Rigged Hilbert Space Theory for Hermitian and Quasi-Hermitian Observables

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Abstract

In this thesis, we study whether the rigged Hilbert space formulation of Quantum Mechanics can be extended to quasi-hermitian operators. The necessary mathematics to understand rigged Hilbert spaces and their representations is presented. Using the mathematics, we give rigorous meaning to Dirac's kets and bras, using the momentum operator as an example. The mathematical theory culminates with the nuclear spectral theorem(Gelfand-Maurin) which guarantees an eigenket decomposition for the wave functions. Next, we illustrate the theory by applying it to the quantum system defined by a potential barrier. We then introduce non-hermitian operators of interest in Quantum Mechanics, specifically PT-symmetric Hamiltonians. It is known that PT-symmetric Hamiltonians are necessarily pseudo-hermitian. We restrict our attention to a subclass of pseudo-hermitian operators, the quasi-hermitian operators, and present an extension of the nuclear spectral theorem. The extension, under certain conditions on the quasi-hermitian operator and the metric operator, guarantees an eigenket decomposition for a dense subset of the Hilbert space on which the operator is defined. We discuss how the extension may help put quasi-hermitian quantum mechanics on a rigorous footing and discuss its drawbacks and possible extensions. Lastly, we present conditions under which a spectral decomposition of quasi-hermitian operators with respect to an operator-valued measure exists. This is an extension of the spectral decomposition of self-adjoint operators with respect to a projection-valued measure.

Contents

1 Introduction

1.1 Introduction(Mathematics)

Functional analysis is an extremely powerful field of mathematics with countless applications to other fields such as physics, statistics, and probability. Notably, it is an invaluable tool to study differential equations. Functional analysis is loosely speaking the study of infinite-dimensional vector spaces endowed with a topological structure and the linear maps between them. The term 'functional analysis' was first used in Hadamard's 1910 book on calculus of variations. However, the concept of a functional is attributed to Volterra some decades before that. The most notable spaces studied in functional analysis are Banach spaces and Hilbert spaces. The former is a complete infinite-dimensional normed vector space while the latter is a complete infinite-dimensional inner product space. Hilbert spaces, in particular, due to their powerful structure are applied widely in applied mathematics. For example, the semi-parametric theory of efficient estimators in statistics is based the study of a collection of interesting Hilbert spaces. Additionally, the mathematical foundations of quantum mechanics heavily rely on Hilbert space theory to describe the space of wavefunctions. The notions of Banach and Hilbert spaces can be further generalised by the general notion of a topological vector space which is just a vector space equipped with an arbitrary general topology. Some notable examples are locally convex spaces where the topology is induced by a family of semi-norms and Fréchet spaces.

In this thesis, the theory of rigged Hilbert spaces and its application to quantum mechanics will be studied. We present the necessary mathematics which includes topological vector spaces, nuclear operators and spaces, and rigged Hilbert spaces . Notably, we discuss the extension of operators on the Hilbert space to the entire rigged Hilbert space, as well as iosmorphisms of rigged Hilbert spaces. Afterwards, we apply the theory to a well-known quantum mechanical problem and demonstrate how it allows the problem to be put on a mathematically rigorous foundation. Before we discuss the main results obtained in this thesis, it is helpful to introduce the notion of a rigged Hilbert space and why it is useful.

In quantum mechanics, one often wishes to find a complete set of eigenvectors for a particular(possibly unbounded) self-adjoint operator defined on the Hilbert space. The eigenvectors are complete in the sense that eigenvectors form some sort of basis that diagonalizes the operator. It is well known that self-adjoint operators do not necessarily have a complete set of eigenvectors in infinite dimensions. Such a complete set is known to exist for compact self-adjoint operators but many operators of interest in applied mathematics do not fit under this description. One result attributed to von Neumann is that all self-adjoint operators can be diagonalized with respect to a projection-valued measure. That is, given a self-adjoint operator $A : H \mapsto H$ defined on a Hilbert space H, one can find a collection of projections E_λ such that

$$(\varphi, A\psi)_H = \int_{\sigma(A)} \lambda d(E_\lambda \varphi, \psi)$$

This result extends the diagonalization of self-adjoint operators in finite-dimensional vector spaces. However, it does so by replacing the complete set of eigenvectors with a projection-valued measure. The reason why arbitrary self-adjoint operators cannot be diagonalized by eigenvectors is simply because its eigenvectors are not necessarily in the Hilbert space. N

The rigged Hilbert space is able to generalise the notion of an eigenvector so that every self-adjoint operator has a complete set of eigenvectors, mimicking the finite-dimensional case. Notable mathematician Israel Gelfand, known for studying partial differential equations and harmonic functions, proved the *nuclear spectral theorem* that proves the existence of a resolution of the identity and diagonalization for an arbitrary self-adjoint operator. These *generalised eigenfunctions* are actually anti-linear functionals defined on the dual space of a topological vector space.

A rigged Hilbert space is a triplet of spaces $\Phi, H, \Phi^\times$ where H is a Hilbert space, Φ is a Fréchet topological vector space densely embedded in H with a finer topology, and $\Phi^\times$ is the anti-dual space of Φ. Note that since Φ has a finer topology than H,

$$H^\times \subset \Phi^\times$$

Furthermore, by Riesz representation theorem

$$H \cong H^\times$$

As a result, one often writes the triplet of spaces as

$$\Phi \subset H \subset \Phi^\times$$

In the nuclear spectral theorem, Gelfand extends a self-adjoint operator on H to an operator on $\Phi^\times$. The generalised eigenfunctions of the operator are simply the eigenvectors of its extension in $\Phi^\times$. Thus, the rigged Hilbert space extends the notion of a Hilbert space to put self-adjoint operators on the same footing.

In this thesis, we will study quasi-hermitian operators and extend the nuclear spectral theorem to describe such operators. Such operators have applications in quantum mechanics and the extension of the theorem is necessary to put such quantum mechanical problems in rigorous footing. A quasi-hermitian operator is an operator that is self-adjoint when defined on a different Hilbert space obtained by completing the original Hilbert space with respect to a different inner product. Equivalently, we say that the quasi-hermitian operator is similar to its adjoint by a positive definite operator.

We show that for a dense subspace of the Hilbert space where the quasi-hermitian operator is defined, one can decompose the elements in terms of the generalised eigenfunctions of the operator. We also show that the operator and its adjoint can be diagonalized by these generalised eigenfunctions. The construction relies on using the rigged Hilbert space induced by the Hilbert space where the operator is self-adjoint. The generalised eigenfunctions are present in this rigged Hilbert space, specifically in the anti-dual space of a dense subspace of the Hilbert space where the operator is self-adjoint. Since there is not necessarily an isomorphism of the original Hilbert space into the anti-dual space where the generalised eigenvectors are located, we were unable to find a natural rigging of the original Hilbert space.

It should also be noted that the dense subspace where our extended nuclear spectral theorem applies is required to be left invariant under the action of the operator and its corresponding positive definite metric operator. The conditions we impose are the minimal conditions necessary so that that the generalised eigenfunction(als) of the operator and its adjoint are in the rigged Hilbert space. In practice, there is no general way of constructing such an invariant subspace. Furthermore, there is no guarantee that the space even exists for a general quasi-hermitian operator. It is possible that the conditions are only satisfied in the trivial case where the operator is hermitian. However, since the conditions required are minimal, if the theorem is only satisfied in the trivial case, it is reasonable to believe that the nuclear spectral theorem can not be extended to the quasi-hermitian case. At least not in its general form and not by our method.

We also discuss how to extend the theory to account for a quantum system described by a collection of quasi-hermitian and hermitian operators. In the case where the operator is non-hermitian but has a complete set of eigenvectors, we present sufficient conditions for a rigged Hilbert space to exist such that the such a collection of operators to have a complete set of generalised eigenvectors. Lastly, we discuss possible extensions of the theory. Specifically, we propose an alternative method of extending the nuclear spectral theorem by means of a spectral representation of quasi-hermitian operators with respect to an operator-valued measure. Lastly, we propose possible extensions to this thesis such as extending the nuclear spectral theorem to pseudo-hermitian operators.

1.2 Historical Background and Introduction(Physics)

The rise of physical theory of Quantum Mechanics in the beginning of the 20-th century drastically changed our understanding of the world. The theory was able to describe a wide array of phenomena at small lengths scales with near perfect accuracy. It led to scientific revolutions countless fields including physics, chemistry, material science, and electronics. Much of the technology we use today from our smart phones and tablets to the medical devices such as MRI's and X-ray are based on quantum mechanical principles.

It began with the ground breaking papers on black-body radiation and the photoelectric effect by Max Planck and Albert Einstein, respectively and was reignited in the mid-1920's by the hands of Schrödinger, Heisenberg, and Born who were key in the development of an all encompassing theoretical framework which described the world at atomic scales. Even though quantum mechanical tools were employed at mass to solve various physical problems, a comprehensive mathematical formalism of the theory was not formed until around the 1920's, beginning with two formulations: Schrödinger's wave mechanics and Heisenberg's matrix mechanics. These two formalisms, while supplying the mathematical framework for which to operate in, was not mathematically rigorous.

In the 1930's, mathematician John von Neumann and Paul Dirac employed the recently developed tools of functional analysis to put the theory on a firm mathematical foundation. Dirac introduced an informal mathematical framework using so-called bra-ket notation which was able to extend the linear algebra of finite dimensional spaces to infinite dimensional spaces. In this framework, wavefunctions and observable eigenfunctions were represented as kets. One could convert a ket into a bra by complex conjugation. Multiplying a bra and a ket led to a result reminiscent of the inner product. On the other hand, multiplying a ket with a bra lead to a projection-like operator. When the bras and kets corresponded to wavefunctions in the Hilbert space, the notation was justified by the inner product.

However, physicists applied the formalism to eigenvectors of continuous observables such as momentum and position. In this case, the eigenvectors were not in the Hilbert space so that the inner product notation no longer applied. With the help of von Neumann, his theory was put on a mathematically rigorous, axiomatic foundation, the so-called Dirac-von Neumann formulation of quantum mechanics. However, the mathematical framework ran into one pitfall. It could only rigorously account for physical phenomena with a discrete spectrum. Many axioms and theorems of the Dirac-von Neumann framework broke down when the system had a continuous spectra. Regardless, physicists were able to apply the theory and Dirac notation with great success by ignoring the mathematical inconsistencies and discrepancies. However to mathematical and theoretical physicists, the inconsistency of the theory was deeply troubling and even today there is active research in extending the Dirac-von Neumann formalism to cover all classes of problems.

The rigged Hilbert space formalism of quantum mechanics is highly suggested to be natural setting of quantum mechanics and is able to successfully account for quantum mechanical problems where the a continuous spectrum is prevalent. Loosely, speaking the rigged Hilbert space is a triple of spaces

$$\Phi \subset H \subset \Phi^{\times}$$

where Φ is a dense subspace of H with a finer topology than H, H is a Hilbert space, and $\Phi^{\times}$ is the anti-dual space of Φ. The space assigns rigorous definitions to Dirac's bras and kets and provides justification for its use by physicists in continuous spectra problems. A key result from the rigged Hilbert space formalism is the *nuclear spectral theorem*. The theorem ensures that self-adjoint operators have a complete set of eigenkets in the rigged Hilbert space. That is, wavefunctions can be decomposed in terms of the eigenkets. Furthermore, it allows the observables to be diagonalized by the eigenkets which justifies the representation of wavefunctions induced by observables.

In this thesis, we illustrate the theory by applying it to the potential barrier. Our illustration is largely based on a more in-depth treatment by de la Madrid that can be found in [1].

Recently, non-hermitian observables, such as PT-symmetric Hamiltonians, have become of interest in quantum mechanics. A notable example is that of the imaginary cubic harmonic oscillator given by

$$H = \frac{-\hbar^2}{2m}\frac{d}{dx} + ix^3$$

For some time, it was believed that observables in quantum mechanics must be hermitian, as this ensures the spectrum is real. In 1998, Physicist Carl Bender discovered a class of non-hermitian operators that have a real spectrum, the so called PT-symmetric operators. There was no longer any reason to believe that nature is restricted to only hermitian observables and it was soon discovered that the field had far-reaching applications in optics and electronics. Specifically, PT-symmetric Hamiltonians corresponded to balanced gain and loss in optical systems. Currently, the field primarily restricted itself to special classes of PT-symmetric operators that satisfy certain nice properties. Common assumptions on the operators are that they have a discrete spectrum and are diagonalizable from which it follows that the operator has a complete eigenbasis in the Hilbert space. The mathematical properties of this restricted class of PT-symmetric operators has been thoroughly studied by Mostafazadeh et al. One especially nice result proven by Mostafazadeh is that the class of diagonalizable PT-symmetric operators with a discrete spectrum are necessarily pseudo-hermitian[2]. He further states that nearly all classes of non-hermitian operators studied by physicists in the field fall under the class of pseudo-hermitian operators.

While diagonalizable PT symmetric operators with discrete spectrum have been rigorously studied in literature, there has been little attention given to putting the general class of PT-symmetric operators in a rigorous framework. We attempt to rectify this by putting non-hermitian quantum mechanics in the rigged Hilbert space framework. Specifically, we offer a possible extension of the nuclear spectral theorem to the class of quasi-hermitian operators. An operator $A : H \mapsto H$ is called quasi-hermitian if its similar to its adjoint by a bounded positive definite operator.

$$A^* = \eta A \eta^{-1}$$

When the requirement for η to be positive definite is removed, we call the operator pseudo-hermitian. We restrict ourselves to the class of quasi-hermitian operators which encompass a large number of PT-symmetric operators treated in literature[3][4][2]. The more general case of pseudo-hermitian operators where the metric operator is indefinite will not be treated and likely cannot be treated by the methods developed in this thesis. It should be noted that even in the case where the Hamiltonian is discrete and diagonalizable to its eigenvectors are in the Hilbert space, a rigged Hilbert space formulation is necessary to incorporate the momentum and position observables and their wavefunction representations.

The fundamental result of this thesis is the extension of the nuclear spectral theorem to quasi-hermitian operators. We show that for a dense subspace of the Hilbert space where the quasi-hermitian operator is defined, one can decompose the wave-function kets in terms of the eigenkets and eigenbras of the operator. We also show that the observable and its adjoint can be diagonalized by these eigekets. The construction relies on using the rigged Hilbert space induced by the Hilbert space where the operator is hermitian. The eigenkets are present in this rigged Hilbert space, specifically in the anti-dual space of a dense subspace of the Hilbert space where the observable is hermitian. Since there is not necessarily an isomorphism of the original Hilbert space into the anti-dual space where the eigenkets are located, we were unable to find a natural rigging of the original Hilbert space. It should also be noted that the dense subspace where our extended nuclear spectral theorem applies is required to be left invariant under the action of the observable and its corresponding metric operator. The conditions we impose are the minimal conditions necessary so that that the eigenkets of the observable and its adjoint are in the rigged Hilbert space. In practice, there is no general way of constructing such an invariant subspace. Furthermore, there is no guarantee that the space even exists for a general quasi-hermitian operator. It is possible that the conditions are only satisfied in the trivial case where the operator is hermitian. However, since the conditions required are minimal, if the theorem is only satisfied in the trivial case, it is reasonable to believe that the nuclear spectral theorem can not be extended to the quasi-hermitian case. At least not in its general form and not by our method. We also discuss how to extend the theory to account for a quantum system described by a collection of quasi-hermitian and hermitian observables. In the case where the Hamiltonian is non-hermitian but has a complete set of eigenvectors, we present sufficient conditions for a rigged Hilbert space to exist such that the Hamiltonian, momentum, and position operator have a complete set of eigenkets. Lastly, we discuss possible extensions of the theory. Specifically, we propose an alternative method of extending the nuclear spectral theorem by means of a spectral representation of quasi-hermitian operators with respect to an operator-valued measure.

1.3 Dirac formulation of Quantum Mechanics

In this section, we will briefly discuss how quantum mechanical problems are solved. For simplicity, we will consider the case of a single particle restricted to move in one dimension.

In general, a particle of mass m in one dimension is described by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi \tag{1}$$

where

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

By separation of variables, one can obtain definite energy solutions of equation (1). The eigensolutions are given by:

$$\hat{H}\psi_E(x) = E\psi_E(x)$$

The general solution with definite energy is then

$$\psi(x,t) = e^{-\frac{i}{\hbar}Et}\psi_E(x) \tag{2}$$

In general, a quantum mechanical problem is solved when the solutions of the time-independent equation are known. Since equation (1) is linear, all solutions of (1) are linear combinations of solutions of form (2).

The solutions ψ of (1) are called wave functions which can be interpreted as probability distributions as follows:

$$|\psi|^2 \text{ is a probability density.}$$

We thus require wave functions to satisfy

$$\int |\psi|^2 dx = 1$$

The Dirac Formalism relies on the following key assumptions:[5]

1. To each quantum mechanical system, there is a corresponding separable Hilbert Space containing all realisable states of the system. We call the possible states of the system wave functions and require them to be normalised to 1 under integration.

2. To each Observable of the system, there is a corresponding self-adjoint operator defined on some domain contained in the Hilbert Space. The possible measurements of the observable are exactly the necessarily real spectra of the self-adjoint operator.

3. To each element λ in the spectrum Λ of the observable A, there exists a corresponding ket $|\lambda\rangle$ that is an eigenvector of A with eigenvalue λ.

$$A\,|\lambda\rangle = \lambda\,|\lambda\rangle$$

4. Every wave function φ can be expanded by these eigenkets as

$$\varphi = \int_{Spectrum(A)} d\lambda \left|\lambda\right\rangle \left\langle\lambda|\varphi\right\rangle$$

5. The eigenkets are normalised to satisfy

$$\langle\lambda|\lambda'\rangle = \delta(\lambda - \lambda')$$

where $\delta(\lambda - \lambda')$ is the Dirac delta function.

