$\begin{aligned} \rho^{growing}_{outgoing}(r; z_n^*; t) = |u^{growing}_{outgoing}(r; z_n^*; t)|^2 &= |\mathcal{J}_4|^2 e^{-2\mathrm{Im}(k_n)r + \Gamma_n t/\hbar} \\ &= |\mathcal{J}_4|^2 e^{\Gamma_n/\hbar(t - r/v_n)}\,, \quad r > b\,, \end{aligned} \tag{6.6.8}$$

that we call the outgoing growing probability density. For this growing part, the condition $\mathcal{J}_4 = 0$ leads to the conclusion that in the growing stage of a resonance only waves with purely incoming probability density are allowed.

In short, the purely outgoing boundary condition (6.3.6d) must be read as *purely outgoing* (in phase or in probability density) only for the decaying part of the resonance and as *purely incoming* (in phase or in probability density) for the growing part of the resonance.

6.7 Exponential Decay Law of the Gamow Vectors

If we are dealing with a scattering system with resonances, the complex basis vector expansion allows us to isolate the contribution of each resonance. To illustrate this, we are going to see how the exponential decay law holds if only the contribution of a resonance is taken into account.

We want to determine the probability $\mathcal{P}_{\Delta r_0}(t)$ of detecting the decaying state within a shell of width Δr_0 outside the potential region ($r > b$). This is the probability that is measured by the counting rate of a detector placed, for example, outside a radioactive nucleus from which an α particle is emitted. We assume that the detector surrounds the nucleus completely and that is at a distance $r_0 > b$ from the center $r = 0$.

Theoretically, the probability $\mathcal{P}_{\Delta r_0}(t)$ to observe an in-state φ^+ at time t within the interval Δr_0 around the surface $r = r_0$ is given by

$$\mathcal{P}_{\Delta r_0}(t) = \int d\Omega \int_{\Delta r_0} r^2 dr |\langle r, \theta, \phi | \varphi^+(t) \rangle|^2\,. \tag{6.7.1}$$

Experimentally, the probability of finding the decaying state particle around r_0, that is, the counting rate of the detector, is not defined for all times t: a resonance must be first prepared before the system can decay. The time at which the preparation of the resonance is finished and at which the decay starts can be chosen arbitrarily (we choose it to be 0). For example, the α particle emitted by an α-unstable nucleus travels at speed $v = \Gamma_R/(2\hbar\mathrm{Im}(k))$ and reaches the point r_0 at the time $t(r_0) = r_0/v$. For times less than $t(r_0)$, the α particle

is not there yet, and therefore the counting rate measured by a detector placed at r_0 is zero for times $t < r_0/v$. Whatever would have been counted by the detector before the instant $t(r_0)$ at r_0 cannot be connected with the decaying state. Thus the theoretical probability to detect a resonance at r_0 should be zero for $t < r_0/v$. This is an instance of the time asymmetry built into a decaying process.

Experimentally as well, the decay of unstable systems usually follows the exponential law (cf. Refs. [44, 45, 46, 47]).

The Hilbert space cannot accommodate either the time asymmetry of $\mathcal{P}_{\Delta r_0}(t)$ [89] or the exponential decay law [90]. To account for these two features, we should use the Rigged Hilbert Space. In the RHS formulation, the Gamow vectors have an asymmetric time evolution given by a semigroup $e^{-iH^\times t/\hbar}$ (cf. Section 6.5 above), which accounts for the time asymmetry of a resonant process. The behavior of the semigroup evolution is in contrast to the time-symmetric Hilbert space time evolution, which is given by a group.

We are going to show that the exponential decay law holds if we consider only the resonance (Gamow vector) contribution to the probability (6.7.1). In Section 6.4, we used the Gamow vectors as basis vectors to expand the normalized in-state φ^+ in terms of the background and the resonance contribution (see Eq. (6.4.3)). In order to compute the n-th resonance contribution to the probability (6.7.1), we approximate φ^+ by the Gamow vector by neglecting the background term and the contribution of the rest of the resonances in (6.4.3),

$$\varphi^+(r,\theta,\phi) \simeq \psi_n^D(r,\theta,\phi) = \frac{u_n(r;z_n)}{r} Y_{0,0}(\theta,\phi)\,. \tag{6.7.2}$$

Thus the n-th resonance contribution to the probability is

$$\mathcal{P}_{\Delta r_0}(t) \simeq \int d\Omega \int_{\Delta r_0} r^2 dr |\langle r,\theta,\phi|\psi_n^D(t)\rangle|^2\,. \tag{6.7.3}$$

The time evolution of the n-th Gamow vector is given by

$$\psi_n^D(t) = e^{-iH^\times t/\hbar}\psi_n^D = e^{-i(E_n t - i\Gamma_n/2)t/\hbar}\psi_n^D\,, \tag{6.7.4}$$

and therefore

$$\langle r,\theta,\phi|\psi_n^D(t)\rangle = e^{-i(E_n - i\Gamma_n/2)t/\hbar}\,\frac{u_n(r;z_n)}{r} Y_{0,0}(\theta,\phi)\,. \tag{6.7.5}$$

Inserting (6.7.5) into (6.7.3) yields

$$\begin{aligned}
\mathcal{P}_{\Delta r_0}(t) &\simeq |e^{-\Gamma_n/(2\hbar)t}|^2 \int_{\Delta r_0} dr |u_n(r;z_n)|^2 \\
&= e^{-\Gamma_n t/\hbar} \int_{\Delta r_0} dr |2iN_n|^2 |e^{i(\mathrm{Re}(k_n) - i\mathrm{Im}(k_n))r}|^2 \\
&= e^{-\Gamma_n t/\hbar} |2N_n|^2 \int_{r_0}^{r_0+\Delta r_0} dr e^{2\mathrm{Im}(k_n)r} \\
&= e^{-\Gamma_n t/\hbar} |2N_n|^2 e^{2\mathrm{Im}(k_n)r_0}\,\frac{e^{2\mathrm{Im}(k_n)\Delta r_0} - 1}{2\mathrm{Im}(k_n)}
\end{aligned}$$

$$\begin{aligned} &\simeq \quad e^{-\Gamma_n t/\hbar}|2N_n|^2 e^{2\mathrm{Im}(k_n)r_0}\,\Delta r_0\,, \\ &= \quad |2N_n|^2 \Delta r_0\, e^{-\Gamma_n/\hbar\,(t-r_0/v_n)}\,, \quad t > r_0/v_n\,, \end{aligned} \tag{6.7.6}$$

where we have used the approximation Δr_0 small in the next to the last step. Therefore,

$$\mathcal{P}_{\Delta r_0}(t) \simeq |2N_n|^2 \Delta r_0 e^{-\Gamma_n/\hbar\,(t-r_0/v_n)}\,, \qquad t > r_0/v_n\,. \tag{6.7.7}$$

Equation (6.7.7) represents the n-th resonance contribution to the counting rate measured by a detector placed at r_0. This counting rate reaches its maximum at $t = r_0/v_n$, and decreases exponentially as time goes on. Therefore, the n-th Gamow vector (resonance) contribution to the probability $\mathcal{P}_{\Delta r_0}(t)$ follows the exponential decay law.

6.8 Conclusion to Chapter 6

In this chapter, we have constructed the Gamow vectors of the square barrier potential resonances, and studied their properties. We have defined a decaying Gamow vector $|z_n^-\rangle$ as the solution of the integral equation (6.3.1), whereas a growing Gamow vector $|z_n^{*+}\rangle$ has been defined as the solution of (6.3.3). We have seen that in the radial representation the Gamow eigenfunction $\langle r|z_n^-\rangle$ satisfies the Schrödinger equation subject to a *purely outgoing* boundary condition, whereas the growing Gamow eigenfunction $\langle r|z_n^{*+}\rangle$ satisfies a *purely incoming* boundary condition. We have also seen that the purely outgoing boundary condition produces the same resonance spectrum as the S-matrix spectrum of Figure 6.2. The $[0,\infty)$-energy representation of the eigenfunction $\langle r|z_n^-\rangle$ has been shown to be the complex delta function multiplied by a normalization factor $A_n\delta(E-z_n)$. The $(-\infty,\infty)$-energy representation of the eigenfunction $\langle r|z_n^-\rangle$ has been shown to be the Breit-Wigner amplitude multiplied by a normalization factor $-1/(2\pi i)\,A_n/(E-z_n)$.