6. All algebraic operations such as commutator relations, products of observable, expectations and variances are well-defined.

In general, the dynamics of a quantum system are described by its (time independent) Hamiltonian. The Hamiltonian is defined as a self-adjoint operator on a Hilbert space and whose structure is given by Schrödinger's equation. The eigenvectors of the Hamiltonian are possible energy eigenstates that the particle can be in and the corresponding spectra represents the possible energy values that can be measured. When the Hamiltonian has a discrete spectrum, as in the case of the infinite well potential, the eigenstates are functions in the Hilbert Space and thus are realisable particle states. Furthermore, the eigenstates of the Hamiltonian form a complete orthogonal basis of the Hilbert space. Thus by decomposing arbitrary wave functions in this basis by use of the inner product, we obtain the expansion given in rule (4). Further by orthogonality of the eigenstates, rule (5) is satisfied. The other rules can like-wise be satisfied.

In this case, bras and kets can be interpreted as the left and right halves of the inner product. Multiplying a bra by a ket is simply the inner product. Similarly, Multiplying a ket by a bra gives a linear operator such that it acts on wave functions by projection on the kets (as functions in the Hilbert space) using the inner product.

We see that in the discrete spectrum case, as expected, the Dirac formulation holds. One may ask where it goes wrong in the continuous spectra case?

To this end, consider the momentum operator which can be defined on a dense subset of the Hilbert space such that it is self-adjoint.

$$\hat{P} = i\hbar\frac{d}{dx}$$

It can be checked that the eigenstates are pure waves of the form

$$|p\rangle = e^{ikx}$$

which are non-normalisable and not in the Hilbert space. As a result, the eigenfunctions certainly cannot be a basis for the Hilbert space. Thus, we are unable to use the inner product structure to obtain decomposition in rule 4 as before. However, by using the Fourier transform of the wave function and the delta function, we can obtain rule (4) and (5). In this case, it is incorrect to interpret bras and kets as halves of the inner product as they are not even in the Hilbert space. Instead the eigenkets and eigenbras are anti-linear and linear functionals respectively on the Hilbert space.

Where for the case of the momentum operator, the eigenkets are the following linear maps:

$$|p\rangle : H \longmapsto \mathbb{C}$$

$\varphi(x) \mapsto |p\rangle\,(\varphi) = \int_{-\infty}^{\infty} \frac{1}{2\pi\hbar} e^{ipx/\hbar}\,\overline{\varphi}\,dx$

Since the map exists for all p, we can define a function $\hat{\varphi}(p) := |p\rangle\,(\varphi(x))$. It is easy to see that this corresponds exactly with the Fourier transform of the wave function. We will later see that such maps will let us define the position, momentum, and energy representations of wavefunctions in a rigorous way.

1.4 Introduction to the Mathematics of Rigged Hilbert Spaces

If one lacks the mathematical background, one should first consult the mathematical framework section before attempting to read this section. This section is presented to offer a short concise overview of the rigged Hilbert space and how it relates to quantum mechanics.

In this thesis, the rigged Hilbert space formulation of quantum mechanics is presented. The rigged Hilbert space formulation of quantum mechanics allows for the bras and kets of the Dirac notation to be rigorously defined. Furthermore, the space is constructed to contain a complete set of eigenkets for all observables. This is in contrary to the Hilbert space formulation where only observables with discrete spectrum have eigenvectors in the space. Loosely speaking, the rigged Hilbert space

A rigged Hilbert space is a triplet of spaces $\Phi, H, \Phi^{\times}$ where H is the Hilbert space, Φ is the space of realizable wavefunctions equipped with a finer topology than H, and $\Phi^{\times}$ is the space of anti-linear continuous functions on Φ. The finer topology essentially tells us that $H^{\times} \subset \Phi^{\times}$. In physics, one often writes a wave function φ as a ket $|\varphi\rangle$. Similarly, one can write it as a bra $\langle\varphi| := \overline{|\varphi\rangle}$. Given two wave functions φ and ψ, written as kets as $|\varphi\rangle$ and $|\psi\rangle$, one takes their inner product by multiplying the bra $\langle\varphi|$ with the ket $|\psi\rangle$. We have

$$(\varphi, \psi)_H = \langle\varphi|\psi\rangle .$$

While $|\varphi\rangle$ and $\langle\varphi|$ are often interpreted as being wave functions, this is technically incorrect. While all wave functions can be written as kets, not all kets are wave functions. There are kets that are not in the Hilbert space that are essential in quantum mechanics. To see this, consider the momentum operator. One can show that the momentum operator $P = -i\hbar\frac{d}{dx}$ has eigenfunctions written e^{ikx} where $k = p/\hbar$. One often writes these as eigenkets (incorrectly) as $|p\rangle = e^{ikx}$. These eigenfunctions are not normalizable and not in the Hilbert space. As a result, they are not realizable particle states and are not wavefunctions. However, by means of the Fourier transform, one can decompose wavefunctions in terms of momentum eigenkets. The momentum eigenkets act like an orthonormal basis for the Hilbert space and can be used to, in a way, diagonalize the momentum operator.

A better description of a ket is as an element of the anti-dual space $\Phi^{\times}$ in the rigged Hilbert space. One can associate with each wave function $\varphi \in \Phi$ an anti-linear functional $|\varphi\rangle \in H^{\times} \subset \Phi^{\times}$ by use of Riesz representation theorem. We write

$$|\varphi\rangle := (\cdot, \varphi)_H .$$

By definition, the bra $\langle\varphi|$ is written

$$\langle\varphi| = (\varphi, \cdot)_H$$

In the case of the momentum operator, one writes the eigenkets as

$$|p\rangle\,(\,\cdot\,) = \int_{\mathbb{R}} (\,\cdot\,) e^{ipx/\hbar} dx.$$

Similarly to how we associated wave functions to elements of the anti-dual space. We can extend continuous operators defined on Φ to operators on $\Phi^{\times}$. For example, the momentum operator when considered as a map on Φ has no eigenfunctions. However, if we extend it to a map on $\Phi^{\times}$, we can find a system of eigenkets which are exactly $|p\rangle$. A similar construction can be made for the position operator and Hamiltonian operators with continuous spectrum. It is necessary to extend the operator so that it acts on kets and bras rather than just wave functions.

Let $A : \Phi \mapsto \Phi$ be continuous and for simplicity self-adjoint on H then we define its extension by $A^{\times} : \Phi^{\times} \mapsto \Phi^{\times}$ as follows. Let $|\varphi\rangle \in \Phi^{\times}$ and $\psi \in \Phi$

$$A^{\times} |\varphi\rangle\,(\psi) := |\varphi\rangle\,(A\psi)$$

When $|\varphi\rangle$ is the ket associated to a wavefunction $\varphi \in \Phi$, one can check that the above can be written

$$A^{\times} |\varphi\rangle\,(\psi) := |A\varphi\rangle\,(\psi)$$

We call the eigenfunctions of the extension $A^\times$ of an operator A generalised eigenfunctions of A. The eigenkets of A are exactly these generalised eigenfunctions.

In physics, one often sandwiches an observable A in between a bra and a ket. This is generally written as

$$\langle\psi| A |\varphi\rangle$$

However, the above is only well defined when φ and ψ are in the Hilbert space so that we can rewrite the above equation as an inner product. It is better written as $\langle\psi| A^\times |\varphi\rangle$. One can compute this to be

$$\langle\psi| A^\times |\varphi\rangle = (\psi, A\varphi)_H$$

where the result is what we would expect.

Given a self-adjoint observable $A : H \mapsto H$ and a rigged Hilbert space $\Phi \subset H \subset \Phi^\times$ such that $A\Phi \subset \Phi$, one can show that A has a complete set of eigenkets in $\Phi^\times$. This is the essence of the nuclear spectral theorem. The eigenkets are complete in the sense that the elements of φ can be written in terms of these eigenkets, and the operator A can be diagonalized in terms of these eigenkets. For the momentum operator, the decomposition is intimately linked with the Fourier transform. The nuclear spectral theorem ensures that given an observable and a possible wavefunction for the quantum mechanical system, we can find the probability of measuring some value of the observable for the quantum system.

2 Mathematical Framework

In this thesis, the necessary mathematics needed to rigorously describe quantum mechanics in the rigged Hilbert space formulation is presented. The basic theory of linear spaces is essential and will be briefly treated in Appendix A. An important topic is that of topological vector spaces which is the study of linear spaces equipped with a topology. Such spaces generalise the usual notions of Banach and Hilbert spaces. We are especially interested in locally convex spaces which are topological vector spaces in which the topology is generated by a family of semi-norms. We will require the family of semi-norms to countable and the space to be complete. A locally convex space satisfying these conditions is an example of a Fréchet space. In the case where the semi-norms in the family are simply norms induced by a family of inner products, the space is called a countably Hilbert space. For quantum mechanical applications, we will restrict ourselves to such spaces. We will further present various classes of operators and notions of their spectrum. These include bounded, unbounded, compact, Hilbert-Schmidt, and nuclear operators. Notably, closed, symmetric, essentially self-adjoint, and self-adjoint operators will be discussed. Afterwards, we will present the concept of the rigged Hilbert space and the nuclear spectral theorem. Also, we will study representations(isomorphisms) of rigged Hilbert spaces. We will provide formal definitions for bras and kets and justify the manipulations often used by physicists. The momentum operator will be used as a case study to give meaning to the various notions.

2.1 Topological Vector Spaces

A topological vector space generalises the notion of a normed vector space by equipping the linear space with an arbitrary topology rather than the topology induced by the norm.

Definition 2.1. Let Φ be a set and let $P(\Phi)$ denote the power set of Φ. A subset $\tau_\Phi \subset P(\Phi)$ is a *topology* if all its elements satisfy the following conditions:

1. $\emptyset \in \tau_\Phi$ and $\Phi \in \tau_\Phi$
2. The union of arbitrarily many elements of τ_Φ is in τ_Φ
3. The intersection of finitely many elements of τ_Φ is in τ_Φ

We call the pair (Φ, τ_Φ) a topological space. Further, the elements of τ_Φ are called *open* sets.

With this notion, we can generalise the definition of continuity of functions to arbitrary topological spaces.

Definition 2.2. Let (X, τ_X) and (Y, τ_Y) be topological spaces and $f : X \mapsto Y$ a function between them. We say f is continuous if

$$\forall\, O_{\tau_Y} \in \tau_Y, \ \ f^{-1}(O_{\tau_Y}) \in \tau_X$$

In other words, the pre-image of an open set is open.

The notions of convergence of sequences in metric spaces can be extended to topological spaces as follows:

Definition 2.3. A sequence $\{\varphi\}_n \in (X, \tau_X)$ converges to $\varphi \in X$ if for all open sets $O \in \tau_X$ where $\varphi \in O$, we have that there exists a $N \in \mathbb{N}$ such that $\forall n \geq N$, $\varphi_n \in O$.

We then say that $\lim_{\tau_X} \varphi_n = \varphi$

Given two topologies τ_{X_1}, τ_{X_2} of a set X, we say that τ_{X_1} is finer than τ_{X_2} if $\tau_{X_2} \subset \tau_{X_1}$. Similarly, we say that τ_{X_1} is courser than τ_{X_2} if $\tau_{X_1} \subset \tau_{X_2}$

Remark. Note that continuous functions between two topological spaces X and Y will remain continuous when X is given a finer topology. It is not guaranteed that the functions will remain continuous when X is given a courser topology. On the other hand, when Y is given a courser topology, continuous functions will remain continuous. Once again, when Y is given a finer topology, it is not guaranteed that the functions remain continuous.

We are now ready to state the definition of a Topological Vector Space(T.V.S).

Definition 2.4. The algebraic operations $+$ and $\cdot$ on a topological vector space (Φ, τ_Φ) are continuous if they are continuous as functions

$$+ : \Phi \times \Phi \mapsto \Phi \text{ given by } (\varphi, \psi) \mapsto \varphi + \psi$$

and

$$\cdot : \mathbb{C} \times \Phi \mapsto \Phi \text{ given by } (c, \psi) \mapsto c \cdot \psi$$

Where the space $\Phi \times \Phi$ is endowed with the product topology induced by Φ

Definition 2.5. A space Φ is a topological vector space if

- Φ is a linear space.
- Φ is a topological space.
- The algebraic operations on Φ are continuous.

For our purposes, we will be interested in a special class of topological vector spaces known as locally convex vector spaces. These spaces are similar to normed vector spaces except the topology is induced by a family of semi-norms rather than a single norm.

2.1.1 Locally Convex Linear Spaces

We will begin by studying linear spaces on which semi-norms are defined. The following definitions and theorems are taken from [6] and [7] We refer to these sources for a more in-depth treatment.

A semi-norm is simply a norm with the condition of non-degeneracy removed.

Lemma 2.1. *Let $p : X \mapsto \mathbb{R}$ be a semi-norm on a linear space X. Then the following properties hold $\forall x, y \in X$*

1. $p(0) = 0$
2. $p(x) \geq 0$
3. $|p(x) - p(y)| \leq p(x - y)$

Definition 2.6. Given a semi-norm p on a linear space X, we call

$$B_{y,\varepsilon}(p) = \{x \in X : p(y - x) < \varepsilon\}$$

a p-semiball of radius ε centered at $y \in X$.

Given a finite collection of semi-norms $p_1, \ldots, p_n$, we call

$$B_{y,\varepsilon}(p_1, \ldots, p_n) = B_{y,\varepsilon}(p_1) \cap \cdots \cap B_{y,\varepsilon}(p_n)$$

the $(p_1, \ldots, p_n)$-semi-ball of radius $\varepsilon > 0$ centered at $y \in X$

The above notion of semi-balls will allow us to definite a topology on a linear space as follows:

Definition 2.7. Let X be a linear space and $\mathcal{P}$ be a family of semi-norms on X. We define a topology on X by calling $A \subset X$ *open* if $\forall x \in X, \exists \varepsilon > 0$ and $p_1, \ldots, p_k \in \mathcal{P}$ such that $B_{x,\varepsilon}(p_1, \ldots, p_k) \subseteq A$. The space $(X, \mathcal{P})$ with the above topology is called a locally convex space.

The above definition can be simplified by the following claim.

Lemma 2.2. *Let $(X, \mathcal{P})$ be a locally convex space and $p_1, \ldots, p_k \in \mathcal{P}$. Let $p(x) : X \mapsto \mathbb{R}$ be defined as*

$$p(x) = \max\{p_1(x), \ldots, p_k(x)\}$$

then p(x) is a seminorm.

Theorem 2.3. *Let $\overline{\mathcal{P}} = \mathcal{P} \bigcup \{\max\{p_1(x), \ldots, p_k(x)\}, p_1, \ldots, p_k \in \mathcal{P}\}$ then $\tau_{\overline{\mathcal{P}}} = \tau_{\mathcal{P}}$. Thus $(X, \mathcal{P})$ and $(X, \overline{\mathcal{P}})$ are topologically equivalent.*

By the above theorem, given any locally convex space, we can always work with the so-called closure of $\mathcal{P}$. This is convenient since $B_{y,\varepsilon}(p_1, \ldots, p_n) = B_{y,\varepsilon}(p)$ where $p = \max\{p_1, \ldots, p_n\}$. Thus we the locally convex topology is induced purely by p-semi-balls. We will from now on always assume that the set of semi-norms is closed.

Using the definition of convergence in topological spaces, it can be readily checked that the following lemma holds.

Lemma 2.4. *Let $(X, \mathcal{P})$ be a locally convex space. A sequence $x_k \in X$ converges to $x \in X$ if and only if*

$$p(x_k - x) \to 0, \forall p \in \mathcal{P}$$

in the topology of $\mathbb{R}$

By the above results, we can now prove necessary and sufficient conditions for functions on locally convex spaces to be continuous.

Theorem 2.5. *Let (X, P) and $(Y, \mathcal{Q})$ be locally convex spaces.*

- *$f : X \mapsto Y$ is continuous iff $\forall x \in X, \varepsilon > 0, q \in \mathcal{Q}, \exists p \in \mathcal{P}, \delta > 0$ such that*

$$z \in B_{x,\delta}(p) \implies q(f(x) - f(z)) < \varepsilon$$

- *If f is linear, then f is continuous iff $\forall q \in \mathcal{Q}, \exists p \in \mathcal{P}, C > 0$ such that*

$$q(f(x)) \leq Cp(x)$$

- *an arbitrary semi-norm $q : X \mapsto \mathbb{R}$ on X is continuous iff $\exists p \in \mathcal{P}, C > 0$ such that*

$$q(x) \leq Cp(x)$$

Corollary 2.5.1. *Let $(X, \mathcal{P})$ and $(Y, \mathcal{Q})$ be locally convex spaces such that $X \subset Y$. The following statements are equivalent:*

1. *The embedding $i : X \mapsto Y$ is continuous.*
2. *$\forall q \in \mathcal{Q}, \exists p \in \mathcal{P}, C > 0$ such that*
$$q(x) \leq Cp(x)$$
3. *The restriction of every semi-norm of $(Y, \mathcal{Q})$ to $(X, \mathcal{P})$ is continuous.*

For our purposes, we wish to add further properties to our locally convex space in order for it to be *nicely* behaved. This will lead us to study *Fréchet* spaces.

2.2 Fréchet Spaces

A Fréchet space is a locally convex space such that the family of semi-norms is countable and the space is complete with respect to its topology. Furthermore, we impose a *separating* condition so that the induced topology is Hausdorff. Under these conditions, the space is metrizable, meaning it is well enough behaved that we can define a metric on the space.

Definition 2.8. A sequence $\{x_n\}$ in a locally convex space is Cauchy if it satisfies

$$\forall p \in \mathcal{P}, p(x_j - x_k) \to 0 \text{ as } j, k \to \infty$$

A locally convex space $(X, \mathcal{P})$ is *complete* if all Cauchy sequences have a limit in X.