The time evolution of the Gamow kets has been shown to be governed by a semigroup, expressing the time asymmetry built into a resonance.

The Gamow vectors have been used as basis vectors in the complex basis vector expansions (6.4.3) and (6.4.4). However, they do not form a complete basis, and therefore a continuous set of Dirac kets was added to complete them. The expansions (6.4.3) and (6.4.4) extract the resonance contribution out of the in- and out-states, respectively.

We have uncovered the time asymmetry that arises from the purely outgoing boundary condition. We have seen that the purely outgoing boundary condition should read as *purely outgoing* only for the decaying part of the resonance, and as *purely incoming* for the growing part of the resonance.

The exponential law has been shown to hold if the background term of the complex basis vector expansion is neglected—only the resonance (Gamow vector) contribution to the probability is taken into consideration.

6.9 Appendix 9: Figures

In this Appendix, we show the graphics of the square barrier potential resonance poles, both in the momentum and energy complex planes. We also show the contours that where used to obtain the complex basis vector expansion.

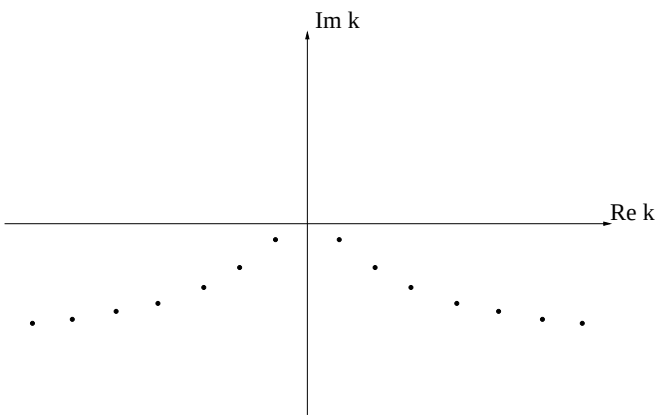

Figure 6.1: The resonance momenta of the square barrier potential.

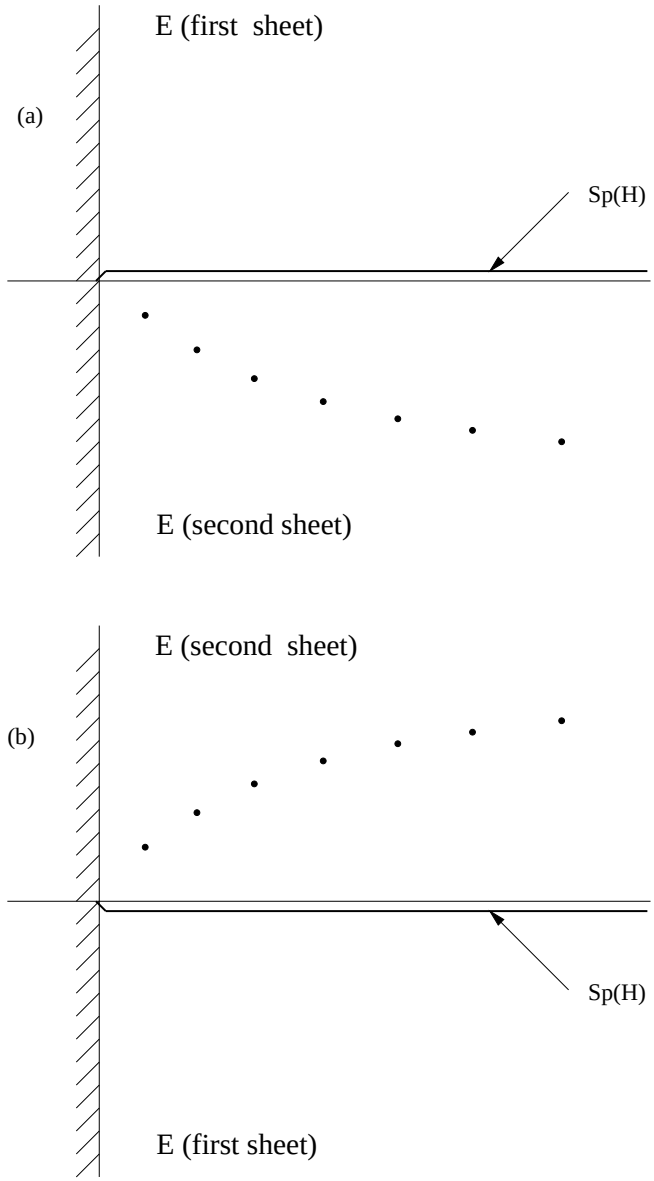

Figure 6.2: The resonance energies of the square barrier potential.

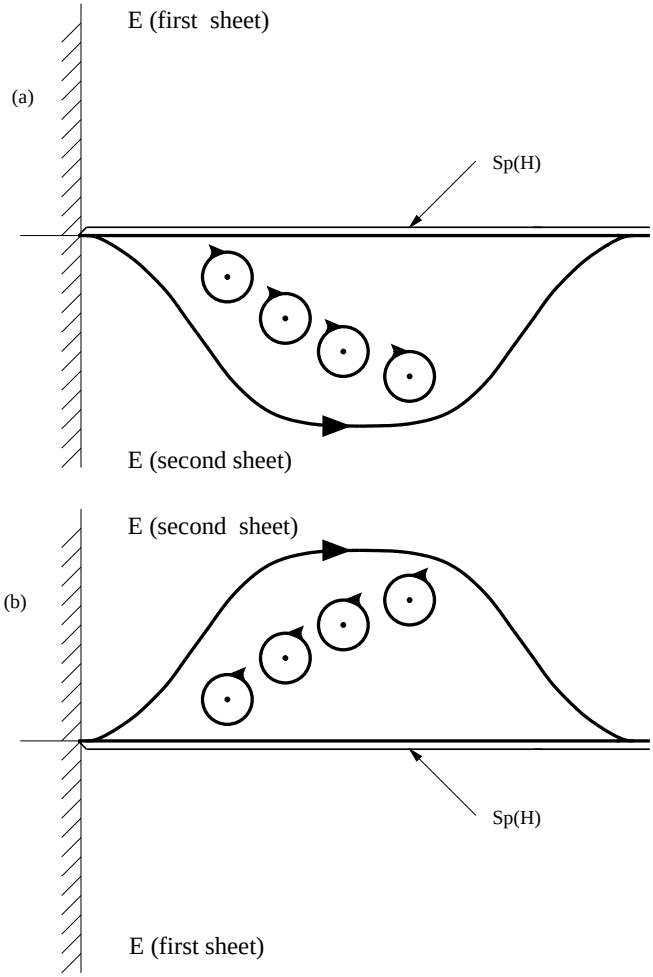

Figure 6.3: Deformation of the path of integration into the second sheet of the energy Riemann surface; (a) for the decaying states and (b) for the growing states.

Chapter 7

The Time Reversal Operator in the Rigged Hilbert Space

In this chapter, we study the behavior of resonances under the time reversal operation. We shall study the standard time reversal operator and also a non-standard one, which yields a doubling of the RHS.

VLADIMIR: We've nothing more to do here.

ESTRAGON: Nor anywhere else.

VLADIMIR: Ah Gogo, don't go like that.
To-morrow everything will be better.

ESTRAGON: How do you make that out?

VLADIMIR: Did you not hear what the child said?

ESTRAGON: No.

VLADIMIR: He said that Godot was sure to come
to-morrow. (*Pause*). What do you say to that?

ESTAGRON: Then all we have to do is to wait here.

Samuel Beckett, *Waiting for Godot*

7.1 Introduction

In the previous chapter, we have seen that the time evolution of the Gamow vectors is given by a semigroup and therefore is time asymmetric. We now want to discuss how this time asymmetry behaves under the action of the time reversal operator in the nonrelativistic domain [59]. We shall forget about our beloved square barrier potential and work with a "general" potential.

We have seen in the previous two chapters that a scattering process should be described by two RHSs. One RHS corresponds to the states φ^+,

$$\mathbf{\Phi}_- \subset \mathcal{H}_{\rm ac} \subset \mathbf{\Phi}_-^\times \,, \tag{7.1.1}$$

whereas the other RHS corresponds to the observables ψ^-,

$$\mathbf{\Phi}_+ \subset \mathcal{H}_{\rm ac} \subset \mathbf{\Phi}_+^\times \,. \tag{7.1.2}$$

In both RHSs, the space $\mathcal{H}_{\rm ac}$ represents the Hilbert space of scattering states of the total Hamiltonian H ("ac" stands for absolutely continuous). On $\mathcal{H}_{\rm ac}$, H has absolutely continuous spectrum only. We shall assume that this spectrum coincides with the positive real line.

Suppose the S-matrix has a pair of simple poles at $z_R = E_R - i\Gamma_R/2$ and at $z_R^* = E_R + i\Gamma_R/2$, and denote their corresponding Gamow vectors as $|z_R^-\rangle$ and $|z_R^{*\,+}\rangle$. These Gamow vectors have the following properties:

i.) The Gamow vectors are functionals,

$$|z_R^-\rangle \in \mathbf{\Phi}_+^\times \,, \tag{7.1.3a}$$
$$|z_R^{*\,+}\rangle \in \mathbf{\Phi}_-^\times \,. \tag{7.1.3b}$$

ii.) They are generalized eigenvectors of the total Hamiltonian H,

$$H^\times |z_R^-\rangle = z_R |z_R^-\rangle \,, \tag{7.1.4a}$$
$$H^\times |z_R^{*\,+}\rangle = z_R^* |z_R^{*\,+}\rangle \,. \tag{7.1.4b}$$

iii.) The time evolution operator e^{-iHt} can be continuously extended to $\mathbf{\Phi}_+^\times$ for *positive* values of time and to $\mathbf{\Phi}_-^\times$ for *negative* values of time. The continuity of the extensions refers to the weak topology [93]. In addition we have:

$$e^{-iH^\times t}|z_R^-\rangle = e^{-iz_R t}|z_R^-\rangle = e^{-iE_R t}e^{-\Gamma_R t/2}|z_R^-\rangle \,, \quad \text{for } t > 0 \,, \tag{7.1.5a}$$
$$e^{-iH^\times t}|z_R^{*\,+}\rangle = e^{-iz_R^* t}|z_R^{*\,+}\rangle = e^{-iE_R t}e^{\Gamma_R t/2}|z_R^{*\,+}\rangle \,, \quad \text{for } t < 0 \,. \tag{7.1.5b}$$

The action of $e^{-iH^\times t}$ on $|z_R^-\rangle$ for $t < 0$ and on $|z_R^{*\,+}\rangle$ for $t > 0$ is, however, not defined. Thus the Hilbert space group evolution splits into two semigroups. This splitting is a consequence of the choice of $\mathbf{\Phi}_\pm$ and the properties of Hardy functions. The choice of Hardy functions is related to a causality condition, and therefore the splitting is also related to causality. The

splitting of the group of evolution into two semigroups shows the *irreversible* character of a resonance [52, 54, 55].

In his study of the representations of the Poincaré group extended by time reversal and parity, Wigner found four different possibilities (cf. Table I of Appendix 7.4 and Refs. [61, 62]). The first possibility is the standard one, but the other three imply a doubling of the space that supports the representation. J. F. Cariñena and M. Santander constructed the projective representations of the Galilei group extended by time inversion and parity [63]. They also found four possibilities for the case with mass. As for the Poicaré group, the standard case does not yield a doubling of the space that supports the representation, while the other three do yield a doubling. Bohm [64] has studied the latter time reversal ($\epsilon_T = \epsilon_I = -1$) in the relativistic case, which yields a doubling. One of our goals is to construct an analog to this doubling in the non-relativistic case for s-waves ($j = 0$).

In the next section, we discuss the effect of the time reversal operator on Gamow vectors in the standard case. This standard case is labeled by $\epsilon_T = \epsilon_I = 1$ (see Table I of Appendix 7.4). In Section 7.3, we study the the case $\epsilon_T = \epsilon_I = -1$ (see Table I of Appendix 7.4) and present the idea of *time reversal doubling*. In Appendix 7.4, we review some general aspects of the time reversal operation.

7.2 The Standard Time Reversal Operator ($\epsilon_T = \epsilon_I = 1$)

In this section, we present the effect of the standard time reversal operation on scattering systems having (simple pole) resonances. The notation we are using here does not differ essentially from that in Ref. [59], although there is a couple of differences:

i.) The restriction to the positive real semiaxis of intersections of Hardy spaces with the Schwartz space are denoted here by

$$\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \ . \tag{7.2.1}$$

The plus sign stands for Hardy functions on the upper half plane and the minus sign for Hardy functions on the lower half plane. $\mathcal{S}$ is the Schwartz space on the real line.

ii.) The extension of the evolution operator e^{-iHt} to the space $\mathbf{\Phi}^\times_+$ is denoted as $\mathcal{U}^\times_+(t)$ for $t > 0$, and the extension of e^{-iHt} to $\mathbf{\Phi}^\times_-$ is denoted as $\mathcal{U}^\times_-(t)$ for $t < 0$. These are the two semigroups discussed in the introduction.

For simplicity, we shall work with a spherically symmetric potential and consider particles without spin or any other possible degrees of freedom. We restrict ourselves to zero values of the angular momentum, and denote the corresponding Hilbert space by $\mathcal{H}_0$. If the system does not have bound states, the space $\mathcal{H}_0$ coincide with $\mathcal{H}_{\rm ac}$.

Let us recall that the unitary operators $U_\pm$ diagonalize the total Hamiltonian H (or its restriction to its absolutely continuous space $\mathcal{H}_{\rm ac}$, if H has bound states), in the sense that these operators give a unitary equivalence between H and the multiplication operator on $L^2(\mathbb{R}^+, dE)$. They are a product of the inverses of the Møller operators times the operator U_0 that diagonalizes the free Hamiltonian, $U_\pm = U_0 \Omega^\dagger_\pm$.

For s waves ($j = 0$), the standard choice of the time reversal operation is $\epsilon_T = \epsilon_I = 1$ (see Table I of Appendix 7.4). Therefore, in the energy representation the time reversal operator A_T acts as the complex conjugation C. Since the mapping C transforms any function of E into its complex conjugate, we have

$$C : \mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \longmapsto \mathcal{H}^2_\mp \cap \mathcal{S}\big|_{\mathbb{R}^+} \ . \tag{7.2.2}$$

Moreover, one can show that this map is continuous.

Our next goal is to define time reversal operators $A_{T\pm}$ on $\mathbf{\Phi}_\pm$. These operators should be equivalent to C and the equivalence should be given by $U_\pm$. Their definition is:

$$A_{T\pm} := U^\dagger_\pm \, C \, U_\mp \, . \tag{7.2.3}$$

This definition makes the following diagram:

$$\begin{array}{ccc} \mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} & \xrightarrow{C} & \mathcal{H}^2_\mp \cap \mathcal{S}\big|_{\mathbb{R}^+} \\ U^\dagger_\mp \downarrow & & \downarrow U^\dagger_\pm \\ \mathbf{\Phi}_\pm & \xrightarrow[A_{T\pm}]{} & \mathbf{\Phi}_\mp \end{array} \tag{7.2.4}$$

These operators have the following properties:

1. $A_{T\pm}$ are continuous antilinear mappings from $\mathbf{\Phi}_\pm$ onto $\mathbf{\Phi}_\mp$.
2. They can be extended to (continuous) antiunitary mappings from $\mathcal{H}_{\rm ac}$ onto itself.
3. Their adjoints are given by

$$A^\dagger_{T\pm} = \Big[U^\dagger_\pm \, C \, U_\mp\Big]^\dagger = U^\dagger_\mp \, C \, U_\pm = A_{T\mp} \, ; \tag{7.2.5}$$

   that is, they are adjoint to each other.