Definition 2.9. A family of semi-norms $\mathcal{P}$ on X is called separating if for any $x \in X - \{0\}$, there exists a $p \in \mathcal{P}$ such that $p(x) \neq 0$. Under this condition, the space $(X, \tau_{\mathcal{P}})$ is Hausdorff.

Definition 2.10. A *Fréchet space* is a locally convex space where $(X, \mathcal{P})$ has countable and separating $\mathcal{P}$, and is complete.

Theorem 2.6. *Open Mapping Theorem for Frechét Spaces*

Let $A : X \mapsto Y$ be a continuous surjective map between the Frechét spaces X, Y. Then, A is an open mapping. It follows that if A is bijective then it has a bounded inverse A^{-1}.

Example 2.7. *A well-known example of a Fréchet space that plays a key role in quantum mechanics is the Schwartz space. This space is handy since many expectation values and differential operators used in quantum mechanics are well defined. Furthermore, the Fourier distribution is well-defined on the space.*

The Schwartz space[7] is defined as

$$S(\mathbb{R}^n) = \{f \in C^\infty(\mathbb{R}^n) : ||f||_{\alpha,\beta} < \infty \; \forall \alpha, \beta \in \mathbb{N}^n\}$$

where $||f||_{\alpha,\beta}$ is a family of norms given by

$$||f||_{\alpha,\beta} = \sup_{x \in \mathbb{R}^n} |x^\alpha D^\beta f(x)|$$

where the α, β are to be read in the multi-index notation.

2.3 Countably Hilbert Space

A countably Hilbert Space is a special case of a Fréchet space where the semi-norms are induced by inner products. These spaces and their dual spaces will be key in defining the notions of a Rigged Hilbert Space. To this end, we will explore these spaces in detail.

Definition 2.11. A *countably Hilbert space* is a linear space Φ on which a countable number of inner products is defined. In other words, for any $\varphi, \psi \in \Phi$, we have that there exists

$$\langle \varphi, \psi \rangle_1, \langle \varphi, \psi \rangle_2, \langle \varphi, \psi \rangle_3, \ldots$$

Further, we require the induced norms to be compatible so that if a sequence is Cauchy in $||\cdot||_p$ and $||\cdot||_q$ and it converges to zero in one of the norms, then it also converges to zero in the other. Without loss of generality[8], it can be assumed that the inner products satisfy

$$\langle \varphi, \varphi \rangle_1 \leq \langle \varphi, \varphi \rangle_2 \leq \langle \varphi, \varphi \rangle_3 \leq \ldots \tag{3}$$

Note that from the inner-products, the following countable family of norms can be defined as

$$||\varphi||_p = \sqrt{\langle \varphi, \varphi \rangle}_p$$

We can turn the countably Hilbert space into a locally convex space by equipping it with a family of (semi)norms $\mathcal{P} := \{||\cdot||_p\}_{p \in \mathbb{N}}$. The theory of the previous sections can then be used to induce a topology from these norms. We will always assume that the countably Hilbert space is equipped with the induced locally convex topology. Since the family of semi-norms $\mathcal{P}$ is actually a countable family of norms, it follows that a countably Hilbert space is a countable, separating locally convex space.

As a result, by taking the completion of a countably Hilbert space, we obtain a Fréchet space.

Theorem 2.8. *The completion of a countably Hilbert space is Fréchet.*

We are only interested in complete countably Hilbert spaces, therefore we will always assume that our countably Hilbert space is Fréchet.

It is interesting to know whether a (complete) countably Hilbert space is equivalent to some Hilbert space with respect to its topology. It turns out that there is a topologically equivalent Hilbert space only when the countably Hilbert space topology can be induced by a finite family of semi-norms.[8]

2.3.1 Dual space of a countably Hilbert Space

Let Φ_n denote the completion of a countably Hilbert space Φ with respect to the topology induced by its nth inner product. Equip the set Φ_n with the nth inner product so that Φ_n is a Hilbert space.

Now, since

$$||\phi||_1 \leq ||\phi||_2 \leq ||\phi||_3 \ldots$$

a sequence that converges in Φ with respect to the $||\cdot||_n$ norm must also converge with respect to $||\cdot||_k$ for all $k \leq n$. Thus the completed spaces Φ_i satisfy the following nested relation:

$$\Phi_1 \supset \Phi_2 \supset \Phi_3 \supset \ldots$$

We can obtain a similar relation for their dual spaces. Recall that,

Definition 2.12. *A (anti)linear functional $f : \Phi_n \mapsto \mathbb{C}$ is continuous iff*

$$\exists C > 0 \textit{ such that } f(\varphi) \leq C||\varphi||_n \textit{ for all } \varphi \in \Phi_n$$

If a linear functional f is continuous as a map from Φ_n then it must also be continuous as a map from Φ_k, $\forall k \geq n$ by the compatibility of the inner products in (3). In other words, continuous functionals on Φ_n are continuous functionals on $\Phi_m, \forall m \geq n$.

It follows, after identifying a function with the function obtained from restricting its domain, that the dual and anti-dual space satisfy the following relation:

$$\Phi_1' \subset \Phi_2' \subset \Phi_3' \subset \cdots \subset \Phi'$$

$$\Phi_1^\times \subset \Phi_2^\times \subset \Phi_3^\times \subset \cdots \subset \Phi^\times$$

To find the dual space of the countably Hilbert space Φ, we use the following result.

By Theorem 2.5, a linear functional $f : \Phi \mapsto \mathbb{C}$ is a continuous iff it is bounded with respect to one norm in the countably Hilbert space. That is,

$$\exists p \in \mathbb{N}\,, C > 0 \text{ such that } f(\varphi) \leq C||\varphi||_p \text{ for all } \varphi \in \Phi$$

Any continuous functional on Φ that is bounded with respect to the norm $||\cdot||_n$, where n is arbitrary, can be uniquely extended to a continuous functional on Φ_n since Φ is dense in Φ_n. Identifying the functional with its extension, we find

$$\Phi' \subset \bigcup_{n=1}^{\infty} \Phi_n' \tag{4}$$

Similarly, by Theorem 2.5 the restriction of continuous functionals of Φ_n to Φ are necessary continuous with respect to Φ. Thus identifying elements of the dual space of Φ_n with its restriction to Φ, we find that

$$\bigcup_{n=1}^{\infty} \Phi_n' \subset \Phi' \tag{5}$$

Combining equations 4 and 5 gives

$$\Phi' = \bigcup_{n=1}^{\infty} \Phi_n'$$

Similarly, we find

$$\Phi^\times = \bigcup_{n=1}^{\infty} \Phi_n^\times$$

From the above it follows that the (anti)dual space of a countably Hilbert space is larger than the dual space of the Hilbert spaces Φ_n.

2.4 Linear operators on Linear Spaces and their Spectrum

In quantum mechanics, observables are represented as self-adjoint linear maps defined on a Hilbert space. We will introduce the necessary notions of bounded, unbounded, and compact operators; as well as the notion of the adjoint of an operator. Further, we will study the eigenvalues and eigenvectors of special types of operators. Nuclear operators which are key in the construction of Nuclear Fréchet spaces and Rigged Hilbert spaces will be introduced as well.

Definition 2.13. A *linear operator* A on a Hilbert space H is a linear map $A : H \mapsto H$. We call the map A *bounded* if $\exists C > 0 : \forall x \in H$, $||Ax|| \leq C||x||$. Otherwise, the map is *unbounded*.

We will denote by $B(H)$ to be the set of all bounded operators on the space H that map to H.

2.4.1 Bounded operators In Hilbert spaces

Definition 2.14. We say that a bounded linear operator $A \in B(H)$ is invertible if A has a bounded inverse.

Theorem 2.9. *If an operator $A : H \mapsto H$ is bounded then there exists a unique operator $A^* : H \mapsto H$ such that*

$$\langle Ax, y\rangle = \langle x, A^*y\rangle$$

$\forall x, y \in H$

The operator A^* is called the *adjoint* of A.

Definition 2.15. if $A = A^*$ then we call A *self-adjoint* or *hermitian*

Definition 2.16. We call a bounded operator A *normal* if satisfies

$$A^*A = AA^*$$

It is easy to see that all self-adjoint operators are normal. However, the converse is not necessarily true.

A special case of a normal operator is the so called unitary operator.

Definition 2.17. A *unitary* operator U on a Hilbert space H is an operator that satisfies

$$||Uf|| = ||f||, \forall f \in H$$

Further, it can be shown that U satisfies

$$UU^* = U^*U = I$$

A similar notion is that of partial isometries. It is trivial that unitary operators are a special case of partial isometries.

Definition 2.18. An operator U on H is a *partial isometry* if it is unitary on the orthogonal compliment of its kernel. Equivalently, we say that there is some closed subspace $M \subset H$ such that the restriction of U to M is unitary.

In other words,

$$U^*U = P_M$$

where P_M is the orthogonal projection onto the subspace M.

Definition 2.19. We call an operator $A \in B(H)$ *compact* if for every bounded sequence $\{\varphi_n\} \in H$, the sequence $\{A\varphi_n\}$ has a convergent subsequence in H.

Definition 2.20. An operator $A \in B(H)$ is *positive definite* if it is a self-adjoint operator such that

$$\langle A\varphi, \varphi\rangle > 0, \forall \varphi \in H \text{ such that } \varphi \neq 0$$

2.4.2 The Spectrum of Bounded Operators

Definition 2.21. Let A be in $B(H)$. The *resolvent set* of A is

$$Re(A) = \{\lambda \in \mathbb{C} : (A - \lambda I) \text{ is invertible }\}$$

The spectrum of A is the complement of the resolvent set given by

$$\sigma(A) = \mathbb{C} \setminus Re(A)$$

It is known that the resolvent set is open and thus the spectrum is closed in $\mathbb{C}$. [9]

Definition 2.22. We call an element $\varphi \in H$ an eigenvector of an operator $A \in B(H)$ and $\lambda \in \mathbb{C}$ its corresponding eigenvalue if

$$A\varphi = \lambda\varphi$$

Clearly, eigenvalues are in $\sigma(A)$.

Theorem 2.10. *The spectrum of a bounded operator $A \in B(H)$ is a bounded closed set in $\mathbb{C}$. Additionally,*

$$|\lambda| \leq ||A||$$

where $||A||$ is the operator norm of A given by

$$||A||_{B(H)} = \sup_{\varphi \in H} \frac{||A\varphi||_H}{||\varphi||_H}$$

In quantum mechanics, the spectrum can be divided into two groups called the discrete spectrum and continuous spectrum. The discrete spectrum of an operator A consists of all its eigenvalues. The remaining elements of $\sigma(A)$ are in the continuous spectrum. This is departure from the spectral theory of operators on finite dimensional spaces where the spectrum is always discrete. We see that elements in the spectrum do not necessarily have a corresponding eigenvector.

Theorem 2.11. *The spectrum of a self-adjoint operator is always real.*

2.4.3 Bounded Operator decompositions and Nuclear Operators

In general, self-adjoint operators(not necessarily bounded) can be diagonalised in its so-called spectral decomposition.

The spectral decomposition is given below for the special case of a compact self-adjoint operator.

Theorem 2.12. *Let $A \in B(H)$ be a compact self-adjoint operator then A can be decomposed in terms of its eigenvectors e_n and eigenvalues λ_n as*

$$A\varphi = \sum_{n=1}^{\infty} \lambda_n \langle \varphi, e_n \rangle$$

In general, a compact operator can be decomposed as the product of a partial isometry and a positive definite operator.

Theorem 2.13. *Let A be a compact operator in $B(H)$. Then A can be written as*

$$A = U|A|$$

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

The decomposition allows us to define a diagonal decomposition of compact operators.

Theorem 2.14. *Any compact operator $A \in B(H)$ can be written as*

$$A\varphi = \sum_{n=1}^{\infty} \lambda_i \langle \varphi, e_n \rangle h_n$$

where e_n are eigenvectors of $|A|$ and h_n are given by $h_n = Ue_n$. The e_n are normalized so that $\{e_n\}$ and $\{h_n\}$ each form an orthonormal basis of H.

Stricter conditions on the above decomposition give a new class of operators.

Definition 2.23. A compact operator $A = U|A|$ is called *Hilbert-Schmidt* if $\sum_{n=1}^{\infty} \lambda_n^2 < \infty$ where λ_n are the eigenvalues of $|A|$. Furthermore, we call the operator decomposition given in theorem 2.14, the *Hilbert Schmidt decomposition.*

An even stricter class of operators are the *nuclear operators* which are key in the construction of Nuclear Hilbert spaces.

Definition 2.24. A compact operator A is called *nuclear or trace class* if $\sum_{i=1}^{\infty} \lambda_n < \infty$ where λ_n are the eigenvalues of $|A|$ in the Hilbert-Schmidt decomposition.

It can be seen that all nuclear operators are necessarily Hilbert-Schmidt.

With the notion of nuclear operators, one can extend the definition of trace in finite dimensional of spaces to infinite dimensional spaces.

Definition 2.25. The trace of an operator A that can be written in the form given in theorem 2.14 denoted by $Tr(A)$ is defined as

$$\sum_{n=1}^{\infty} \langle e_n, Ae_n \rangle$$

where e_n form an orthonormal basis of H. It is known that its value is independent of the choice of basis.

Theorem 2.15. *An operator admitting a Hilbert-Schmidt decomposition is nuclear if and only if it has finite trace. Further, the trace of a nuclear operator is given by*

$$Tr(A) = \sum_{i=1}^{\infty} \lambda_n$$

2.4.4 Unbounded Linear Operators

In quantum mechanics, possible measurement values are given by the spectrum of a self-adjoint operator. The spectrum is necessarily real and so are our measurements. In many cases, it is known that the possible measurement values are unbounded. For example, an electron's energy and momentum is unbounded from above. Since bounded operators have a bounded spectrum, these are not ideal candidates to describe quantum systems. Thus one generally requires that the observables are unbounded self-adjoint operators defined on a Hilbert space. Unfortunately, there are a few caveats that arise from this as we will see. The existence of an adjoint for unbounded operators is not guaranteed unlike in the case of the bounded operators. Furthermore, self-adjoint unbounded operators must be defined on a strict subspace (ideally dense) of the Hilbert space. From now on, we will always assume the operators are densely defined in H.

Definition 2.26. Let A and B be two operators defined on a (dense) subset of H. Denote their respective domains by $D(A)$ and $D(B)$. A is an *extension* of B if $D(B) \subset D(A)$ and $A\varphi = B\varphi$, $\forall \varphi \in D(B)$. We then say that $B \subset A$ and further that B is the *restriction* of A to $D(B)$

For a special class of operators, one can define its unique extension called its *closure.*

Let A be an unbounded operator on H. We will denote its extension by $\overline{A}$ which will be constructed as follows. The following argument is based on the construction given in [8]. Let $\{\varphi_n\} \in H$ be a Cauchy sequence. Suppose $\{A\varphi_n\}$ is also Cauchy, then since both Cauchy sequences must converge in H, we can define $\varphi = \lim \varphi_n$ and $\psi = \lim A\varphi_n$. We then say that $\overline{A}\varphi = \psi$. However, for this extension to be well defined, we require that the limit of the Cauchy sequence $A\varphi_n$ is independent of the chosen Cauchy sequence that converges to φ. If A is continuous/bounded then it is trivial that if any two Cauchy sequences φ_n and φ_n' converge to φ then $A\varphi_n$ and $A\varphi_n'$ both converge to ψ. In the case of unbounded operators, this is not guaranteed.

The class of operators A for which the above extension $\overline{A}$ exists are called *closable.* The definition of a closable operator can be put in a more rigorous form by use of its graph.

Definition 2.27. The graph of an operator A denoted by $G(A)$ is defined as the set

$$G(A) = \{(\varphi, A\varphi) : \varphi \in D(A)\} \subset D(A) \times D(A)$$

Definition 2.28. An operator A is *closed* if its graph $G(A)$ is closed in the product topology. If there exists an operator $\overline{A}$ such that $G(\overline{A}) = \overline{G(A)}$ then we say that $\overline{A}$ is the *closure* of A. Clearly, $\overline{A}$ extends A.

Definition 2.29. An operator A is *closable* if its extension $\overline{A}$ exists. Further, an operator A is called *closed* if

$$A = \overline{A}$$

2.4.5 Spectral notions and classes of Unbounded Operators

Definition 2.30. Let A be a closed unbounded operator on H. The resolvent set $Re(A)$ is defined as

$$Re(A) := \{\lambda \in \mathbb{C} : (A - \lambda I) \text{ is a bijection from } D(A) \mapsto H \text{ with bounded inverse}\}$$

The definition of spectrum, discrete spectrum, and continuous spectrum are the same as in the bounded case.

Whenever an unbounded operator is densely defined, we can define its *adjoint*.

Definition 2.31. Let $A : D(A) \subset H \mapsto H$ be an unbounded densely defined operator. We define the domain of the adjoint of A, A^* by

$$D(A^*) = \{f \in H : \exists z \in H \text{ such that } \langle f, Ag\rangle = \langle z, g\rangle, \forall g \in H\}$$

We define A^* by $A^*f = z$. The element z is unique by the denseness of $D(A)$ so A^* is well defined. Thus

$$\langle f, Ag\rangle = \langle A^*f, g\rangle, \forall f \in D(A), \forall g \in D(A^*)$$

Theorem 2.16. *The adjoint A^* of A is always closed.*

The notion of a self-adjoint operator can be generalised by *symmetric* operators.

Definition 2.32. An operator A on H is *symmetric* if $D(A)$ is dense in H and

$$\langle Af, g\rangle = \langle f, Ag\rangle, \forall f, g \in D(A)$$

An operator is symmetric iff $A \subset A^*$. A is called *self-adjoint* if $D(A)$ is dense in H and $A = A^*$. We call A *essentially self-adjoint* if $\overline{A}$ is self-adjoint.

Theorem 2.17. *If A is a symmetric operator then it is closable.*
The closure of a symmetric operator A is exactly A^{**}

Proof. See previous theorem. Uniqueness follows from construction. □

Since essentially self-adjoint operators are symmetric, it follows that $\overline{A} = A^{**}$. However by definition, $\overline{A}$ is self-adjoint so that $A^* = A^{**}$.

The following summary taken from [8] illustrates the above nicely.

- A is symmetric iff $A \subset \overline{A} = A^{**} \subset A^*$
- A is essentially self adjoint iff $A \subset \overline{A} = A^{**} = A^*$
- A is self-adjoint iff $A = \overline{A} = A^{**} = A^*$

It should be noted that essentially self-adjoint operators have a unique self-adjoint extension. The same is not necessarily true for symmetric operators. An interesting consequence of the above results is that higher order adjoints of operators are not interesting. For example, from Corollary 3.18.1, $A^{**} = \overline{A^{**}} = A^{****}$ and $A^{*} = \overline{A^{*}} = A^{***}$.

The following theorem entirely classifies self-adjoint operators defined on the entire Hilbert space. It tells us that unbounded self-adjoint operators must be defined on a strict subspace of the Hilbert space.

Theorem 2.18 (Helllinger-Toeplitz). *Let A be an everywhere defined operator on a Hilbert space H with $\langle f, Ag\rangle = \langle Af, g\rangle$, $\forall f, g \in H$. Then A is bounded. In other words, unbounded symmetric operators cannot be defined on all of H. [9]*

2.5 Nuclear Rigged Hilbert Space

We are now ready to define the notion of nuclear Rigged Hilbert spaces. We will proceed by defining a special class of countably Hilbert spaces known as nuclear spaces. [10]

2.5.1 Nuclear Spaces

Let Φ be a countably Hilbert space with the sequence of inner products

$$\langle \varphi, \varphi\rangle_1 \leq \langle \varphi, \varphi\rangle_2 \leq \ \dots$$

Denote Φ_n as the completion of Φ with respect to the norm $||\varphi||_n = \sqrt{\langle \varphi, \varphi\rangle_n}$. We then obtain the sequence of spaces

$$\Phi_1 \supset \Phi_2 \supset \ \cdots \supset \Phi$$

Φ is dense in each Φ_n by construction. We define $\varphi^{[n]}$ and $\varphi^{[m]}$ to be the element $\varphi \in \Phi$ considered as an element of Φ_n and Φ_m, respectively. The following identity mapping is well defined,

$$id^n_m : \Phi \subset \Phi_n \mapsto \Phi \subset \Phi_m,$$

$$\phi^{[n]} \mapsto \phi^{[m]}$$

Furthermore, for $m \leq n$, the mapping is continuous in their respective topologies. Thus we can uniquely extend id^n_m to be defined on all of Φ_n by denseness of Φ. Denote this extension by T^n_m.

Definition 2.33. A countably Hilbert space Φ is called *nuclear* if for any n there exists an m such that the inclusion map T^n_m is *nuclear* i.e.

$$T^n_m \varphi = \sum_{k=1}^{\infty} \lambda_k \langle e_k, \varphi\rangle_n h_k$$

$$\sum_{k=1}^{\infty} \lambda_k < \infty$$

for all $\phi \in \Phi_n$ where $\{e_k\}$ and $\{h_k\}$ are orthonormal systems of Φ_n and Φ_m, respectively.

From this it follows that T^n_m is necessarily of class Hilbert-Schmidt and thus necessarily compact. Nuclear spaces have a number of interesting properties that are similar to finite dimensional spaces. Because of this, they are convenient to work with. In general, proving that a space is nuclear is a difficult task. We will in general assume that the spaces we work with are nuclear. For more information on nuclear spaces, we refer to [10].

2.5.2 Nuclear Rigged Hilbert Spaces, bras, kets and its Application to Momentum

Let Φ be a nuclear countably Hilbert space. We introduce a primary inner product $\langle \cdot, \cdot \rangle$ on Φ such that the inclusion map of Φ into H is continuous with respect their topology. By completing Φ with respect to the topology induced by $\langle \cdot, \cdot \rangle$, we obtain a Hilbert space H. By continuity of the inner product, the inclusion map $i : \Phi \mapsto H$ is continuous so that we may identify the elements of Φ with those of H giving

$$\Phi \subset^i H \tag{6}$$

It is known[8] that if $\langle \cdot, \cdot \rangle$ is continuous with respect to the countably Hilbert space topology that we can construct a countably Hilbert space Φ^0 with the sequence of inner products

$$\langle \cdot, \cdot \rangle \leq \langle \cdot, \cdot \rangle_1^0 \leq \langle \cdot, \cdot \rangle_2^0 \dots \tag{7}$$

such that Φ^0 has the same countably Hilbert space topology as Φ. We will without loss of generality assume that Φ has a sequence of inner products of the form (7). It is now clear that the topology on Φ is finer than that of H so that

$$H^\times \subset^{i^*} \Phi^\times \tag{8}$$

where $i^* : H^\times \mapsto \Phi^\times$

Since H is isomorphic to $H^\times$ by Riesz representation theorem, we can identify the elements of H with those of $H^\times$. Now, by combining (6) and (8), we obtain the *Gelfand Triplet.*

$$\Phi \subset^i H \subset^{i^*} \Phi^\times$$

Definition 2.34. A *nuclear rigged Hilbert space* is a triple of spaces Φ, H, $\Phi^\times$ where Φ is a countably nuclear Hilbert space, H is a Hilbert space obtained by the completion of Φ with respect to one of its inner products, and $\Phi^\times$ is the anti-dual space of Φ. Equivalently, we say that the triple of spaces is a *rigging* of the Hilbert space H if Φ is a dense nuclear space with a finer topology such that the inclusion map into H is continuous.

Remark. Using this framework, we can assign a mathematical meaning to Dirac's bras and kets. We say that the antilinear functionals of $\Phi^\times$ are *kets* and that the linear functionals of Φ' are *bras.* We will denote kets by $|f\rangle$ and bras by $\langle f|$.

Further, we will define the complex conjugate of a ket $|f\rangle \in \Phi^\times$ as the complex conjugate of whatever it evaluates to. The complex conjugate of a bra is defined similarly. That is.

$$\overline{|f\rangle}(\varphi) = \overline{|f\rangle\,(\varphi)}$$

It can be easily seen that the conjugate of a ket is a bra and the conjugate of a bra is a ket. Thus, there is a one to one pairing between kets and bras. For this reason, we will use the following convention,

$$\langle f| := \overline{|f\rangle}$$
$$|f\rangle := \overline{\langle f|}$$

In addition, we use the following notation for the action of a bra and ket on the elements of Φ.

$$\langle \varphi | f \rangle := |f\rangle\,(\varphi) \tag{9}$$
$$\langle f | \varphi \rangle := \langle f|\,(\varphi) \tag{10}$$

The above notation should not be confused with the inner product which is given by $\langle \cdot, \cdot \rangle$. One may notice that the notation of (9) and (10) is rather ambiguous as there is no way to tell whether a bra $\langle \phi|$ is acting on a function f or whether a ket $|f\rangle$ is acting on a function ϕ. In general, it should be clear from the context what is meant. However, in quantum mechanics, we are only interested in kets $|f\rangle$ that are integral operators so that $|f\rangle = \int f \cdot (\,.\,)dx$. Furthermore, the inner product we work with is similarly given by $\langle f, g\rangle = \int f(x)g(x)dx$. In this case, (9) and (10) can be evaluated both ways and give the same answer. Technically, the integrand f of $|f\rangle$ may not actually be in Φ or H so that $\langle\varphi|\,(f)$ is not well defined as an element of the dual space. However, if one ignores domain issues and just computes $\langle\varphi|\,(f)$ treating $\langle\varphi|$ as a bra, one will obtain the correct answer.

It is no coincidence that (9) and (10) are strikingly similar to the inner product of H. In certain cases (9) and (10) exactly correspond with the inner product. This is when f and φ are both elements of the Hilbert space. Given an element $\varphi \in \Phi$, we can assign it to a ket and bra by means of the inner product using the following maps,

$$|\varphi\rangle := \langle\cdot, \varphi\rangle$$

$$\langle\varphi| := \langle\varphi, \cdot\rangle$$

The action of the above ket and bra on an element $\psi \in \Phi$ is given by

$$\langle\psi|\varphi\rangle = \langle\psi, \varphi\rangle$$

$$\langle\varphi|\psi\rangle = \langle\varphi, \psi\rangle$$

We see that in this case, the ambiguity can safely be ignored as $|\varphi\rangle$ and $\langle\psi|$ are well defined elements in $\Phi^\times$ and Φ', respectively. The above concepts will be further illuminated in the following example.

Example 2.19. *Let $S(\mathbb{R})$ be the Schwartz space. We can define an inner product as*

$$\langle\varphi, \psi\rangle = \int_{-\infty}^{\infty} \overline{\varphi(x)}\psi(x)dx$$

$S(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ so that the completion of $S(\mathbb{R})$ gives $L^2(\mathbb{R})$. $S(\mathbb{R})$ can be equipped with a locally convex topology such that it is nuclear[8]. Therefore we have the rigged Hilbert space

$$S(\mathbb{R}) \subset L^2(\mathbb{R}) \subset S(\mathbb{R})^\times$$

We call the elements of $S(\mathbb{R})^\times$ distributions. The momentum operator $-i\hbar\frac{d}{dx}$ is well defined on $S(\mathbb{R})^\times$ and its (generalized) eigenfunctions can easily be computed to be $e^{ix/\hbar}$. However, these functions are not members of the Hilbert space $L^2(\mathbb{R})$ since they are not normalizable. Instead, we can consider them as members of $S(\mathbb{R})^\times$ by the following map,

$$|e^{ipx/\hbar}\rangle(\varphi) = \langle\varphi|e^{ipx/\hbar}\rangle := \int_{-\infty}^{\infty} \overline{\varphi(x)}e^{ipx/\hbar}dx$$

We call such anti-linear functionals generalised eigenfunctions of the momentum operator since they are not in on the Hilbert space.

By use of the Gelfand Triplet, we can generalise the notion of eigenvectors of (possibly unbounded) self-adjoint operators so that each element of the continuous spectrum can be assigned a *generalised eigenfunction.* To do so, we define the extension of an operator defined on Φ to an operator defined on $\Phi^\times$.

Definition 2.35. Let $A : \Phi \mapsto \Phi$ be a continuous operator. We define the map $A^\times : \Phi^\times \mapsto \Phi^\times$ by

$$|f\rangle(\varphi) \mapsto A^\times|f\rangle(\varphi) := |f\rangle(A\varphi),\ \forall|f\rangle \in \Phi^\times$$

We call $A^\times$ the conjugate of A.

We can also define the conjugate of A as a map on the dual space Φ' as follows.

Definition 2.36. Let $A : \Phi \mapsto \Phi$ be a continuous operator. We define the map $A^\times : \Phi' \mapsto \Phi'$ by

$$\langle f|(\varphi) \mapsto \langle f|(\varphi)A^\times := \langle f|(A^*\varphi),\ \forall \langle f| \in \Phi^\times$$

Remark. In physics, often we identify A with its conjugate and use the following notation,

$$\langle\varphi|\, A\, |\psi\rangle := A^\times\, |\psi\rangle\, (\varphi) = \langle\varphi|\, A^\times(\psi)$$

This is only strictly correct when φ and ψ are in Φ so that the bra-ket corresponds with the inner product. In this case, we see that by the definition of $A^\times$ that we obtain the same result whether we have $A^\times$ act on the bras or kets. In general, it should be clear from the context whether $A^\times$ is meant to act from the left or from the right.

Here, we employ the bra-ket notation and use the convention that operators act on the right of bras and the left of kets. In practice, one often identifies A with its conjugate. This is justified by the following result.

Theorem 2.20. *The space Φ can be embedded in $\Phi^\times$ and Φ'. As a result, we can identify elements of Φ with those in its dual and anti-dual space.*

Proof. We prove by construction. Consider the two maps,

$$i : \Phi \mapsto \Phi^\times,\ \ i(\varphi) \mapsto |\varphi\rangle := \langle\cdot, \varphi\rangle \tag{11}$$

$$i : \Phi \mapsto \Phi',\ \ i(\varphi) \mapsto \langle\varphi| := \langle\varphi, \cdot\rangle \tag{12}$$

where $\langle\cdot, \varphi\rangle$ and $\langle\varphi, \cdot\rangle$ are inner products with an empty slot. The continuity of the functionals with respect to the countably Hilbert space topology follows from the continuity of the inner product. It can be checked that the maps are algebraic isomorphisms of the linear structure of Φ. □

The action of $A^\times$ on the images of the maps (11) and (12) behave exactly like the action of A^* and A on their respective pre-images. This can be seen by noting that

$$A^\times|\varphi\rangle(\psi) = \langle A\psi|\varphi\rangle = \langle A\psi, \varphi\rangle = \langle\psi|A^*\varphi\rangle$$

Now by identifying the domain and image of (11), we find

$$A^\times|\varphi\rangle = |A^*\varphi\rangle =^i A^*\varphi$$

A similar computation shows that

$$\langle\varphi|A^\times = \langle A\varphi| =^i A\varphi$$

which also follows from

$$(A^*)^\times|\varphi\rangle = |A\varphi\rangle =^i A\varphi$$

The above results warrant their own theorem.

Theorem 2.21. *The map $A^\times : \Phi^\times \mapsto \Phi^\times$ is an extension of $A^* : \Phi \mapsto \Phi$ to the anti-dual space. Similarly, the map $(A^*)^\times : \Phi^\times \mapsto \Phi^\times$ is an extension of $A : \Phi \mapsto \Phi$ to the anti-dual space. If A is hermitian then $A^\times$ extends A to the anti-dual space.*

Notice that if A is not hermitian then $A^\times$ does not extend A and the notation is misleading. In quantum mechanics, the observables are generally hermitian so that we do not need to worry about this. We will see when we look at non-hermitian observables that this will be of importance.

In the case that A is self-adjoint so that $A = A^*$ then we have that $A^\times$ extends A to $D(\Phi^\times)$. We say that $A \subset A^\times$. Now that this extension is well defined and using it, we can generalize the notion of eigenvectors.

Definition 2.37. Let $A : \Phi \subset H \mapsto \Phi \subset H$ be a densely defined self-adjoint operator on H. Let $A^\times : \Phi^\times \mapsto \Phi^\times$ be the extension of A. We say that $|\lambda\rangle \in \Phi^\times$ is a *generalised eigenvector* or *eigenket* of A with *generalised eigenvalue* $\lambda \in \mathbb{C}$ if

$$A^\times|\lambda\rangle = \lambda|\lambda\rangle$$

Lemma 2.22. *Let $A : \Phi \subset H \mapsto \Phi \subset H$ be a densely defined self-adjoint operator. Let $\varphi \in \Phi$ be an eigenvector of A with eigenvalue λ. Then $|\varphi\rangle := i(\varphi)$ is a generalised eigenvector i.e.*

$$A^\times|\varphi\rangle = \lambda|\varphi\rangle$$

Proof. We prove this by considering the action of the functional on an arbitrary element $\psi \in \Phi$. We then use the fact that the action of these linear functionals is defined in terms of their inner product. Note,

$$A^\times|\varphi\rangle(\psi) = \langle A\psi, \varphi\rangle = \langle \psi, A\varphi\rangle = \langle \psi, \lambda\varphi\rangle = \lambda\langle \psi, \varphi\rangle = \lambda|\varphi\rangle(\psi)$$

Thus,

$$A^\times|\varphi\rangle = \lambda|\varphi\rangle$$

It follows that $|\varphi\rangle$ is a generalised eigenvector.

□

The above proof shows that the notion of a *generalized eigenvector* is indeed a *generalization* of eigenvectors. It follows that all eigenvectors are generalised eigenvectors when identified with its functional. However, the converse is not necessarily true. The spectrum of $A^\times$ can be defined in the usual way. However, for our purposes, we are only interested in the discrete spectrum.

Definition 2.38. The *generalized (discrete) spectrum* of a self-adjoint operator $A : \Phi \mapsto \Phi$ is

$$\sigma^\times(A) := \{\lambda \in \mathbb{C} :\ \exists|\lambda\rangle \in \Phi^\times \text{ such that } A^\times|\lambda\rangle = \lambda|\lambda\rangle\}$$

It follows that

$$\sigma(A) \subset \sigma^\times(A)$$

We will now present the Nuclear Spectral Theorem on which the foundation of rigged Hilbert space quantum mechanics is based.

2.5.3 Nuclear Spectral Theorem and Momentum Operator as Example

The following theorem guarantees a diagonal decomposition of a self-adjoint operator in terms of its generalised eigenvectors. Further, it states that the generalized eigenvectors form a basis for Φ and in a sense are complete. The theorem only guarantees the existence of the decomposition and gives no way of actually constructing it. For given operators, there are techniques to directly compute the generalized eigenvectors and Borel measures[11].

Theorem 2.23 (Nuclear Spectral Theorem)**.** *Let Φ be a nuclear Fréchet space and $\Phi \subset H \subset \Phi^\times$ a Gelfand triple. Let $(A, D(A))$ be a self-adjoint operator on the Hilbert space H such that $\Phi \subset D(A)$ and $A\Phi \subset \Phi$. Then for some countable set K the operator A has a complete system $\{|\lambda\rangle_k\}$of generalised eigenvectors in $\Phi^\times$. Further, there exists finite Borel measures $\{\mu_k\}_{k\in K}$ such that for $\varphi \in \Phi$,*

$$|\varphi\rangle = \sum_{k\in K} \int_{\mathbb{R}} \langle\lambda|\varphi\rangle|\lambda\rangle d\mu_k(\lambda) \tag{13}$$

and

$$|A\varphi\rangle = \sum_{k\in K} \int_{\mathbb{R}} \lambda\langle\lambda|\varphi\rangle|\lambda\rangle d\mu_k(\lambda) \tag{14}$$

It should be noted that the same result holds if $\Phi^\times$ is replaced with Φ'. The generalised eigenvectors of the two spaces are related by their complex conjugation.