4. They are inverse to each other,

$$A_{T+}A_{T-} = U^\dagger_+ C U_- U^\dagger_- C U_+ = I \, , \quad \text{on } \mathbf{\Phi}_- \, , \tag{7.2.6}$$
$$A_{T-}A_{T+} = U^\dagger_- C U_+ U^\dagger_+ C U_- = I \, , \quad \text{on } \mathbf{\Phi}_+ \, . \tag{7.2.7}$$

Consider now a densely defined continuous antilinear operator A on $\mathcal{H}$ with the following property: there are two RHSs $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times$ and $\mathbf{\Psi} \subset \mathcal{H} \subset \mathbf{\Psi}^\times$ such that $A^\dagger$ maps continuously $\mathbf{\Phi}$ into $\mathbf{\Psi}$. Then, A can be extended by continuity to $\mathbf{\Phi}^\times$ using the following formula:

$$\langle \psi | A^\times F \rangle := \overline{\langle A^\dagger \psi | F \rangle} = \langle F | A^\dagger \psi \rangle \, , \quad \forall F \in \mathbf{\Phi}^\times \, , \ \forall \psi \in \mathbf{\Psi} \, . \tag{7.2.8}$$

Thus $A^\times$ is a weak continuous antilinear mapping from $\mathbf{\Phi}^\times$ into $\mathbf{\Psi}^\times$. The proof of this goes exactly as the proof for the linear case [93].

It is straightforward to apply this definition to the time reversal operator, after making the identification $\mathbf{\Phi} = \mathbf{\Phi}_\pm$, $\mathbf{\Psi} = \mathbf{\Phi}_\mp$, $A = A_{T\pm}$, and $A^\dagger = A_{T\mp}$. Thus, we have the following continuous antilinear extensions:

$$A^\times_{T\pm} : \mathbf{\Phi}^\times_\pm \longmapsto \mathbf{\Phi}^\times_\mp \,. \tag{7.2.9}$$

These extensions are one-to-one, onto mappings with continuous inverses, and they indeed extend $A_{T\pm}$ as originally defined in (7.2.3).

We now obtain the images of Lippmann-Schwinger kets and of the Gamow vectors by $A^\times_{T\pm}$. To this end, let us consider two arbitrary vectors $\varphi^\mp \in \mathbf{\Phi}_\pm$.[1] Their wave functions in the energy representation are given by

$$\widehat{\varphi}^\pm(E) = \langle {}^\pm E|\varphi^\pm\rangle = (U_\pm\varphi^\pm)(E) \in \mathcal{H}^2_\mp \cap \mathcal{S}\big|_{\mathbb{R}^+} \,. \tag{7.2.10}$$

Using the definition of $A_{T\pm}$ we obtain

$$\langle\varphi^\pm|A^\times_{T\pm}|E^\mp\rangle = \langle {}^\mp E|A^\dagger_{T\pm}\varphi^\pm\rangle = C\widehat{\varphi}^\pm(E) = \overline{\widehat{\varphi}^\pm(E)} = \langle\varphi^\pm|E^\pm\rangle\,; \tag{7.2.11}$$

that is,

$$A^\times_{T\pm}|E^\mp\rangle = |E^\pm\rangle\,. \tag{7.2.12}$$

Take now the Gamow vectors $|z_R^-\rangle$ and $|z_R^{*}{}^+\rangle$. Then

$$\langle\varphi^+|A^\times_{T+}|z_R^-\rangle = \langle {}^-z_R|A^\dagger_{T+}\varphi^+\rangle = C\widehat{\varphi}^+(z_R) = \overline{\widehat{\varphi}^+(z_R)} = \langle\varphi^+|z_R^{*+}\rangle\,; \tag{7.2.13}$$

that is,

$$A^\times_{T+}|z_R^-\rangle = |z_R^{*}{}^+\rangle\,. \tag{7.2.14}$$

Analogously

$$A^\times_{T-}|z_R^{*}{}^+\rangle = |z_R^-\rangle\,. \tag{7.2.15}$$

Next, we study the action of the standard time reversal operator on the time evolution semigroups. We know that $e^{iHt}\mathbf{\Phi}_+ \subset \mathbf{\Phi}_+$ if $t > 0$. Then,

$$\begin{aligned} A_{T+}e^{iHt}A_{T-}\varphi^+ &= U_+^\dagger C U_- e^{iHt} U_-^\dagger C U_+\varphi^+ \\ &= U_+^\dagger C e^{itE} C U_+\varphi^+ \\ &= U_+^\dagger e^{-itE} U_+\varphi^+ \\ &= e^{i(-t)H}\varphi^+\,, \quad \varphi^+ \in \mathbf{\Phi}_-\,,\ t > 0\,. \end{aligned} \tag{7.2.16}$$

Analogously, if $t < 0$, we have that $e^{iHt}\mathbf{\Phi}_- \subset \mathbf{\Phi}_-$. Then

$$A_{T-}e^{iHt}A_{T+}\varphi^- = e^{i(-t)H}\varphi^-\,, \quad \varphi^- \in \mathbf{\Phi}_+\,,\ t < 0\,. \tag{7.2.17}$$

Therefore,

$$A_{T+}\mathcal{U}_+^\dagger(t)A_{T-} = \mathcal{U}_-^\dagger(-t)\,, \quad t > 0\,, \tag{7.2.18a}$$

$$A_{T-}\mathcal{U}_-^\dagger(t)A_{T+} = \mathcal{U}_+^\dagger(-t)\,, \quad t < 0\,. \tag{7.2.18b}$$

[1] In this chapter, we shall denote the observables ψ^- by φ^- in order not to repeat the formulas twice.

We see that the operators $A_{T\pm}$ transform one semigroup into the other. The extension of these formulas to the dual spaces yields

$$A^{\times}_{T+}\mathcal{U}^{\times}_{+}(t)A^{\times}_{T-} = \mathcal{U}^{\times}_{-}(-t)\,, \quad t > 0\,, \tag{7.2.19a}$$
$$A^{\times}_{T-}\mathcal{U}^{\times}_{-}(t)A^{\times}_{T+} = \mathcal{U}^{\times}_{+}(-t)\,, \quad t < 0\,. \tag{7.2.19b}$$

One could expect that the operators $A_{T\pm}$ are the same operator restricted to different subdomains. That is true. As a matter of fact, their extensions to $\mathcal{H}_{\rm ac}$ coincide:

The proof of this statement is rather simple. Write

$$A^2_{T+} = U^{\dagger}_{+}CU_{-}U^{\dagger}_{+}CU_{-}\,. \tag{7.2.20}$$

Since $U_{\pm} = U_0\Omega^{\dagger}_{\pm}$, one has

$$A^2_{T+} = \Omega_{+}U^{\dagger}_0CU_0\Omega^{\dagger}_{-}\Omega_{+}U^{\dagger}_0CU_0\Omega^{\dagger}_{-}\,. \tag{7.2.21}$$

The S operator is given by

$$S = \Omega^{\dagger}_{-}\Omega_{+}\,, \tag{7.2.22}$$

and its adjoint is given by

$$S^{\dagger} = \Omega^{\dagger}_{+}\Omega_{-}\,. \tag{7.2.23}$$

Since

$$U_0SU_0^{-1} = U_0SU_0^{\dagger} = S(E) \quad (= S(E+i0)\,, \quad E > 0)\,, \tag{7.2.24}$$

we have that

$$U_0S^{\dagger}U_0^{\dagger} = (U_0SU_0^{\dagger})^{\dagger} = \overline{S(E)}\,. \tag{7.2.25}$$

Plugging Eqs. (7.2.22)-(7.2.25) into (7.2.21) we obtain

$$\begin{aligned} A^2_{T+} &= \Omega_{+}U^{\dagger}_0CU_0SU^{\dagger}_0CU_0\Omega^{\dagger}_{-} \\ &= \Omega_{+}U^{\dagger}_0CS(E)CU_0\Omega^{\dagger}_{-} \\ &= \Omega_{+}U^{\dagger}_0\overline{S(E)}U_0\Omega^{\dagger}_{-} \\ &= \Omega_{+}S^{\dagger}\Omega^{\dagger}_{-} \\ &= \Omega_{+}\Omega^{\dagger}_{+}\Omega_{-}\Omega^{\dagger}_{-} \\ &= I\,, \end{aligned} \tag{7.2.26}$$

where I is the identity on $\mathcal{H}_{\rm ac}$. The same is true for A_{T-}. Therefore A_{T+} is an invertible bounded operator such that $A_{T+} = A^{-1}_{T+}$ on $\mathcal{H}_{\rm ac}$. Since A^{-1}_{T+} and A_{T-} coincide on the dense subspace $\mathbf{\Phi}_{-}$, they are equal on $\mathcal{H}_0$, and we have that $A_{T-} = A^{-1}_{T+} = A_{T+}$.

7.3 The Time Reversal Doubling ($\epsilon_T = \epsilon_I = -1$)

In this section, we present the construction of the time reversal doubling. According to Wigner [61, 62], there are three other possible representations of the Poincaré group extended by time reversal and parity besides the (standard) one of the previous section. All four possibilities are listed in Table I of Appendix 7.4.

Let us consider the following pair of RHSs:

$$\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \otimes \mathbb{C}^2 \subset L^2(\mathbb{R}^+) \otimes \mathbb{C}^2 \subset \left(\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+}\right)^\times \otimes \mathbb{C}^2 \,, \tag{7.3.1}$$

where $\mathbb{C}^2$ denotes the two-dimensional linear space of column vectors whose entries are complex numbers. The elements of each space of the triplet (7.3.1) can be expressed as two-dimensional vectors whose entries belong to the space in the left hand side of the tensor product. In the case $\epsilon_T = \epsilon_I = -1$, the time reversal operator in the energy representation is defined by (cf. Table I of Appendix 7.4)

$$\mathcal{C} := \begin{pmatrix} 0 & C \\ -C & 0 \end{pmatrix} , \tag{7.3.2}$$

where C denotes the complex conjugation. This operator is antilinear and continuous from $\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \otimes \mathbb{C}^2$ onto $\mathcal{H}^2_\mp \cap \mathcal{S}\big|_{\mathbb{R}^+} \otimes \mathbb{C}^2$. By duality, it can be extended to a continuous antilinear mapping $\mathcal{C}^\times$ from $\left(\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+}\right)^\times \otimes \mathbb{C}^2$ onto $\left(\mathcal{H}^2_\mp \cap \mathcal{S}\big|_{\mathbb{R}^+}\right)^\times \otimes \mathbb{C}^2$.

Each space $\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \otimes \mathbb{C}^2$ has two distinguished subspaces,

$$\Sigma^+_\pm = \mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \otimes \begin{pmatrix} \alpha \\ 0 \end{pmatrix} , \tag{7.3.3a}$$

$$\Sigma^-_\pm = \mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+} \otimes \begin{pmatrix} 0 \\ \beta \end{pmatrix} , \tag{7.3.3b}$$

where α and β are arbitrary complex numbers. We have, therefore, two new RHSs that can be written in the following form:

$$\Sigma^\pm_\pm \subset L^{2\pm}(\mathbb{R}^+) \subset (\Sigma^\pm_\pm)^\times \,, \tag{7.3.4}$$

where

$$L^{2+}(\mathbb{R}^+) = L^2(\mathbb{R}^+) \otimes \begin{pmatrix} \alpha \\ 0 \end{pmatrix} , \tag{7.3.5a}$$

$$L^{2-}(\mathbb{R}^+) = L^2(\mathbb{R}^+) \otimes \begin{pmatrix} 0 \\ \beta \end{pmatrix} . \tag{7.3.5b}$$

The dual of the spaces (7.3.3) can be written as

$$(\Sigma^+_\pm)^\times = \left(\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+}\right)^\times \otimes \begin{pmatrix} \alpha \\ 0 \end{pmatrix} , \tag{7.3.6a}$$

$$(\Sigma^-_\pm)^\times = \left(\mathcal{H}^2_\pm \cap \mathcal{S}\big|_{\mathbb{R}^+}\right)^\times \otimes \begin{pmatrix} 0 \\ \beta \end{pmatrix} . \tag{7.3.6b}$$

It is not difficult to show that $\mathcal{C}$ is a continuous antilinear bijection from $\Sigma^{\pm}_{\pm}$ onto $\Sigma^{\mp}_{\mp}$,

$$\mathcal{C}\Sigma^{\pm}_{\pm} = \Sigma^{\mp}_{\mp} \,. \tag{7.3.7}$$

Thus $\mathcal{C}$ can be continuously extended to the dual spaces,

$$\mathcal{C}^{\times}(\Sigma^{\pm}_{\pm})^{\times} = (\Sigma^{\mp}_{\mp})^{\times} \,. \tag{7.3.8}$$

As an operator on $\mathcal{H}_{\rm ac} \otimes \mathbb{C}^2$, the square of $\mathcal{C}$ is proportional to the identity,

$$\mathcal{C}^2 = -\mathbb{I} = \epsilon_T \mathbb{I} \,, \tag{7.3.9}$$

where $\mathbb{I}$ represents the identity on $\mathcal{H}_{\rm ac} \otimes \mathbb{C}^2$.

In order to clarify the notation, we replace the superscript signs by r, with $r = +, -$. That is, we shall write $\Sigma^{r}_{\pm}$, and so on. This notation makes it clear that the signs above are independent of the signs below.

Let us define the operators

$$\mathfrak{U}_{\pm} := U_{\pm} \otimes I \,, \tag{7.3.10}$$

where I is the identity on $\mathbb{C}^2$. We can write these operators as

$$\mathfrak{U}_{\pm} = \begin{pmatrix} U_{\pm} & 0 \\ 0 & U_{\pm} \end{pmatrix} , \tag{7.3.11}$$

and their adjoints as

$$\mathfrak{U}^{\dagger}_{\pm} = \mathfrak{U}^{-1}_{\pm} = \begin{pmatrix} U^{\dagger}_{\pm} & 0 \\ 0 & U^{\dagger}_{\pm} \end{pmatrix} . \tag{7.3.12}$$

It is clear that $\mathfrak{U}_{\pm}$ maps $\mathcal{H}_{\rm ac} \otimes \mathbb{C}^2$ onto $L^2(\mathbb{R}^+) \otimes \mathbb{C}^2$. Using those operators, we can define the following spaces:

$$\mathbf{\Phi}^{r}_{\pm} := \mathfrak{U}^{\dagger}_{\mp}\, \Sigma^{r}_{\pm} \,. \tag{7.3.13}$$

Clearly, the spaces $\mathbf{\Phi}^{r}_{\pm}$ are subspaces of $\mathcal{H}_{\rm ac} \otimes \mathbb{C}^2$. It is obvious that

$$\mathbf{\Phi}^{r=+}_{\pm} = \mathbf{\Phi}_{\pm} \otimes \begin{pmatrix} \alpha \\ 0 \end{pmatrix} , \tag{7.3.14a}$$

$$\mathbf{\Phi}^{r=-}_{\pm} = \mathbf{\Phi}_{\pm} \otimes \begin{pmatrix} 0 \\ \beta \end{pmatrix} . \tag{7.3.14b}$$

The operators $\mathfrak{U}_{\pm}$ and their respective inverses $\mathfrak{U}^{\dagger}_{\pm}$ can be continuously extended to the dual spaces.

We are now in a position to introduce the time reversal operators for our $\epsilon_T = \epsilon_I = -1$ choice. They can be defined as

$$\mathcal{A}_{T\pm} := \pm\mathfrak{U}^{\dagger}_{\pm}\mathcal{C}\mathfrak{U}_{\mp} \,. \tag{7.3.15}$$

These two operators have similar properties to those satisfied by $A_{T\pm}$. We list here these properties without proofs, since these proofs do not differ much from those for $A_{T\pm}$:

1. $\mathcal{A}_{T\pm}$ are continuous antilinear mappings from $\mathbf{\Phi}^r_\pm$ onto $\mathbf{\Phi}^{-r}_\mp$, respectively. They can be continuously extended to antilinear mappings between the respective duals.