Remark. Often in physics, we have an observable A with a discrete and continuous spectrum. In this case, the decomposition is usually of the form

$$|\varphi\rangle = \sum_{\lambda_n \in \sigma(A)} \langle \lambda_n, \varphi\rangle \, |\lambda_n\rangle + \int_{\lambda \in \sigma(A)} \langle \lambda|\varphi\rangle |\lambda\rangle d\mu(\lambda)$$

where we have a sum over the discrete spectrum λ_n and an integral over the continuous spectrum λ. Notice that the first term of the sum contains the inner product since $|\lambda_n\rangle$(technically its integrand) is an eigenvector in the Hilbert space. One can clearly see that when the spectrum is purely discrete it corresponds with the standard spectral decomposition in terms of its eigenvectors.

Definition 2.39. The Fourier transform is a unitary map

$$\mathcal{F} : S(\mathbb{R}) \mapsto \mathcal{F}(S(\mathbb{R}))$$

given by

$$\varphi(x) \mapsto \widetilde{\varphi}(p) = \mathcal{F}(\varphi) := \sqrt{\frac{1}{2\pi\hbar}} \int_{-\infty}^{\infty} \overline{\varphi(x)} e^{ipx/\hbar} dx \tag{15}$$

Its inverse is given by

$$\widetilde{\varphi}(p) \mapsto \varphi(x) = \mathcal{F}^{-1}(\widetilde{\varphi}) := \sqrt{\frac{1}{2\pi\hbar}} \int_{-\infty}^{\infty} \overline{\widetilde{\varphi}(p)} e^{ipx/\hbar} dp \tag{16}$$

Example 2.24. *Consider the momentum operator $P = -i\hbar\frac{d}{dx}$ and the Gelfand Triple as defined in Example 2.19. It can be shown that the anti-linear functionals*

$$|e^{ipx/\hbar}\rangle(\varphi) = \langle \varphi | e^{ipx/\hbar}\rangle := \int_{-\infty}^{\infty} \overline{\varphi(x)} e^{ipx/\hbar} dx \tag{17}$$

are generalised eigenfunctions. In fact, they are a complete set of generalised eigenfunctions.

Further, it is known that the Fourier transform $\mathcal{F}$ is a well-defined map on $S(\mathbb{R})$ that can be extended to all of $L^2(\mathbb{R})$.

Now, note that $|p\rangle := \int_{\mathbb{R}} dp \sqrt{\frac{1}{2\pi\hbar}}\, e^{ipx/\hbar}$ is also a generalised eigenvector with eigenvalue p. Comparing (17) *and* (16) *gives $\langle \phi | p\rangle = \widetilde{\varphi}(p)$. We can obtain the decompositions* (13) *and* (14) *by substituting* (15) *into* (16) *which gives*

$$\varphi(x) = \int_{-\infty}^{\infty} \overline{\langle \varphi | p\rangle} e^{ipx/\hbar} dp$$

which implies

$$|\varphi(x)\rangle = \int_{-\infty}^{\infty} \langle p|\varphi\rangle |p\rangle dp$$

Further by checking the action of the momentum operator P on $\varphi(x)$, it can be shown that

$$P^\times \, |\varphi\rangle = |P\varphi\rangle = \int_{-\infty}^{\infty} p \langle p|\varphi\rangle |p\rangle dp$$

Note in the above that we identify ϕ with $|\phi\rangle$ to obtain a diagonal expansion in Φ.

It is interesting to note that the generalized eigenfunctions are normalized in the sense of the Dirac function,

$$\int_{-\infty}^{\infty} e^{ipx/\hbar} e^{iqx/\hbar} dx = 2\pi\hbar \cdot \delta(p-q)$$

For this reason, we define

$$\langle p|q\rangle := \delta(p-q)$$

Because of the above example, the decomposition 14 is often called a *generalised Fourier transform*

2.6 Representations of Rigged Hilbert Spaces

One can define a class of *isomorphic* rigged Hilbert spaces by means of unitary maps between their respective Hilbert Spaces. The unitary map of the Hilbert spaces can be extended to be a map on the anti-dual space of Φ and restricted to be unitary on Φ with respect to the Hilbert space inner product. In the next section, we will see how this gives rise to the momentum, position, and energy representation in Quantum Mechanics.

Definition 2.40. A *representation* of a rigged Hilbert space is an element of the equivalence class of isomorphic rigged Hilbert spaces. We say two representations are *isomorphic* if there exists a unitary map between their Hilbert spaces such that its restriction to the countably Hilbert spaces are homeomorphic under the countably Hilbert topologies.

Let

$$\Phi \subset H \subset \Phi^{\times}$$

be a nuclear Rigged Hilbert space. Furthermore, Suppose

$$U : H \mapsto \mathcal{H}$$

is a unitary map between two Hilbert spaces. Let $\Psi = U(\Phi)$ then we claim that Ψ is also a nuclear countably Hilbert space.

Theorem 2.25. *Let $\Phi \subset H$ be a nuclear countably Hilbert space compatible with the inner product of H and $U : H \mapsto \mathcal{H}$ a unitary map then $\Psi := U(\Phi)$ is a nuclear countably Hilbert space.*

Proof. Note that U be definition is invertible so that $U^{-1} : \mathcal{H} \mapsto H$ exists. One can restrict the map to $\mathcal{H}$ to obtain a unitary map(under the inner product of H) $U^{-1} : \Psi \mapsto \Phi$. Since U and U^{-1} are bounded, their restrictions are as well. Let the countable sequence of inner products on Ψ be induced from Φ as follows. Let $\varphi, \psi \in \Psi$, define

$$\langle \varphi, \psi\rangle_{n,\Psi} := \langle U^{-1}\varphi, U^{-1}\psi\rangle_{n,\Phi} \tag{18}$$

Without loss of generality, we can assume that $n = 0$ corresponds with

$$\langle \varphi, \psi\rangle_{\mathcal{H}} = \langle U^{-1}\varphi, U^{-1}\psi\rangle_{H}$$

So that, equation 18 is compatible with the inner product of $\mathcal{H}$. Thus Ψ with the induced topology forms a countably Hilbert space. The nuclearity will follow if we can show that the restriction of U to Φ and Ψ is continuous and invertible. By construction, U^{-1} is a continuous map with respect to the τ_Φ and τ_Ψ topologies. By the open mapping theorem for Fréchet spaces(we assume our countably Hilbert space is complete), we have that U^{-1} has a bounded and thus continuous inverse. Thus Φ and Φ are topologically equivalent which implies that they are necessarily both nuclear. In total, we have that Ψ when endowed with the induced topology is a nuclear countably Hilbert space.

□

We will now show that the map U as defined above can be extended to a map $U^{\times} : \Phi^{\times} \mapsto \Psi^{\times}$.

Theorem 2.26. *Let $\Phi \subset H$ be a nuclear countably Hilbert space such that its image under a unitary map $U : H \mapsto \mathcal{H}$ is also a nuclear countably Hilbert space $\Psi \subset \mathcal{H}$. Then, there exists an bijective map $U^{\times} : \Phi^{\times} \mapsto \Psi^{\times}$.*

Proof. Let $|f\rangle \in \Phi^\times$ and $\psi \in \Psi$. Define the extension of U to $U^\times$ as $U^\times |f\rangle(\psi) = |f\rangle(U^{-1}\psi)$. Clearly, the image is an antilinear map on Ψ. Furthermore, it is actually continuous since if $\psi_n = U\varphi_n \to_{n\to\infty} \psi = U\varphi$ then $U^\times |f\rangle(\psi_n) = |f\rangle(\varphi_n) \to |f\rangle(\varphi) = U^\times |f\rangle(\psi_n)$. Where we employ the continuity of $|f\rangle$ to obtain the limit. Thus, $U^\times |f\rangle \in \Psi^\times$. In fact, it is easy to show that the map is actually bijective so that $U^\times \Phi = \Psi$.

□

By the above theorems, we can obtain the following result.

Theorem 2.27. *Let $\Phi \subset H \subset \Phi^\times$ be a nuclear rigged Hilbert space and $U : H \mapsto \mathcal{H}$ a unitary map between two Hilbert spaces. Then $U\Phi \subset UH \subset U^\times\Phi$ is a nuclear rigged Hilbert space which we denote by $\Psi \subset \mathcal{H} \subset \Psi^\times$.*

3 Rigged Hilbert Space Formulation of Potential Barrier

We will now employ the mathematical theory laid out in section 2 to rigorously formulate and solve the quantum mechanical system where the potential is a finite barrier. The goal of this section is to illustrate the necessary steps in rigorously solving a quantum mechanical problem by means of rigged Hilbert spaces. As a result, we will justify the bra and ket notation, spectral decompositions of observables, and the representations of wavefunctions with respect to certain observables. We will not compute the eigenfunctions directly as this require Sturm-Liouville theory. Their existence is sufficient for our purposes. The following theory is based on [8] and we refer to them for a more in-depth treatment.

3.1 Introduction

The time-independent Schrödinger equation describing the finite potential barrier is given by

$$H\varphi = E\varphi$$

where H is the differential operator given by

$$H = \frac{\hbar^2}{2m}\frac{d}{dx} + V(x)$$

where

$$V(x) = \begin{cases} 0, & \text{if } x < a \\ V_0 > 0, & \text{if } a \leq x \leq b \\ 0, & \text{if } x > b \end{cases}$$

Let $\mathcal{H} := L^2(\mathbb{R}, dx)$ be a Hilbert space where

$$L^2(\mathbb{R}, dx) = \left\{ f(x) | \int_{\mathbb{R}} dx \, |f(x)|^2 < \infty \right\}$$

Other operators of interest are the position and momentum operators given by

$$Q := x$$

$$P := -i\hbar\frac{d}{dx}$$

We will now seek a domain dense in $\mathcal{H}$ such that our operator is self-adjoint and densely defined. We do the same for the position and momentum operators.

3.2 Self-adjoint Extension

It is clear that for H on $D(H)$ to be well defined we require certain smoothness conditions. We denote by $D^0(H)$ the *maximal* domain on which H can be defined.

$$D^0(H) = \{f(x) \in L^2(\mathbb{R}, dx)|\ f(x) \in AC^2,\ Hf \in L^2(\mathbb{R}, dx)\}$$

where AC^2 is the set of differentiable functions whose derivative is absolutely continuous. In other words, $f(x)$ is second order differentiable almost everywhere.

We begin by finding a subdomain where H is symmetric. Let H^* be the adjoint. Let $f, g \in D^0(H)$. We can integrate by parts since f and g are sufficiently smooth. We find

$$\int_{\mathbb{R}} f \frac{d^2}{dx^2} g dx = f(x)\frac{dg}{dx}|_{-\infty}^{+\infty} - \int_{\mathbb{R}} \frac{df}{dx}\frac{dg}{dx} dx = f(x)\frac{dg}{dx}|_{-\infty}^{+\infty} - g(x)\frac{df}{dx}|_{-\infty}^{+\infty} + \int_{\mathbb{R}} \frac{d^2 f}{dx^2} g dx$$

Since f and g are in L^2 and AC^2, they tend to zero for sufficiently large $|x|$. This gives

$$\int_{\mathbb{R}} f \frac{d^2}{dx^2} g dx = \int_{\mathbb{R}} \frac{d^2 f}{dx^2} g$$

From which is follows that

$$\int_{\mathbb{R}} f(Hg) dx = \int_{\mathbb{R}} (Hf) g$$

Define

$$D(H) := D^0(H)$$

Then $H = H^*$ on $D(H)$ so that H is symmetric.

The following theorem[12] guarantees the existence of a unique self-adjoint extension of H. It turns out that $D^0(H)$ is exactly the domain on which H is self-adjoint [**?**].

Theorem 3.1. *A Hamiltonian H for a free particle($V(x) = 0$) defined on a dense domain $D(X)$ of $L^2(\mathbb{R}, dx)$ such that it is symmetric has a unique self-adjoint extension.*

Since our Hamiltonian differs from the Hamiltonian of a free particle by only a constant, one can show that the set of all possible domains on which the two operators are well-defined coincide. Further, one can easily verify that if one of the operators is self-adjoint on a domain then the other is as well. Thus, we know that our Hamiltonian H can be defined on a dense domain so that it is self-adjoint. We will now assume that $D(H)$ is this domain. It is not necessary to explicitly compute the domain. The self-adjoint domains of the position and momentum operators are[1]

$$D(Q) = \left\{ f \in L^2 \middle| xf \in L^2 \right\}$$

$$D(P) = \left\{ f \in AC \middle| Pf \in L^2, xf \in L^2 \right\}$$

3.2.1 Spectrum and Energy Representation

The self-adjoint operator H is of the form *Sturm-Liouville* which is a well studied class of differential operators. From the theory of such operators, it is known that

$$\sigma(H) = [0, \infty)[1]$$

Furthermore, it is known that there exists two *fundamental solutions* Θ_1^E and Θ_2^E[1] which satisfy

$$H\Theta_1^E = E\Theta_1^E$$

$$H\Theta_2^E = E\Theta_2^E$$

These two solutions form a basis for the eigenspace of H however they are not necessarily in L^2. They can be computed explicitly using Green's function techniques and Sturm-Liouville theory.[8] Furthermore, by a spectral theorem of ODE's[11], there exists for H a unitary map U given by[1]

$$\begin{gathered}U : L^2(\mathbb{R}, dx) \mapsto L^2(\sigma(A)), dE) \\ \varphi \mapsto \widetilde{\varphi}(E) := \int_0^\infty dx\, \varphi(x)\, \overline{\sigma(x, E)}\end{gathered}$$

for some $\sigma(x, E) \in span(\Theta_1^E, \Theta_2^E)$. We refer to [13] for the exact form of these solutions.

Definition 3.1. We call $\widetilde{\varphi}(E)$ the *energy representation* of $\varphi(x)$

The spectrum of P and Q are[8]

$$\sigma(P) = (-\infty, \infty)$$

$$\sigma(Q) = (-\infty, \infty)$$

Now with the definition of H and knowledge of its spectrum, we can construct the rigged Hilbert space formulation.

3.3 Rigged Hilbert Space of Q,P,H

By use of Sturm-Liouville theory, one can obtain a domain on which H is self-adjoint, as well as unitary map that diagonalizes H. However, this is not sufficient to describe the quantum mechanical system. We, generally, wish to compute the expectation of our wavefunctions with respect to various operators such as momentum, position, and energy. Furthermore, we wish to be able to compute commutation relations which require products and differences between operators. The wavefunctions in the domain of H do not satisfy all these requirements and therefore we need to find a smaller subdomain on which all of these operations make sense. It is useful to use the domain on which the action of Q, P and H are invariant.(This also is a necessary requirement to employ the *nuclear spectral theorem*). This problem is analysed in complete detail in [13]. We will summarize the main points in [13] and use the results to see how rigged Hilbert spaces work in practice.

3.3.1 Invariant subspace

The following requirements are necessary for the necessary operations to be well defined on a domain $\Phi \subset L^2$.[8]

- The functions should be infinitely differentiable so that all powers H and P are well defined.
- The functions vanish at the boundaries of the potential so that Hf is differentiable at the boundaries for all $f \in \Phi$
- The action of all powers of Q, P, and H remain in L^2

The above conditions are satisfied by

$$\Phi = \left\{ \varphi \in L^2 \middle| \varphi \in C^\infty(\mathbb{R}),\, \varphi^{(n)}(a) = \varphi^{(n)}(b) = 0,\, n \in \mathbb{N} \cup 0,\, P^n Q^m H^l \varphi \in L^2,\, n, m, l \in \mathbb{N} \cup 0 \right\}$$

It is easy to see that this is indeed a subdomain of the self-adjoint domain of the operators.

We will now install a topology on Φ such that it becomes a countably Hilbert space.

Let

$$\langle \varphi, \psi \rangle_{n,m,l} := \langle P^n Q^m H^l \varphi,\, P^n Q^m H^l \psi \rangle_{L^2}$$

Theorem 3.2. *$\langle \varphi, \psi \rangle_{n,m,l}$ is an inner product*

Proof. This proof can be found in [1]. The inner product inherits the linearity and anti-linearity of its components from the inner product of L^2. It only remains to show that it is positive definite so that it induces a norm.

It suffices to show that if the

$$\langle \varphi, \varphi \rangle_{n,m,l} = 0$$

then $\varphi = 0$. First, note that P and Q have no eigenvectors in Φ as they are non-normalizable. Also, it can be checked that the H has no eigenvectors corresponding to the eigenvalue 0 in Φ.

Suppose that φ is not zero while its induced (semi)norm is. Then,

$$\int_{\mathbb{R}} |P^n Q^m H^l \varphi|^2 dx = 0$$

Using that the integrand is differentiable a.e. and continuous everywhere, we find that $|P^n Q^m H^l \varphi|^2 = 0$. This implies that specifically $P^n Q^m H^l \varphi = 0$. However, we know that P and Q have no zero eigenvectors in Φ so we must conclude $H^l \varphi = 0$. This is a contradiction since 0 is not an eigenvalue of H . The same argument can be applied to H^l. Thus, we conclude $\varphi = 0$. □

We now have a countable family of inner products on Φ. Furthermore, the inner product corresponding with $n = m = l = 0$ corresponds with that of L^2. It can further be shown that the sequence of inner products are compatible and that Φ is complete. We will assume that this is the case. Thus, we can endow Φ with a countable Hilbert space topology τ_Φ such that it is continuously embedded in L^2.