2. They are adjoint to each other,
$$\mathcal{A}^\dagger_{T\pm} = \mathcal{A}_{T\mp}\,. \tag{7.3.16}$$

3. As operators on $\mathcal{H}_{\rm ac}\otimes\mathbb{C}^2$, they are antiunitary. In addition, they are inverse to each other,
$$\mathcal{A}_{T+}\mathcal{A}_{T-} = \mathbb{I}\,, \tag{7.3.17a}$$
$$\mathcal{A}_{T-}\mathcal{A}_{T+} = \mathbb{I}\,. \tag{7.3.17b}$$

4. On the Hilbert space $\mathcal{H}_{\rm ac}\otimes\mathbb{C}^2$, we have that
$$\mathcal{A}^2_{T\pm} = -\mathbb{I} \implies \mathcal{A}_{T-}\mathcal{A}_{T+}\mathcal{A}_{T+} = -\mathcal{A}_{T-} \implies \mathcal{A}_{T+} = -\mathcal{A}_{T-}\,. \tag{7.3.18}$$

Formulas (7.3.16)-(7.3.18) are a consequence of the definition chosen in (7.3.15) for $\mathcal{A}_{T-}$ (with minus sign), which has its origin in the fact that $\mathcal{C}^\dagger = -\mathcal{C}$. If we redefined $\mathcal{A}_{T-}$ without the minus sign in (7.3.15), we would have

$$\mathcal{A}^\dagger_{T\pm} = -\mathcal{A}_{T\mp}\,, \tag{7.3.19a}$$
$$\mathcal{A}_{T+}\mathcal{A}_{T-} = -\mathbb{I}\,, \tag{7.3.19b}$$
$$\mathcal{A}_{T-}\mathcal{A}_{T+} = -\mathbb{I}\,, \tag{7.3.19c}$$
$$\mathcal{A}_{T+} = \mathcal{A}_{T-}\,. \tag{7.3.19d}$$

We can choose either (7.3.16)-(7.3.18) or (7.3.19). The choice (7.3.19) has the advantage of having a unique time reversal operator, and the distinction between $\mathcal{A}_{T+}$ and $\mathcal{A}_{T-}$ indicates the restriction of a unique time reversal operator to different subspaces $\mathbf{\Phi}^r_\pm$. As we shall see later, this choice has the disadvantage of leading to the appearance of a minus sign in the formulas of the action of the time reversal operator on the semigroups.

The importance of the above construction lies on the possibility of extending the time reversal operator to the dual spaces, which contain the Lippmann-Schwinger kets and the Gamow vectors.

We define the Lippmann-Schwinger kets in the $\epsilon_T = \epsilon_I = -1$ case as

$$|E^\pm; r=+\rangle = \begin{pmatrix} |E^\pm\rangle \\ 0 \end{pmatrix} \in (\mathbf{\Phi}^{r=+}_\mp)^\times\,, \tag{7.3.20a}$$
$$|E^\pm; r=-\rangle = \begin{pmatrix} 0 \\ |E^\pm\rangle \end{pmatrix} \in (\mathbf{\Phi}^{r=-}_\mp)^\times\,. \tag{7.3.20b}$$

The kets in Eqs. (7.3.20) are generalized eigenvectors of the operator $H\otimes I$ (H is the exact Hamiltonian, and I is the identity on $\mathbb{C}^2$) with generalized eigenvalue $E>0$. We now

determine the action of $\mathcal{A}_{T\pm}$ on those eigenkets. We start with the following definition, which has its origin in (7.2.8):

$$\langle \Xi^{\pm} | \mathcal{A}^{\times}_{T\pm} | E^{\mp}; r \rangle = \langle {}^{\mp}E; r | \mathcal{A}^{\dagger}_{T\pm} \Xi^{\pm} \rangle \,, \quad \Xi^{\pm} \in \mathbf{\Phi}^{r}_{\mp} \,. \tag{7.3.21}$$

From (7.3.15) we obtain

$$\mathcal{A}_{T\pm} = \pm \begin{pmatrix} 0 & A_{T\pm} \\ -A_{T\pm} & 0 \end{pmatrix} . \tag{7.3.22}$$

Let us write

$$\Xi^{\pm} = \begin{pmatrix} \varphi^{\pm} \\ \psi^{\pm} \end{pmatrix} , \tag{7.3.23}$$

where $\varphi^{\pm}$, $\psi^{\pm} \in \mathbf{\Phi}_{\mp}$. We shall study separately the cases $r = \pm$. Take first $r = +$. Then

$$\begin{aligned} \langle {}^{\mp}E; r = + | \mathcal{A}^{\dagger}_{T\pm} \Xi^{\pm} \rangle &= \pm (\langle {}^{\mp}E|, 0) \begin{pmatrix} A^{\dagger}_{T\pm} \psi^{\pm} \\ -A^{\dagger}_{T\pm} \varphi^{\pm} \end{pmatrix} \\ &= \pm \langle {}^{\mp}E | A^{\dagger}_{T\pm} \psi^{\pm} \rangle \\ &= \pm \langle \psi^{\pm} | A^{\times}_{T\pm} | E^{\mp} \rangle \\ &= \pm \langle \psi^{\pm} | E^{\pm} \rangle \\ &= \pm (\varphi^{\pm}, \psi^{\pm}) \begin{pmatrix} 0 \\ |E^{\pm}\rangle \end{pmatrix} \\ &= \pm \langle \Xi^{\pm} | E^{\pm}; r = - \rangle \,. \end{aligned} \tag{7.3.24}$$

This and Eq. (7.3.21) yield

$$\mathcal{A}^{\times}_{T\pm} | E^{\mp}; r = + \rangle = \pm | E^{\pm}; r = - \rangle \,. \tag{7.3.25}$$

The $\pm$ signs appear as the coefficient of $|E^{\pm}; r = -\rangle$ in Eq. (7.3.25) only if we make the choice $\mathcal{A}_{T-} = -\mathfrak{U}^{\dagger}_{-} \mathcal{C} \mathfrak{U}_{+}$. The choice $\mathcal{A}_{T-} = \mathfrak{U}^{\dagger}_{-} \mathcal{C} \mathfrak{U}_{+}$ replaces the $\pm$ signs in (7.3.25) by plus. Now take $r = -$. An analogous calculation to (7.3.24) yields

$$\mathcal{A}^{\times}_{T\pm} | E^{\mp}; r = - \rangle = \mp | E^{\pm}; r = + \rangle \,, \tag{7.3.26}$$

where the $\mp$ signs have the same origin as in the case $r = +$. The choice $\mathcal{A}_{T-} = \mathfrak{U}^{\dagger}_{-} \mathcal{C} \mathfrak{U}_{+}$ replaces them by minus.

The next step is to define the Gamow vectors and to obtain their images under time reversal. The Gamow vectors $|z^{-}_{R}\rangle$ and $|z^{*+}_{R}\rangle$ can be used to define the following Gamow vectors for our $\epsilon_T = \epsilon_I = -1$ case:

$$|z^{-}_{R}; r = + \rangle := \begin{pmatrix} |z^{-}_{R}\rangle \\ 0 \end{pmatrix} , \tag{7.3.27a}$$

$$|z^{-}_{R}; r = - \rangle := \begin{pmatrix} 0 \\ |z^{-}_{R}\rangle \end{pmatrix} , \tag{7.3.27b}$$

$$|z^{*+}_{R}; r = + \rangle := \begin{pmatrix} |z^{*+}_{R}\rangle \\ 0 \end{pmatrix} , \tag{7.3.27c}$$

$$|z^{*+}_{R}; r = - \rangle := \begin{pmatrix} 0 \\ |z^{*+}_{R}\rangle \end{pmatrix} . \tag{7.3.27d}$$

The Gamow vectors (7.3.27a) and (7.3.27b) are generalized eigenvectors of the operator $H \otimes I$ with generalized eigenvalue z_R, while the Gamow vectors (7.3.27c) and (7.3.27d) are generalized eigenvectors of $H \otimes I$ with generalized eigenvalue z_R^* . One can also show that

$$\begin{aligned}
\mathcal{A}_{T+}^{\times}|z_R^-; r=+\rangle &= -|z_R^{*+}; r=-\rangle\,, && (7.3.28a)\\
\mathcal{A}_{T+}^{\times}|z_R^-; r=-\rangle &= |z_R^{*+}; r=+\rangle\,, && (7.3.28b)\\
\mathcal{A}_{T-}^{\times}|z_R^{*+}; r=+\rangle &= |z_R^-; r=-\rangle\,, && (7.3.28c)\\
\mathcal{A}_{T-}^{\times}|z_R^{*+}; r=-\rangle &= -|z_R^-; r=+\rangle\,. && (7.3.28d)
\end{aligned}$$

The overall signs on the right hand side of Eqs. (7.3.28c) and (7.3.28d) correspond to the choice

$$\mathcal{A}_{T-} = -\mathfrak{U}_+^\dagger \mathcal{C} \mathfrak{U}_-\,. \tag{7.3.29}$$

For the choice

$$\mathcal{A}_{T-} = \mathfrak{U}_+^\dagger \mathcal{C} \mathfrak{U}_-\,, \tag{7.3.30}$$

the overall signs on the right hand side of Eqs. (7.3.28c) and (7.3.28d) are the opposite.