3.3.2 Gelfand Triple and Generalized Eigenvectors

Now, that we have shown that Φ is a nuclear countably Hilbert space, we can construct its corresponding nuclear Rigged Hilbert space.

By taking its anti-dual space, we find the triple

$$\Phi \subset L^2(\mathbb{R}) \subset \Phi^\times$$

The nuclear spectral theorem implies the existence of generalised eigenvectors of Q, P, H. However, we can do more than that. We claim that the following anti-linear functionals form generalized eigenvectors of Q, P, H, respectively

$$\langle \varphi | x \rangle := \int_{\mathbb{R}} dx' \, \overline{\varphi}(x') \, \delta(x - x') = \varphi(x) \tag{19}$$

$$\langle \varphi | p \rangle := \int_{\mathbb{R}} dx \, \overline{\varphi}(x) \, \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{20}$$

$$\langle \varphi | E \rangle := \int_{\mathbb{R}} dx \, \overline{\varphi}(x) \, \sigma(x, E) \tag{21}$$

Theorem 3.3. $|x\rangle, |p\rangle, |E\rangle$ *form generalized eigenvectors* $\in \Phi^\times$

Proof. The proof can be found in [13]. It follows immediately that the kets are anti-linear. To show they are continuous in the Φ topology requires more work. □

Theorem 3.4. *The generalized eigenvectors* $|p\rangle, |x\rangle, |E\rangle$ *are complete in the sense of the nuclear spectral theorem*

Proof. Note that $\overline{\varphi(x')} = \langle x'|\varphi\rangle$ so that by integrating both sides of 19 with respect to x' gives

$$|\varphi\rangle = \int_{\mathbb{R}} dx' \, |x'\rangle \, \langle x'|\varphi\rangle$$

where $|\varphi\rangle := \int_{\mathbb{R}} dx \, \langle \varphi|x\rangle \, (\overline{\cdot})$ is the anti-linear functional of $\varphi(x)$.

By the fact that the Fourier transform is a unitary map, we obtain

$$|\varphi\rangle = \int_{\mathbb{R}} dp \, |p\rangle \, \langle p|\varphi\rangle$$

Lastly, since the energy transformation is unitary as well,

$$|\varphi\rangle = \int_{(0,\infty)} dE \, |E\rangle \, \langle E|\varphi\rangle$$

□

3.4 Representations of a Rigged Hilbert Space

We can obtain decompositions directly for $\varphi = \langle \varphi|x\rangle \in \Phi$ by introducing the following notation.

Definition 3.2. Let

$$\begin{aligned} \langle x|E\rangle &:= \sigma(x, E) \\ \langle x|p\rangle &:= \tfrac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \\ \langle x|x'\rangle &:= \delta(x - x') \end{aligned}$$

Then

$$\begin{aligned} \langle \varphi|x\rangle &= \textstyle\int_{\mathbb{R}} dx' \, \langle \varphi|x'\rangle \, \langle x'|x\rangle \\ \langle \varphi|x\rangle &= \textstyle\int_{\mathbb{R}} dp \, \langle \varphi|p\rangle \, \langle p|x\rangle \\ \langle \varphi|x\rangle &= \textstyle\int_{(0,\infty)} dE \, \langle \varphi|E\rangle \, \langle E|x\rangle \end{aligned} \tag{22}$$

The above decompositions allows us to consider the below *operators* as a resolution of the identity for wave functions. Note that the below equations are treated as identity operators in physics.

$$\begin{gathered} \textstyle\int_{\mathbb{R}} dx' \, |x'\rangle \, \langle x'| \\ \textstyle\int_{\mathbb{R}} dp \, |p\rangle \, \langle p| \\ \textstyle\int_{(0,\infty)} dE \, |E\rangle \, \langle E| \end{gathered} \tag{23}$$

That is, given a wave function $\langle \varphi|x\rangle$, we can stick any of the above identity operators in between the bra and the ket and obtain the same answer.

We can actually obtain an even stronger result given by

$$\begin{aligned} \langle \varphi|\psi\rangle &= \textstyle\int_{\mathbb{R}} dx' \, \langle \varphi|x'\rangle \, \langle x'|\psi\rangle \\ &= \textstyle\int_{\mathbb{R}} dp \, \langle \varphi|p\rangle \, \langle p|\psi\rangle \\ &= \textstyle\int_{(0,\infty)} dE \, \langle \varphi|E\rangle \, \langle E|\psi\rangle \end{aligned} \tag{24}$$

The above follows from the fact that the Fourier transform, and the energy diagonalization map are unitary and thus preserve the inner product of Φ. This can be checked by a simple computation. The *operators* given by equation (23) should be interpreted as sesquilinear forms defined on Φ. It happens to be that they coincide with the inner product on H. In general, one can construct sesquilinear forms on Φ by taking the tensor products of a bra and a ket. Consider $\langle E| \in \Phi'$ and $|F\rangle \in \Phi^{\times}$. Their tensor product is defined as

$$\langle \varphi|F\rangle \langle E|\psi\rangle := \langle F| \otimes |E\rangle (\varphi, \psi) = \langle F| (\varphi) \cdot |E\rangle (\psi)$$

So that

$$|F\rangle \langle E| := |F\rangle \otimes \langle E|$$

It should be highlighted that the above interpretation only makes sense when we only operate on elements of Φ. The interpretation fails if we try to use the notation of definition 3.2.

3.5 Position, Momentum Energy Representation

The unitary maps can be extended to the whole rigged Hilbert space such that its image is also a rigged Hilbert space. We call this an isomorphism of rigged Hilbert spaces. Each element in the class of isomorphic rigged Hilbert spaces, we call a representation.

The rigged Hilbert Space we constructed in section 4.3 is what we call the *position representation.* In this representation, the wavefunctions and operators, when explicitly written, depend on x. However, this is just one representation of the Rigged Hilbert Space. In practical applications the momentum and energy representations are also of interest.

Recall that the Fourier transform $\mathcal{F} : L^2(\mathbb{R}, dx) \mapsto L^2(\mathbb{R}, dp)$ is a unitary map so that by section 3.8, the map induces a nuclear Rigged Hilbert space

$$\Psi_p = \mathcal{F}(\Phi) \subset L^2(\mathbb{R}, dp) \subset \Psi_p^{\times}$$

which we call the momentum representation.

Furthermore, by the nuclear spectral theorem, and using (22) and (24), there exists a unitary map $U_E : L^2(\mathbb{R}, dx) \mapsto L^2((0, \infty), dE)$ which leads to the energy representation given by

$$\Psi_E = U_E(\Phi) \subset L^2((0, \infty), dE) \subset \Psi_E^{\times}$$

Recall, how in the position representation, the eigenkets of Q given by $|x\rangle$ form dirac delta distributions. It turns out that the same holds true for $|p\rangle$ and $|E\rangle$ in the momentum and energy representations, respectively.

Theorem 3.5.

$$\mathcal{F}^{\times} |p\rangle = \int_{\mathbb{R}} dp' \delta(p - p')$$

$$U_E^{\times} |E\rangle = \int_{(0,\infty)} dE' \delta(E - E')$$

Proof. By definition,

$$\mathcal{F}^{\times} |p\rangle (\varphi(p)) = |p\rangle (\mathcal{F}^{-1}(\varphi)(x))$$

Furthermore, by definition of $|p\rangle$ we have that

$$|p\rangle (\mathcal{F}^{-1}(\varphi)(x)) = \mathcal{F}(\mathcal{F}^{-1}(\varphi(p)))(p) = \varphi(p)$$

which gives the desired result.

The result for $|E\rangle$ is obtained completely analogously. □

3.5.1 δ normalization of eigenkets

The unitary maps $\mathcal{F}$ and U_E diagonalize the self-adjoint operators P and H, respectively. Thus, in the momentum and energy representations, we have

$$P_p := \mathcal{F}P\mathcal{F}^{-1} = p$$

and

$$H_E := U_E H U_E^{-1} = E$$

It will follow that the eigenkets are $\delta-$ normalized. We will show this for the case of $|E\rangle$.

Consider H in the energy representation which we will denote by E. Then, the eigenket $|E\rangle$ is given by

$$\int_{(0,\infty)} dE' \; \delta(E - E')$$

The eigenfunctions of E which we associate with $|E\rangle$ and $|E^*\rangle$ are given by $\delta(E-E')$ and $\delta(E^*-E')$. Let $\langle E^*|E\rangle = \delta(E^* - E')\delta(E - E')$. If we define the linear functional

$$\int dE' \overline{\varphi(E')} \langle E^*|E\rangle := \int dE \; \overline{\varphi(E')}\delta(E - E')\, \delta(E^* - E') = \int dE \; \overline{\varphi(E)}\delta(E - E^*)$$

We see that $\langle E^*|E\rangle$ is equal to $\delta(E - E^*)$. The same holds for $\langle p|p^*\rangle$. It should be noted that the normalisation is independent of the representation chosen. The normalization can also be shown using the position representation and definition 3.2 by directly computing

$$\int dx \, \langle E|x\rangle \, \langle x|E^*\rangle = \delta(E - E^*)$$

and

$$\int dx \, \langle p|x\rangle \, \langle x|p^*\rangle = \delta(p - p^*)$$

Our definition of $\langle E^*|E\rangle$ and $\langle p|p^*\rangle$ allows us in the distributional sense to say that $\langle E^*|E\rangle = \langle E^*|x\rangle \langle x|E\rangle$ and $\langle p|p^*\rangle = \langle p^*|x\rangle \langle x|p\rangle$. So that the *identity* operators given in equation (23) i.e. $\int dx \; |x\rangle \langle x|$ also work when sandwiched between eigenkets. It should be noted that $\langle p|p^*\rangle$ looks like the inner product of the momentum eigenfunctions, however it should be interpreted and only makes sense as the integrand of a distribution.

3.6 Conclusion to the Potential Barrier

In this section, we put the quantum mechanical problem of a finite potential barrier in one dimension in rigorous footing. Since the spectrum is entirely continuous and there are no eigenvectors in the Hilbert space, we had to construct a nuclear rigged Hilbert space. By doing this, we found eigenkets of the observables of the system as well as a unitary map that diagonalizes the observables. Throughout the section, we rigorously justified the bra-ket manipulations commonly used in practice.

4 Non-Hermitian Operators in Quantum Mechanics

In the previous formulation of quantum mechanics, we require observables to be hermitian as this ensures that the eigenvalues are real. However, it turns out that there are classes of non-hermitian operators that have a real spectrum. Two classes of interest are the pseudo-hermitian and quasi-hermitian operators. In this section, we will discuss whether the rigged Hilbert space formulation can be extended to account for such operators.

4.1 Pseudo-Hermitian and Quasi-Hermitian Operators

As we will see, the class of pseudo-Hermitian operators covers nearly all non-hermitian operators in Quantum Mechanics. Specifically, PT-symmetric operators form a subset of such operators.

Definition 4.1. A linear operator A on a Hilbert space $\big(H, (\cdot,\cdot)\big)$ is called *pseudo-Hermitian* if it is similar to its adjoint by a bounded self-adjoint linear operator $\eta : H \mapsto H$. That is, $A^* = \eta A \eta^{-1}$

Quasi-hermitian operators are a subset of the class of pseudo-hermitian operators. They are particularly of interest since they share many properties that self-adjoint operators have.

Definition 4.2. A linear operator A on a Hilbert space $\big(H, (\cdot,\cdot)\big)$ is called *quasi-Hermitian* if there exists an inner product $\langle\cdot,\cdot\rangle$ on the linear space H such that A is hermitian on $\overline{\big(H, \langle\cdot,\cdot\rangle\big)}$.

Given two inner products on a Hilbert space, we can always express one inner product in terms of the other by means of a positive definite operator. That is,

$$\text{There exists a map } \eta : H \mapsto H \text{ such that } \langle\cdot,\cdot\rangle = \big(\cdot, \eta\,\cdot\big) \tag{25}$$

The following definition for quasi-hermitian operators is equivalent to the former.

Definition 4.3. Equivalently, a linear operator A on a Hilbert space $\big(H, (\cdot,\cdot)\big)$ is *quasi-Hermitian* if

$$A^* = \eta A \eta^{-1}$$

for a bounded positive definite operator $\eta : H \mapsto H$.

Lemma 4.1. *Let η be a positive definite operator defined on a Hilbert space H. Then there exists a hermitian square root $\rho : H \mapsto H$ of η so that $\rho^* \cdot \rho = \rho \cdot \rho = \eta$*

By the existence of ρ, we can rewrite equation (25) as

$$\langle\cdot,\cdot\rangle = \big(\cdot, \eta\,\cdot\big) = \big(\rho\cdot, \rho\,\cdot\big)$$

Definition 4.4. Two sequences φ_n, $\psi_m \in H$ form a *Riesz basis* for the Hilbert space H if they satisfy

$$\langle \varphi_n, \psi_m\rangle_H = \delta_{n,m}$$

and for all elements $x \in H$, we have that

$$x = \sum_n \langle \varphi_n, x\rangle_H \psi_n$$

Theorem 4.2. *The left and right eigenvectors of a quasi-hermitian operator with purely discrete spectrum form a Riesz Basis.*

Proof. See next sections. □

Definition 4.5. We say that a non-hermitian operator A is *diagonalizable* if its eigenvectors form a *Riesz Basis.* It follows that all quasi-hermitian matrices are diagonalizable.

Theorem 4.3. *A quasi-hermitian operator has real spectrum.*

4.2 Pseudo-Hermitian Operators in Quantum Mechanics

A class of non-hermitian Hamiltonians of interest in physics is that of Hamiltonians with PT-Symmetry. Most PT-symmetric systems considered in practice have discrete spectrum and can be diagonalized by a complete set of eigenvectors. Much of the mathematical theory developed, notably by Mostafazadeh[2] and Bender[14], for PT-symmetric systems require this as an assumption. Mostafazadeh[15] showed that all diagonalizable PT-symmetric Hamiltonians with discrete spectrum are necessarily pseudo-hermitian.

Definition 4.6. Let $\mathcal{P} : H \mapsto H$ denote the parity operator where $H = L^2(dx)$. That is, for $f(x) \in H$

$$\mathcal{P}f(x) = f(-x)$$

Furthermore, let $\mathcal{T} : H \mapsto H$ denote the complex conjugate operator defined by

$$\mathcal{T}f(x) = \overline{f(x)}$$

A Hamiltonian is PT-symmetric if it commutes with the $\mathcal{PT}$ operator.

$$\mathcal{PT}H(\mathcal{PT})^{-1} = H$$

Definition 4.7. We say an operator $A : H \mapsto H$ admits an anti-linear symmetry if it commutes with an anti-linear operator X. That is,

$$AX = XA$$

where $X(c\varphi + d\psi) = \bar{c}X\varphi + \bar{d}X\psi$

Theorem 4.4. *A diagonalizable Hamiltonian is pseudo-hermitian if and only if it admits an anti-linear symmetry.*

Proof. See [15] □

Corollary 4.4.1. *Since the $\mathcal{PT}$ operator is anti-linear, all diagonalizable PT-symmetric Hamiltonians admit an anti-linear symmetry and thus are pseudo-hermitian.*

Theorem 4.5. *A diagonalizable Hamiltonian with real spectrum is necessarily quasi-hermitian*

Proof. See [15] □

In practice, given a PT-symmetric Hamiltonian(and pseudo-hermitian operators in general), it is not easy to construct the metric operator. Methods exist and are currently being developed to tackle this problem[2]. In the next section, we will discuss some examples of PT-symmetric systems.

Remark. Quasi-hermitian Hamiltonians are well-understood and easy to work with. They can naturally be studied in the Hilbert space setting. Pseudo-symmetric Hamiltonians on the other hand are not necessarily similar to their adjoint by a positive definite metric operator. In many cases, the metric operator is only nondegenerate and as a result it cannot be used to construct an inner product on the Hilbert space. A generalization of Hilbert spaces, known as *Krein spaces*, are linear spaces equipped with a nondegenerate bi-linear form that satisfy all properties of the inner product except positive-definiteness. Pseudo-hermitian operators emerge as self-adjoint operators on Krein spaces. In the case where one assumes the operator is diagonalizable with discrete spectrum, a form of quantum mechanics can be developed using such spaces[2]. However, general self-adjoint operators and their spectral theory on Krein spaces is beyond the scope of this thesis. For this reason, we will not attempt to extend the theory of rigged Hilbert spaces to general pseudo-hermitian operators. We will restrict our attention to quasi-hermitian operators.

4.2.1 The need for rigged Hilbert space formulation of PT-symmetric quantum mechanics

Currently, PT-symmetric quantum mechanics is not laid on a rigorous mathematical foundation. The bra and ket notation, while justified for conventional quantum mechanics, is not mathematically justified for PT-symmetric Hamiltonians. Even in the case where the PT-symmetric Hamiltonian is discrete so that its eigenvectors are in the Hilbert space, a rigged Hilbert space formulation is needed to be able to incorporate the position and momentum operators in the framework. For conventional quantum mechanics, the momentum and position representation emerge as equivalent representations of the rigged Hilbert space. Furthermore, the momentum and position eigenvectors are represented as anti-linear functionals in the dual space $\Phi^{\times}$ of the space of wave functions Φ. The dual space of H is not sufficient to describe the full system. In the case, where the Hamiltonian has continuous spectrum, the eigenvectors are not in the Hilbert space so we require some sort of rigged Hilbert space construction that accounts for the energy representation of the system.

One might think that a discrete diagonalizable PT-symmetric Hamiltonian can be easily introduced into the Rigged Hilbert space formulation since its eigenvectors are in the Hilbert space. We will see that this is not so simple.

One naive solution is to construct the rigged Hilbert space generated by the self-adjoint operators P and Q. This gives

$$\Phi \subset H \subset \Phi^{\times}$$

where the eigenkets of P and Q are in $\Phi^{\times}$. Let h represent the PT symmetric Hamiltonian with discrete spectrum. By assumption, the left and right eigenvectors φ_n, ψ_m of H form a Riesz basis. The eigenkets $|\varphi_n\rangle$, $|\psi_m\rangle \in H^{\times}$ are well-defined elements of $\Phi^{\times}$. It should be noted that φ_n and $\psi_m \in H$ may not be elements of Φ and thus may not be realizable quantum states. As a result, the eigenfunctions of h are in general best interpreted as anti-linear functionals and not wave functions. Another issue is that Φ is not necessarily an invariant domain of h so that $h : \Phi \mapsto \Phi$ is ill-defined. One will find that the due to domain issues that commutation relations of between P, Q and h are not well-defined which undermines the point of the rigged Hilbert space formulation. One may attempt to solve this by finding a domain contained in Φ such that it is invariant under all the observables however there is no guarantee that h is continuous in the Φ topology. In principle, if possible, constructing Φ such that all the observables are invariant and continuous on Φ would solve the problem. As the eigenvectors of h are in principle already known to exist by assumption, the nuclear spectral theorem need not be applied to h. In a later section, we will discuss this in further detail.

In the case where h is a general PT-symmetric Hamiltonian, the above construction breaks down completely.

4.2.2 Examples of PT-symmetric systems with discrete and continuous spectra

While most PT-symmetric Hamiltonians studied in literature are discrete and diagonalizable, there are quantum systems that are described by a PT-symmetric Hamiltonians with purely continuous spectrum. Furthermore, many examples in literature are quasi-hermitian.

Some examples of PT-symmetric quantum systems that are quasi-hermitian can be found in [4] and [2]. Where the former explicitly constructs the metric operator for a quasi-hermitian Hamiltonian with discrete spectrum, along with its adjoint and eigenvectors. The latter contains various examples of quasi-hermitian operators containing both discrete and continuous spectrum. In general, finding the metric operator for a given Hamiltonian is very difficult and often cannot be computed exactly. Perturbation methods are often employed as seen in [2]. One example of interest is that of the PT-symmetric barrier potential[2].

Example 4.6. *Consider the following scattering potential*

$$\nu(x) = \begin{cases} -i\zeta(x) \text{ } for \text{ } |x| < \frac{L}{2} \\ 0 \text{ } for \text{ } |x| \geq \frac{L}{2} \end{cases}$$

where ζ, L, $x \in \mathbb{R}$, and $L > 0$. The above potential plays a role in describing the propogation of electromagnetic waves in certain diaelectric waveguides[16]. A pertubative expression when ζ is small for the metric η can be found in [2].

Another quasi-hermitian Hamiltonian with continuous spectrum is that of the complex scattering delta function given by

$$v(x) = \beta\delta(x)$$

where $\beta \in \mathbb{C}$.

The potential is analysed in further detail in [2].

In the article [17], the metric operator and adjoint operator for a very general class of non-hermitian complex cubic potentials are found. A class of PT-symmetric Hamiltonians with discrete spectrum of interest in research is given by

$$H_N = p^2 - (ix)^N$$

One famous example is that of the imaginary cubic potential given by $N = 3$ in the above equation. Unfortunately, it is known that the cubic potential is not quasi-hermitian. [3]. It is unknown whether H_N is not quasi-hermitian for all N.

4.2.3 Quasi-Hermitian Operators with Purely Discrete Spectrum

In this section, we will construct the trivial rigged Hilbert space $H \subset H^{\times}$ for quasi-hermitian operators that have a complete set of eigenvectors.

Let $A : H \mapsto H$ be a densely defined quasi-hermitian operator with a discrete (nondegenerate) spectrum so that its eigenvectors are in the Hilbert space H. Let $\eta : H \mapsto H$ be the bounded positive definite metric operator with bounded inverse η^{-1} such that $A^* = \eta A \eta^{-1}$. Let $\mathcal{H}$ be the Hilbert space obtained by completing the set H with respect to the inner product $\langle \cdot, \eta \cdot \rangle$. By construction, it follows that H is dense in $\mathcal{H}$. Since A was densely defined as a map on H, A is also densely defined as a map on $\mathcal{H}$. As a result, $A : \mathcal{H} \mapsto \mathcal{H}$ is a densely defined self-adjoint operator.

By assumption, A has a discrete spectrum so that there exists a complete set of eigenvectors $\varphi_n \in H$ with corresponding eigenvalues E_n. It can be seen as follows that A^* also admits a complete set of eigenvectors with eigenvalues E_n given by $\eta\varphi_n$. Note that

$$A^* \eta\varphi_n = \eta A \eta^{-1} \eta \varphi_n = \eta A \varphi_n = E_n \eta \varphi_n$$

Thus, the pair $\{\varphi_n, \eta\varphi_n\}$ form a set of left and right eigenvectors of A. Now, consider A as a self-adjoint map in $\mathcal{H}$. Since $H \subset \mathcal{H}$, we know that the the eigenvectors φ_n are in $\mathcal{H}$ as well. Thus, A has a complete set of eigenvectors in $\mathcal{H}$. By the self-adjointness of A, the eigenvectors are orthonormal according to the inner product of $\mathcal{H}$. Thus φ_n must satisfy

$$\langle \varphi_n, \varphi_m \rangle_{\mathcal{H}} = \langle \varphi_n, \eta\varphi_m \rangle_H = \delta_{nm}$$

From the above equation, we see that the pair $\{\varphi_n, \eta\varphi_m\}$ are also orthonormal according to the inner product on H. Thus, A admits a set of bi-orthogonal left and right eigenvectors.

One can expand any element in $\psi \in \mathcal{H}$ as

$$\psi = \sum_n \langle \varphi_n, \psi \rangle_{\mathcal{H}} \varphi_n$$

Thus, for any element $\phi \in H$ we have that

$$\phi = \sum_n \langle \eta\varphi_n, \phi \rangle_H \varphi_n \tag{26}$$

Which shows that $\{\varphi_n, \eta\varphi_m\}$ form a complete biorthogonal eigenbasis in H.

Using the canonical mapping of H into $H^\times$, we can find the eigenkets for A and A^*. Note that A and A^* are not necessarily continuous so that their extensions to $H^\times$ are ill-defined. Nonetheless, we will naively apply the extensions to the eigenkets. However, the following is only formally correct when we assume A is a bounded, entirely defined map. The eigenkets for A and A^* are $\eta^\times |\varphi_n\rangle = |\eta\varphi_n\rangle$ and $|\varphi_n\rangle$, respectively. To check this, note

$$A^\times |\eta\varphi_n\rangle (\psi) = |\eta\varphi_n\rangle (A\psi) = \langle A\psi, \eta\varphi_n\rangle_H = \langle \psi, A^*\eta\varphi_n\rangle_H$$

$$= \langle \psi, E\eta\varphi_n\rangle_H = E\langle \psi, \eta\varphi_n\rangle_H = E\,|\eta\varphi_n\rangle (\psi)$$

A similar computation shows that

$$A^{*\times} |\varphi_n\rangle = E\,|\varphi_n\rangle$$

We can construct the trivial rigging of H into a rigged Hilbert space given by $H \subset H \subset H^\times$ which for clarity we will denote $H \subset H^\times$.

From equation (26), it follows that the eigenkets are complete as for any $\psi \in H$, we have that

$$|\psi\rangle = \sum_n \langle \varphi_n|\,\eta^\times\,|\psi\rangle\,|\varphi_n\rangle$$

In conclusion, we find that the quasi-hermitian operator A has a complete set of eigenkets in the rigged Hilbert space $H \subset H^\times$.

Theorem 4.7. *Let $A : H \mapsto H$ be a (nondegenerate) quasi-hermitian operator with a discrete spectrum and complete set of eigenvectors. Then $H \subset H^\times$ is a rigged Hilbert space for A such that A has a complete set of eigenkets in $H^\times$.*

4.3 General case of Quasi-hermitan operators

Theorem 4.7 motivates the possible existence of rigged Hilbert spaces for general quasi-hermitian operators. In this section, we will see to what end such a rigged Hilbert space construction is possible.

Let $A : H \mapsto H$ be a quasi-hermitian operator satisfying $A = \eta^{-1}A^*\eta$ with $\eta : H \mapsto H$ a bounded invertible positive definite operator. It follows immediately that A^* is also a quasi-hermitian operator satisfying $A^* = \eta A \eta^{-1}$. One can verify that A is self-adjoint with respect to the inner product $\langle\cdot, \eta\cdot\rangle_H$ and A^* is self-adjoint with respect to the inner product $\langle\cdot, \eta^{-1}\cdot\rangle_H$.

In the discrete case established in the previous section, we found that in the discrete specturm case, the operator has eigenkets of the form $\eta^\times |\varphi_n\rangle$ where $|\varphi_n\rangle$ are eigenkets of its adjoint. Thus, one may expect that the eigenkets of A denoted by $|E\rangle$ are related to the eigenkets of A^* given by $|F\rangle$ by

$$|F\rangle = \eta^{-1\times}\,|E\rangle \tag{27}$$

Let us for the sake of investigation assume that we have a rigged Hilbert space $\Phi \subset H \subset \Phi^\times$ such that A has a complete set of eigenkets $|E\rangle \in \Phi^\times$. Furthermore, lets assume that η, η^{-1}, A and A^* are all continuous and Φ is left invariant under the maps so that their extensions to $\Phi^\times$ are well defined. I claim that the kets given by equation 27 are actually eigenkets of A^*. To see this, note that

$$A^{*\times}\,|F\rangle (\psi) = (\eta A \eta^{-1})^\times \eta^{-1\times}\,|E\rangle (\psi) = |E\rangle (\eta^{-1}\eta A \eta^{-1}\psi) = |E\rangle (A\eta^{-1}\psi)$$

$$= A^\times\,|E\rangle (\eta^{-1}\psi) = E\,|E\rangle (\eta^{-1}\psi) = E\eta^{-1\times}\,|E\rangle$$

where the first equality in the above equation follows because $\eta^{-1}\psi \in \Phi$. Thus, the assumption that the maps Φ is left invariant is essential. In conclusion, the rigged Hilbert space(if it exists) has a complete system of eigenket pairs given by $\{|E\rangle, \eta^{-1}\,|E\rangle\}$.

The below lemma shows that sufficient conditions that can imposed on Φ to lead to an equivalent space.

Lemma 4.8. *Suppose $\Phi \subset H \subset \Phi^\times$ is a rigged Hilbert space. By definition, Φ is Fréchet. Let $\eta^{-1} : H \mapsto H$ be invertible. Suppose Φ satisfies $A\Phi \subset \Phi$ and $\eta^{-1}\Phi = \Phi$ where A and η^{-1} are bounded and thus continuous maps in the Φ topology. Then, A^* and η are continuous in Φ as well and A^* satisfies $A^*\Phi \subset \Phi$*

Proof. Since $\eta^{-1} : H \mapsto H$ is an invertible map, its restriction to Φ will also have an inverse denoted by η. Since η^{-1} is by assumption surjective and bounded, we have by the open mapping theorem for Fréchet spaces that η^{-1} has a bounded inverse. Thus, $\eta : \Phi \mapsto \Phi$ is invertible and $\eta : \Phi \mapsto \Phi$ is continuous. Recall that $A^* = \eta A \eta^{-1}$. Clearly, A^* when restricted to Φ is a composition of continuous maps whose action on Φ is invariant. Thus, A^* is continuous and satisfies $A^*\Phi \subset \Phi$ $\square$

In the above analysis, we assumed that such a rigged Hilbert space with a complete set of eigenkets exists. However, this is not guaranteed. We do know that generally we can find such a space in the trivial case where A is self-adjoint by means of the nuclear spectral theorem. Next, we will show that using $\mathcal{H}$ and $\mathcal{H}_*$, we can construct a rigged Hilbert space that admits a resolution of the identity and diagonalization in terms of eigenkets of A and A^* for a dense subspace of H.

Theorem 4.9. *Let $A : H \mapsto H$ be quasi-hermitian. Assume that there exist a rigged Hilbert space $\Psi \subset \mathcal{H} \subset \Psi^\times$ such that $A\Psi \subset \Psi$, $\eta^{-1}\Psi \subset \Psi$ and A, η^{-1} are continuous maps on Ψ. Then, there exists an inner product space Σ such that $\Sigma \subset H$ and $\Sigma = \Psi$ element-wise. Furthermore, we have series of maps $\Sigma \mapsto \Psi^\times$, $A^\times, A^{*\times}$, $i^\times$ and $j^\times$ that give a resolution of the identity and diagonalization of A and A^*.*

$$A^\times(\varphi) := |A^*\varphi\rangle_H = \int_{\mathbb{R}} E \langle E| \eta^{-1\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$A^{*\times}(\varphi) := |A\varphi\rangle_H = \int_{\mathbb{R}} E \langle E|\varphi\rangle \eta^{-1\times} |E\rangle \, d\mu(E)$$

$$i^\times(\varphi) := |i\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \eta^{-1\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$j^\times(\varphi) := |j\varphi\rangle_H = \int_{\mathbb{R}} \langle E|\varphi\rangle \eta^{-1\times} |E\rangle \, d\mu(E)$$

where for simplicity, we assume the decomposition to be with respect to a single Borel measure $d\mu$. See Theorem 2.23 for the general form with respect to multiple Borel measures.

Proof. Note that by construction $H \subset \mathcal{H}$. Since $A\Psi \subset \Psi$ and the domain of A is strictly contained in H, it follows that $\Psi \subset H$ as well. Thus, the canonical injection of Ψ into $H^\times$ and $\mathcal{H}^\times$ is well defined.

Denote the canonical injection of $\mathcal{H}$ into $\Psi^\times$ by

$$|\varphi\rangle_{\mathcal{H}} := \langle \cdot, \varphi \rangle_{\mathcal{H}}$$

and the injection of H into $H^\times$ by

$$|\varphi\rangle_H = \langle \cdot, \varphi \rangle_H$$

Lemma 4.10. *The following spectral decompositions in $\mathcal{H}$ hold for the elements in Ψ*

$$|\varphi\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \langle E|\varphi\rangle |E\rangle \, d\mu(E) \tag{28}$$

$$|A\varphi\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \langle E|\varphi\rangle |E\rangle \, d\mu(E)$$

Proof. Under the above assumptions, $\Psi \subset \mathcal{H} \subset \Psi^{\times}$ is a rigged Hilbert space under which $A\Psi \subset \Psi$ and A is self-adjoint. Thus, we can apply the nuclear spectral theorem(2.23) which gives us a complete system of eigenkets $|E\rangle \in \Psi^{\times}$.

Then by the nuclear spectral theorem, for all $\varphi \in \Psi$, we have that

$$|\varphi\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \langle E|\varphi\rangle \, |E\rangle \, d\mu(E) \tag{29}$$

$$|A\varphi\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \langle E|\varphi\rangle \, |E\rangle \, d\mu(E)$$

□

The above resolution of the identity and diagonalization of A is only for the kets $|\varphi\rangle_{\mathcal{H}}$ and therefore will not necessarily hold for $|\varphi\rangle_H$. However, note that for $\varphi \in H$

Lemma 4.11.

$$|\varphi\rangle_H = \left|\eta^{-1}\varphi\right\rangle_{\mathcal{H}}$$

Proof.

$$|\varphi\rangle_{\mathcal{H}} = \langle \cdot, \varphi\rangle_{\mathcal{H}} = \langle \cdot, \eta\varphi\rangle_H = |\eta\varphi\rangle_H$$

so that

$$|\varphi\rangle_H = \left|\eta^{-1}\varphi\right\rangle_{\mathcal{H}}$$

□

Lemma 4.12. *The following resolution of the identity holds for the elements of* Ψ

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \, \eta^{-1\times} \, |\varphi\rangle \, |E\rangle \, d\mu(E)$$

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E|\varphi\rangle \, \eta^{-1\times} \, |E\rangle \, d\mu(E)$$

Proof. Let $\varphi \in \Psi$ then because by assumption $\eta^{-1}\Psi \subset \Psi$, we have that $\eta^{-1}\varphi \in \Psi$. We can now apply the resolution of the identity given in equation 4.3 to $\eta^{-1}\varphi$. This gives

$$|\varphi\rangle_H = \left|\eta^{-1}\varphi\right\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \left\langle E\middle|\eta^{-1}\varphi\right\rangle |E\rangle \, d\mu(E)$$

Is it important to note that $\langle E| \, \eta^{-1\times}$ is a bra in the dual space Ψ'. η^{-1} is self adjoint on $\mathcal{H}$ since $\langle \eta^{-1}\varphi, \varphi\rangle_{\mathcal{H}} = \langle \eta^{-1}\varphi, \eta\varphi\rangle_H = \langle \varphi, \eta^{-1}\eta\varphi\rangle_H = \langle \varphi, \eta\eta^{-1}\varphi\rangle_H = \langle \varphi, \eta^{-1}\varphi\rangle_{\mathcal{H}}$. As a result,

$$\langle E| \, \eta^{-1\times}(\varphi) = \left\langle E\middle|\eta^{-1*}\varphi\right\rangle = \left\langle E\middle|\eta^{-1}\varphi\right\rangle$$

Which lets us write equation 4.3 as a decomposition of the kets $|E\rangle$ and $\eta^{-1\times} \, |E\rangle$. That is,

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \, \eta^{-1\times} \, |\varphi\rangle \, |E\rangle \, d\mu(E)$$

One can obtain the alternate form by passing $\psi \in \Psi$ as argument in the above function. This gives

$$|\varphi\rangle_H(\psi) = \langle \psi, \varphi\rangle_H = \langle \psi|_H(\varphi) = \int_{\mathbb{R}} \langle E| \, \eta^{-1\times} \, |\varphi\rangle \, \langle \psi|E\rangle \, d\mu(E)$$

Now, taking the complex conjugate we get

$$|\psi\rangle_H(\varphi) = \int_{\mathbb{R}} \langle \varphi| \, \eta^{-1\times} \, |E\rangle \, \langle E|\psi\rangle \, d\mu(E)$$

Lastly, removing the argument φ and rearranging gives

$$|\psi\rangle_H = \int_{\mathbb{R}} \langle E|\psi\rangle \, \eta^{-1^\times} \, |E\rangle \, d\mu(E)$$

□

Lemma 4.13. *The following spectral decompositions of A and A^* hold in Ψ.*

$$|A^*\varphi\rangle_H = \int_{\mathbb{R}} E \, \langle E| \, \eta^{-1^\times} \, |\varphi\rangle \, |E\rangle \, d\mu(E)$$

$$|A\psi\rangle_H = \int_{\mathbb{R}} E \, \langle E|\psi\rangle \, \eta^{-1^\times} \, |E\rangle \, d\mu(E)$$

Proof. Let $\varphi \in \Psi$ We know by the nuclear spectral theorem that

$$|A\varphi\rangle_{\mathcal{H}} = \int_{\mathbb{R}} E \, \langle E|\varphi\rangle \, |E\rangle \, d\mu(E)$$

Substituting $\eta^{-1}\varphi$ in the above equation gives

$$\left|A\eta^{-1}\varphi\right\rangle_{\mathcal{H}} = \int_{\mathbb{R}} \left\langle E\middle|\eta^{-1}\varphi\right\rangle |E\rangle \, d\mu(E)$$

Note $A = \eta^{-1}A^*\eta$ where A^* is well-defined since $\Psi \subset H$. Substitution gives

$$\left|\eta^{-1}A^*\eta\eta^{-1}\varphi\right\rangle_{\mathcal{H}} = \left|\eta^{-1}A^*\varphi\right\rangle_{\mathcal{H}} = |A^*\varphi\rangle_H$$

So

$$\left|A\eta^{-1}\varphi\right\rangle_{\mathcal{H}} = |A^*\varphi\rangle_H$$

From the above equation, we can conclude that the ket $|A^*\varphi\rangle_H$ is a member of $\Psi^\times$ and coincides with $\left|A\eta^{-1}\varphi\right\rangle_{\mathcal{H}}$. Furthermore, it tells us that the map $A^{*\times} : H^\times \mapsto H^\times$ is well defined for $|\varphi\rangle_H \in H^\times$ when $\varphi \in \Psi$. Note that A^* is not necessarily bounded(continuous) on H so that the map $A^{*\times} : H^\times \mapsto H^\times$ is not globally well defined.