Now, we obtain the action of the time reversal operator on the time evolution semigroups. The time evolution semigroups are defined on the dual spaces $(\mathbf{\Phi}_\pm^r)^\times$ as

$$\mathcal{W}_\pm^\times(t) := \mathcal{U}_\pm^\times(t) \otimes I = \begin{pmatrix} \mathcal{U}_\pm^\times(t) & 0 \\ 0 & \mathcal{U}_\pm^\times(t) \end{pmatrix}\,. \tag{7.3.31}$$

The operator $\mathcal{W}_+^\times(t)$ is well defined on $(\mathbf{\Phi}_+^r)^\times$ for $t > 0$ only, while $\mathcal{W}_-^\times(t)$ is well defined on $(\mathbf{\Phi}_-^r)^\times$ for $t < 0$ only. From Eqs. (7.2.19) it follows that

$$\begin{aligned}
\mathcal{A}_{T+}^\times \mathcal{W}_+^\times(t) \mathcal{A}_{T-}^\times &= \mathcal{W}_-^\times(-t)\,, \quad t > 0\,, && (7.3.32a)\\
\mathcal{A}_{T-}^\times \mathcal{W}_-^\times(t) \mathcal{A}_{T+}^\times &= \mathcal{W}_+^\times(-t)\,, \quad t < 0\,. && (7.3.32b)
\end{aligned}$$

This result has been obtained for the choice of $\mathcal{A}_{T-}$ as in (7.3.29). If we made the choice (7.3.30), a minus sign would appear on the right hand side of Eqs. (7.3.32). As mentioned above, we prefer the choice (7.3.29), because we want Eqs. (7.3.32) to not have that minus sign.

7.4 Appendix 10: Time Reversal

Textbooks on Quantum Mechanics usually define the time reversal operation in the position representation as

$$C\psi(\vec{x}, t) = \psi^*(\vec{x}, -t)\,, \tag{7.4.1}$$

where the star denotes complex conjugation. We are going to explain what this definition means.

Following Wigner, time reversal is an operation such that the following operations, when performed sequentially, yield the identity:

$$\text{time displacement by } t \times \text{time reversal} \times \text{time displacement by } t \times \text{time reversal}\,. \tag{7.4.2}$$

If we denote the time reversal operator by C, a possible definition would be $C\psi(t) = \psi(-t)$. However, this kind of operation is obviously linear. The need for an antilinear time reversal operation has been nicely shown by Wigner in the following terms:

> Consider a system whose Hamiltonian has a complete set of eigenvectors φ_n (for instance, the Harmonic oscillator, the bound states of the Hydrogen atom, or any system formed by the bound states of the Hamiltonian, if any). Then, any state vector φ can be expanded by those eigenvectors,
>
> $$\varphi = \sum_n a_n \varphi_n\,, \tag{7.4.3}$$
>
> where
>
> $$H\varphi_n = E_n \varphi_n\,. \tag{7.4.4}$$
>
> The operations (7.4.2) yield the identity if and only if:
>
> $$\text{time displacement by } t \times \text{time reversal} = \text{time reversal} \times \text{time displacement by } -t\,. \tag{7.4.5}$$
>
> Let us apply these operations to φ in (7.4.3). If we assume that the time reversal operator C is linear, then
>
> $$C\varphi = \sum_n a_n C\varphi_n\,. \tag{7.4.6}$$
>
> Since $[H, C] = 0$, $C\varphi_n$ is also an eigenvector of the Hamiltonian with the same eigenvalue E_n. Therefore, time displacement by t on (7.4.6) gives
>
> $$\sum_n a_n e^{-iE_n t} C\varphi_n\,. \tag{7.4.7}$$
>
> According to the rule in (7.4.5), this should be equal to the result of performing first the time displacement by $-t$ on φ
>
> $$\sum_n a_n e^{iE_n t} \varphi_n\,, \tag{7.4.8}$$
>
> and then the time reversal operation C, which (assuming that C is linear) leads to
>
> $$\sum_n a_n e^{iE_n t} C\varphi_n\,. \tag{7.4.9}$$
>
> This result does not coincide with the expression given by (7.4.7). However, they do coincide if C is defined as an antilinear operator.

Once we have shown that the time reversal operator must be antilinear, we study its action in the energy representation. In this representation, the Hamiltonian H acts as the multiplication operator. If $\psi(E)$ is a wave function in the energy representation, then the action of the time reversal operator on it is defined by

$$C\psi(E) := \psi^*(E)\,, \tag{7.4.10}$$

where we have chosen the complex conjugation as the time reversal operator (as Wigner does). Time displacement by t on (7.4.10) gives

$$e^{-iEt}\,\psi^*(E)\,. \tag{7.4.11}$$

If we apply time reversal to (7.4.11), which is now equivalent to perform the complex conjugation operation, we obtain

$$e^{iEt}\,\psi(E)\,. \tag{7.4.12}$$

Finally, time displacement by t on (7.4.12) gives

$$e^{-iEt}\,e^{iEt}\,\psi(E) = \psi(E)\,. \tag{7.4.13}$$

Hence, the time reversal operator C defined by (7.4.10) fulfills the above rule (7.4.2) and is antilinear. Obviously,

$$C\left(\psi(E,t)\right) = C\left(e^{-iEt}\psi(E)\right) = e^{iEt}\,\psi^*(E)\,. \tag{7.4.14}$$

We can look at $e^{iEt}\,\psi^*(E)$ as the result of applying time displacement by $-t$ on $\psi^*(E)$. Therefore, $e^{iEt}\,\psi^*(E)$ is what should be identified with the $\psi^*(E,-t)$ (or $\psi^*_{-t}(E)$) that appears in the literature. Note that $\psi^*(E,-t) = e^{iEt}\,\psi^*(E) = [e^{-iEt}\,\psi(E)]^* = [\psi(E,t)]^*$.

The same can be argued in the position representation, where time reversal is given by

$$\widetilde{C}\,\psi(\vec{x}) = \psi^*(\vec{x})\,. \tag{7.4.15}$$

However, in the momentum representation, the time reversal operator, which we denote by C', acts as

$$C'\,\varphi(\vec{p}) = [\varphi(-\vec{p})]^*\,, \tag{7.4.16}$$

since the time reversal changes $\vec{p}$ for $-\vec{p}$.

In order to show it, let $\psi(\vec{x})$ be a wave function in the position representation. Then the corresponding wave function in the momentum representation is given by

$$\widehat{\psi}(\vec{p}) \equiv \mathcal{F}\psi(\vec{p}) := \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\vec{p}\vec{x}}\,\psi(\vec{x})\,d\vec{x}\,. \tag{7.4.17}$$

where $\mathcal{F}$ and hat denote the Fourier transform. The Fourier transform takes the time reversal operator in the position representation into the time reversal operator in the momentum representation,

$$C' = \mathcal{F}\widetilde{C}\mathcal{F}^{-1}\,. \tag{7.4.18}$$

Hence,

$$\begin{aligned}
(C'\widehat{\psi})(\vec{p}) &= (\mathcal{F}\widetilde{C}\mathcal{F}^{-1}\widehat{\psi})(\vec{p}) \\
&= (\mathcal{F}\widetilde{C}\psi)(\vec{p}) \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\vec{p}\vec{x}}(\widetilde{C}\psi)(\vec{x})\,d\vec{x} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\vec{p}\vec{x}}\psi^*(\vec{x})\,d\vec{x} \\
&= [\widehat{\psi}(-\vec{p})]^*\,, \qquad (7.4.19)
\end{aligned}$$

which proves Eq. (7.4.16).

Consider now an arbitrary representation supported by the Hilbert space $\mathcal{H}$. Let U be the unitary operator that transforms from the position into that arbitrary representation. Analogously to (7.4.18), we define the time reversal operator A_T on $\mathcal{H}$ as

$$A_T\phi := U\widetilde{C}U^{-1}\phi \equiv U\widetilde{C}\phi(\vec{x})\,. \qquad (7.4.20)$$

If we denote $\phi^T := A_T\phi$, $\phi(t) := e^{-itH}\phi$, and call $H' = U^{-1}HU$ the Hamiltonian in the position representation, then

$$\begin{aligned}
A_T\phi(t) &= A_T e^{-iHt}\phi \\
&= U\widetilde{C}U^{-1}e^{-iHt}\phi \\
&= U\widetilde{C}U^{-1}e^{-iHt}U\phi(\vec{x}) \\
&= U\widetilde{C}e^{-iH't}\phi(\vec{x}) \\
&= Ue^{iH't}\phi^*(\vec{x}) \\
&= e^{iHt}U\widetilde{C}\phi(\vec{x}) \\
&= e^{iHt}U\widetilde{C}U^{-1}\phi \\
&= e^{iHt}A_T\phi \\
&= (A_T\phi)(-t) \\
&= \phi^T(-t)\,. \qquad (7.4.21)
\end{aligned}$$

Thus $A_T\phi(t) = \phi^T(-t)$, which generalizes the equation $C\psi(\vec{x},t) = \psi^*(\vec{x},-t)$.

However, this is not the whole story. As mentioned above, Wigner [61, 62] realized that, when constructing projective representations of the Poincaré group extended by time inversion and parity, new possibilities exist. These new possibilities are not independent of the representation of the parity and imply a doubling of the space supporting the representation. We do not want to discuss this construction here. Instead, we present a table with the four possibilities (see Table I below). The four possibilities are characterized by two parameters, which also appear among the parameters that characterize the representations of the extended Poincaré group.

Consider the space, time, and total inversion operators on a Hilbert space $\mathcal{H}$, which we denote respectively by U_P, A_T and A_I. The operator U_P is unitary, while A_T and A_I are

antiunitary. From the nature of the corresponding physical operations, it follows that the operators U_P^2, A_T^2, and A_I^2 must be proportional to the unit operator. Since U_P is unitary, we can choose its phase such that

$$U_P^2 = I\,, \tag{7.4.22}$$

while such a normalization is not possible for the antiunitary A_T or A_I. In fact, the antiunitarity and the associative law of the group multiplication dictate that the squares of A_T and A_I must necessarily equal either $+1$ or -1:

$$A_T^2 = \epsilon_T I\,, \qquad \epsilon_T = \pm 1\,, \tag{7.4.23a}$$

$$A_I^2 = \epsilon_I I\,, \qquad \epsilon_I = \pm 1\,. \tag{7.4.23b}$$

Moreover, the phase of A_I can be chosen such that

$$A_I = U_P A_T\,. \tag{7.4.24}$$

Corresponding to the values that ϵ_T and ϵ_I can take, there exist four extensions of the continuous symmetry group. Barring the existence of any additional conditions, all four are possible, and Wigner [61] has derived these four classes of projective representations of the extended Poincaré group. The results are summarized in the following table:[2]

Table I

ϵ_T	ϵ_I	U_P	A_T
$(-1)^{2j}$	$(-1)^{2j}$	1	C
$-(-1)^{2j}$	$(-1)^{2j}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & C \\ -C & 0 \end{pmatrix}$
$(-1)^{2j}$	$-(-1)^{2j}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & C \\ C & 0 \end{pmatrix}$
$-(-1)^{2j}$	$-(-1)^{2j}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & C \\ -C & 0 \end{pmatrix}$

In this table, j refers to the spin of the particle under consideration, while C is the well known $(2j+1)$-dimensional matrix whose entries are $c_{\mu,\nu} = (-1)^{j+\mu}\delta_{\mu,-\nu}$, $-j \le \mu, \nu \le j$. In these representations, the continuous space-time transformations U_g, as well as any other known observables such as the internal symmetry generators B, have the following form:

$$U_g = \begin{pmatrix} U_g & 0 \\ 0 & U_g \end{pmatrix}\,, \quad B = \begin{pmatrix} B & 0 \\ 0 & B \end{pmatrix}\,. \tag{7.4.25}$$

[2] In the non-relativistic case, J. F. Cariñena and M. Santander have obtained a totally analogous result for the Galilei group (in the case with mass) [63].

The representation space of the extensions of the space-time symmetry group by P and T is therefore reducible under the restricted symmetry transformations and observables. From Table I we see that only the case for which $\epsilon_T = \epsilon_I = (-1)^{2j}$ leads to no doubling of the space of the microscopic system under inversions. This is the only case discussed in relativistic quantum field theory, and quantum fields have so far been constructed only for this class of the four classes of projective representations of the extended Poincaré group [94]. In the three other cases, the restricted space-time symmetry transformation is doubled after the time reversal operator is adjoined—*the time reversal doubling*. In these cases, the two subspaces that are left invariant under U_g and B remain invariant also under U_P, albeit they have opposite relative parity in the two cases for $\epsilon_T\epsilon_I = -1$. In these two cases, the two subspaces can in fact be distinguished by their parity eigenvalue, and to the extent that we associate microscopic systems with irreducible representations of the symmetry group, the two subspaces would describe particles with the same mass and spin but opposite parity. This, however, is not the situation for the extended group characterized by $\epsilon_T = \epsilon_I = -(-1)^{2j}$ for which the relative parity of the two subspaces of states is $+1$. It is this class of projective representations which have been used in Ref. [64], because for these representations a label r can be introduced, a two-valued parameter, which was used in Ref. [64] to distinguish between the space of prepared states and the space of time reversed registered observables. These two subspaces (have the same parity and) remain irreducible under U_g and B. From Table I it is clear that A_T changes the value r.

Chapter 8

Conclusions

In this last chapter, we present the conclusions of the dissertation.

> There is never an ending to Paris and the memory of each person who has lived in it differs from that of any other. We always returned to it no matter who we were or how it was changed or with what difficulties, or ease, it could be reached. Paris was always worth it and you received return for whatever you brought to it. But this is how Paris was in the early days when we were very poor and very happy.
>
> Ernest Hemingway, *A movable Feast*

The RHS language has been used to describe Dirac kets, Lippmann-Schwinger kets and Gamow vectors in a consistent way. We have seen that the mathematical image of those objects should be the following:

Physical quantity	Mathematical image	Symbol	Name
Bound state of energy $E_n < 0$	Normalizable eigenvector of H with eigenvalue E_n	$\|E_n)$	Bound state
Scattering state of energy $E > 0$	Generalized eigenvector of H with real eigenvalue E	$\|E^+\rangle$	Lippmann-Schwinger ket
Resonance of energy E_R and width Γ_R	Generalized eigenvector of H with complex eigenvalue z_R	$\|z_R^-\rangle$	Gamow ket

In terms of results, we would like to highlight the following:

• We have presented a systematic review of the mathematical methods of the Rigged Hilbert Space.

• We have reviewed and improved the construction of the RHS of the harmonic oscillator.

• We have shown that the natural framework for the solutions of the Schrödinger equation is the RHS. We have illustrated this point by constructing *a* RHS of the square barrier potential explicitly.

• We have shown that a consistent description of the Lippmann-Schwinger equations needs a pair of RHSs. We have also shown that the Lippmann-Schwinger kets act as anti-linear functionals over spaces of wave functions that are boundary values of functions that can be continued analytically.

• We have translated A. Mondragón *et al.*'s integral equation for the Gamow vectors into the RHS language.

• We have constructed the Gamow vectors of the square barrier potential Hamiltonian. We have shown that the $[0, \infty)$-energy representation of these vectors is the complex delta functional, and that their $(-\infty, \infty)$-energy representation is the Breit-Wigner amplitude.

• We have disclosed the time asymmetry of the purely outgoing boundary condition.

• We have studied the action of the time reversal operator on resonances for the standard case and for one of the cases that lead to a doubling of the space supporting the representation. The doubling has been explicitly constructed within the RHS framework.

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