Putting it all together we find

$$|A^*\varphi\rangle_H = \int_{\mathbb{R}} E \, \langle E| \, \eta^{-1\times} \, |\varphi\rangle \, |E\rangle \, d\mu(E)$$

We can find the expansion for $|A\varphi\rangle_H$ as well. Let $\psi \in \Psi$ then

$$|A^*\varphi\rangle_H (\psi) = \langle \psi, A^*\varphi\rangle_H = \langle A\psi, \varphi\rangle_H = \langle A\psi|_H (\varphi))$$

So

$$\langle A\psi|_H (\varphi)) = \int_{\mathbb{R}} E \, \langle E| \, \eta^{-1\times} \, |\varphi\rangle \, \langle \psi|E\rangle \, d\mu(E)$$

Taking the complex conjugate of both sides gives

$$|A\psi\rangle_H (\varphi)) = \int_{\mathbb{R}} E \, \langle \varphi| \, \eta^{-1\times} \, |E\rangle \, \langle E|\psi\rangle \, d\mu(E)$$

by removing the argument φ and some rearranging, it follows that

$$|A\psi\rangle_H = \int_{\mathbb{R}} E \, \langle E|\psi\rangle \, \eta^{-1^\times} \, |E\rangle \, d\mu(E)$$

□

In conclusion for all elements $\varphi \in \Psi$, we obtain the following identities.

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \eta^{-1^\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E|\varphi\rangle \eta^{-1^\times} |E\rangle \, d\mu(E)$$

$$|A^*\varphi\rangle_H = \int_{\mathbb{R}} E \langle E| \eta^{-1^\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$|A\varphi\rangle_H = \int_{\mathbb{R}} E \langle E|\varphi\rangle \eta^{-1^\times} |E\rangle \, d\mu(E)$$

Define as we usually would $A^\times |\varphi\rangle_H := |A^*\varphi\rangle_H$ and $A^{*\times} |\varphi\rangle_H := |A\varphi\rangle_H$ then one might conclude from the equalities that $|E\rangle$ are generalised eigenvectors of A and $\eta^{-1^\times} |E\rangle$ are generalised eigenvectors of A^*. This is exactly what we found in the discrete spectrum case. However, $A^\times$ and $A^{*\times}$ are ill-defined on the kets in $H^\times$ as A and A^* are not continuous. There action can only be well defined on the kets induced by Ψ.

Formally speaking, the right hand side of the expression are kets in $\Psi^\times$ since they are just a linear combination of $|E\rangle, \eta^{-1^\times} |E\rangle \in \Psi^\times$ and the right hand side we interpret as elements of a dense subspace of $H^\times$.

Lemma 4.14. *There exists an inner product space Σ such that $\Sigma \subset H$ and $\Sigma = \Psi$ element-wise. Furthermore, we have a series of maps, $A^\times : \Sigma \mapsto \Psi^\times, A^{*\times} : \Sigma \mapsto \Psi^\times$, $i^\times : \Sigma \mapsto \Psi^\times$ and $j^\times : \Sigma \mapsto \Psi^\times$ that give a resolution of the identity and diagonalization of A and A^*.*

$$A^\times(\varphi) := |A^*\varphi\rangle_H = \int_{\mathbb{R}} E \langle E| \eta^{-1^\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$A^{*\times}(\varphi) := |A\varphi\rangle_H = \int_{\mathbb{R}} E \langle E|\varphi\rangle \eta^{-1^\times} |E\rangle \, d\mu(E)$$

$$i^\times(\varphi) := |i\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \eta^{-1^\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$j^\times(\varphi) := |j\varphi\rangle_H = \int_{\mathbb{R}} \langle E|\varphi\rangle \eta^{-1^\times} |E\rangle \, d\mu(E)$$

Proof. Let us equip the set Ψ with the inner product $\langle \cdot, \cdot \rangle_H$ then Ψ is an inner product space whose completion coincides with H. For clarity, let us denote this space as Σ. Since $\Sigma \subset H$ and Σ has the same topology as H, we have $H^\times \subset \Sigma^\times$. Since Σ is not complete and thus not a Hilbert space, Reiz representation theorem does not apply. However, we can show that $\Sigma^\times \subset H^\times$ is true as well. Let $f \in \Sigma^\times$ then f is a continuous anti-linear functional on a dense subset of H. By taking limits, we can construct a unique anti-linear functional $F \in H^\times$. Thus, any anti-linear functional in $H^\times$ when restricted to Σ is in $\Sigma^\times$, and any anti-linear functional in $\Sigma^\times$ can be uniquely extended to an anti-linear functional in $\mathcal{H}^\times$. Thus,

$$\Sigma^\times = H^\times$$

Consider $A : \Sigma \mapsto H$ and $A^* : \Sigma \mapsto H$. Let $A^\times : \Sigma \mapsto \Psi^\times$ and $A^{*\times} : \Sigma \mapsto \Psi^\times$ be defined as follows. For all $\varphi \in \Sigma$

$$A^\times(\varphi) := |A^*\varphi\rangle_H = \int_{\mathbb{R}} E \langle E| \eta^{-1\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$A^{*\times}(\varphi) := |A\varphi\rangle_H = \int_{\mathbb{R}} E \langle E|\varphi\rangle \eta^{-1\times} |E\rangle \, d\mu(E)$$

We can also define $i : \Sigma \mapsto \Psi$ as $i(\varphi) = \varphi$ and $i^\times : \Sigma \mapsto \Psi^\times$ by

$$i^\times(\varphi) := |i\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \eta^{-1\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

Similarly, define $j^\times : \Sigma \mapsto \Psi^\times$

$$j^\times(\varphi) := |j\varphi\rangle_H = \int_{\mathbb{R}} \langle E|\varphi\rangle \eta^{-1\times} |E\rangle \, d\mu(E)$$

□

□

Remark. The above theorem can be applied equally well to the quasi-hermitian operator A^*. The construction in the proof will follow similarly accept the Hilbert space $\mathcal{H}$ will be replaced with $\mathcal{H}_*$. Furthermore, the nuclear spectral theorem will give us the existence of eigenkets of A^* denoted by $|F\rangle$. We can find the eigenket corresponding to A to be $\eta^\times |F\rangle$. One might naively think that $|F\rangle = \eta^{-1\times} |E\rangle$. However, this is not necessarily the case. The rigged Hilbert spaces constructed in the cases of A and A^* are not necessarily equivalent. As a result, there is no guaranttee that the eigenkets in one of the rigged Hilbert spaces is also in the other. Furthermore, the Ψ constructed in both may be entirely different. However, both methods give us equally valid resolutions of the identity and diagonlizations of the maps. From a physical perspective, one may prefer the space derived from A since Ψ necessarily satisfies $A\Psi \subset \Psi$. However even so, there is an ambiguity in choosing the set of eigenkets. Another problem is that since A^* is not continuous in the above theorem, its extension to $\Psi^\times$ is ill-defined. As a result, $\eta^{-1\times} |E\rangle$ cannot be formally interpreted as an eigenket of A^*. Another issue is that Φ is not invariant under A^*. Ideally, one would like to find a way to combine the constructions for A and A^* so that they are on equal footing. The next theorem imposes stronger conditions on the rigged Hilbert space in hopes of doing this.

Corollary 4.14.1. *Let $A : H \mapsto H$ be quasi-hermitian. Assume that there exist a rigged Hilbert space $\Psi \subset \mathcal{H} \subset \Psi^\times$ such that $A\Psi \subset \Psi$, $\eta^{-1}\Psi = \Psi$ and A, η^{-1} are continuous maps on Ψ. By lemma 4.8, A, A^*, η^{-1} and η are all continuous invariant maps. In this case, the extensions $A^\times : \Psi^\times \mapsto \Psi^\times$ and $A^{*\times} : \Psi^\times \mapsto \Psi^\times$ are well-defined. As a result, $|E\rangle$ is an eigenket of $A : \mathcal{H} \mapsto \mathcal{H}$ and $\eta^{-1\times} |E\rangle$ is an eigenket of $A^* : \mathcal{H} \mapsto \mathcal{H}$.*

Proof. In this case, $A, A^*, \eta,$ and η^{-1} are all continuous and can all be extended to $\Psi^\times$. All results of the previous theorem follow. Furthermore, $\Psi \subset \mathcal{H} \subset \Psi^\times$ satisfies exactly the assumptions of the *fictional* rigged Hilbert space scenario investigated at the beginning of the section. It was there shown that $\eta^{-1\times} |E\rangle$ is an eigenket of A^*. □

Remark. It would be interesting to see whether a construction according to the corollary above can be made such that when applied to A or A^*, they give equivalent answers. Also, it is entirely possible that the assumption $A\Psi \subset \Psi$ and $\eta^{-1}\Psi = \Psi$ is only satisfied when $\eta = id$. It should be asked whether the class of bounded positive definite operators that admit a dense invariant subset is not trivial. Furthermore, it should be checked whether the subclass of bounded positive definite operators that have an invariant dense subset whose inverse also admits one is not trivial.

It is not difficult to see that the above theorem reverts to the original nuclear spectral theorem when A is self-adjoint($\eta = id_H$).

4.4 Discussion of rigged Hilbert space framework for Quasi-Hermitian Observables in Quantum Mechanics

In the previous section, we obtained, under certain conditions on the observable and metric, a complete set of generalised eigenvectors. Additionally, we found that for a dense subset Φ of the Hilbert space, one can obtain a resolution of the identity and diagonalizations of the observable and its adjoint with respect to the eigenvectors. One caveat is that we required Φ to be left invariant under the action of the observable and the metric operator. In general, we do not know whether such a set Φ can be found. It is possible that such a Φ only exists in the trivial case where the metric operator satisfies $\eta = id_H$. However, these conditions are necessary for generalised left and right eigenvectors to be in the anti-dual space. Thus, if no non-trivial Φ exists, it gives one reason to conclude that there is no rigged Hilbert space formulation for quasi-hermitian operators. If this is the case, an alternate approach is likely needed. Assuming there are non-trivial examples, the obtained result does not give a natural rigged Hilbert space for the quasi-hermitian operator. Specfiically, we require the Hilbert space obtained for the inner product where the observable is self-adjoint to be rigged into a nuclear rigged Hilbert space. The eigenkets of the observable and its adjoint are in this rigged Hilbert space. One can argue that the construction is not canonical since the original Hilbert space where the quasi-hermitian operator is defined does not come into play.

4.4.1 Possible Alternative Approach by using Operator and Projection Valued Measures

It is possible that the approach taken in this thesis is not the most natural one. We tried to generalise the nuclear spectral theorem to the quasi-hermitian case by applying the nuclear spectral theorem in the Hilbert space where the operator is self-adjoint. One may have more luck if they attempt to generalise the proof of the nuclear spectral theorem itself. Such a proof will likely require some sort of spectral decomposition of the quasi-hermitian operator. Specifically, one likely will need to generalise the decomposition of self-adjoint operators in terms of projection valued measures to the quasi-hermitian case. One possible method of doing this is by considering the spectral decomposition of the operator in the Hilbert space where it is self-adjoint.[18] The spectral theorem says that a self-adjoint operator $A : \mathcal{H} \mapsto \mathcal{H}$ can be written as follows, where $(\cdot, \cdot)_{\mathcal{H}}$ represents the inner product. Let $A : \mathcal{H} \mapsto \mathcal{H}$ be a densely defined self-adjoint map then for $\varphi, \psi \in D(A)$, we have

$$(\varphi, \psi)_{\mathcal{H}} = \int_{\Lambda(A)} d(E_\lambda \varphi, \psi)_{\mathcal{H}} \tag{30}$$

$$(\varphi, A\psi)_{\mathcal{H}} = \int_{\Lambda(A)} \lambda d(E_\lambda \varphi, \psi)_{\mathcal{H}} \tag{31}$$

where φ, $\psi \in H \subset \mathcal{H}$. Note that $E_\lambda : \mathcal{H} \mapsto \mathcal{H}$ is an orthogonal projection defined on all of $\mathcal{H}$ and $d(E_\lambda \varphi, \psi)_{\mathcal{H}}$ is a projection valued measure.

If we let $A : H \mapsto H$ be quasi-hermitian in the Hilbert space H so that $(\varphi, \psi)_{\mathcal{H}} = (\varphi, \eta\psi)_H$, then A can be considered a self-adjoint map in $\mathcal{H}$ with a domain $D(A)$ that remains dense. As a result, we can apply (30) and (31). Note

$$(\varphi, A\psi)_{\mathcal{H}} = (\varphi, \eta A\psi)_H = (\varphi, A^*\eta\psi)_H$$

where we $\psi, \varphi \in D(A)$ and we use that $\eta A = A^*\eta$ from being quasi-hermitian. Note that

$$|A^*\eta\psi\rangle_H (\varphi) := (\varphi, A^*\eta\psi)_H$$

Let $\Phi \subset D(A)$ be such that $\eta\Phi = \Phi$ and $A\Phi \subset \Phi$. It follows that $A^*\Phi \subset \Phi$. Furthermore, suppose $E_\lambda \Phi \subset H$, $\forall \lambda \in \Lambda(A)$. Thus, similar as in the proof of the extension of the nuclear spectral theorem, we require the existence of a subspace invariant under the actions of the operators.

Then for all $\psi \in \Phi$, we can find a $\phi \in \Phi$ such that $\eta^{-1}\phi = \psi$. Substitution in (31) gives,

$$\langle \varphi | A^* \phi \rangle_H = \int_{\Lambda(A)} \lambda d(E_\lambda \varphi, \eta^{-1}\phi)_{\mathcal{H}}$$

but $(E_\lambda \varphi, \eta^{-1}\phi)_{\mathcal{H}} = (E_\lambda \varphi, \phi)_H$ assuming $E_\lambda \Phi \subset H$.

So

$$\langle\varphi|A^*\phi\rangle_H = \int_{\Lambda(A)} \lambda d(E_\lambda\varphi, \phi)_H$$

Remark. We see that the requirement $E_\lambda\Phi \subset H$ is necessary in order for the spectral measure to be written in terms of the inner product of H.

Using the fact that $\langle\varphi|A^*\phi\rangle_H = \langle A\varphi|\phi\rangle_H$ gives

$$\langle A\varphi|\phi\rangle_H = \int_{\Lambda(A)} \lambda d(E_\lambda\varphi, \phi)_H$$

and taking the complex conjugate, we find a similar expression for A.

$$\langle\phi|A\varphi\rangle_H = \int_{\Lambda(A)} \lambda d(\phi, E_\lambda\varphi)_H$$

where we use that λ is real.

It can similarly be shown from the self-adjoint case that

$$\langle\phi|\varphi\rangle_H = \int_{\Lambda(A)} d(\phi, E_\lambda\varphi)_H$$

Note that in the above spectral decompositions if E_λ is a self-adjoint orthogonal projection then the operator is necessarily self-adjoint. This is not a contradiction since E_λ is not self-adjoint in the inner product of H. Thus, we have found a spectral decomposition for A and A^*. By removing the λ, in the integral we obtain the resolution of the identity. In this case, we decompose the operator with respect to an operator valued measure. The E_λ is no longer an orthogonal projection.(It may be a non-orthogonal projection but this needs to be checked).

In conclusion, we present the following theorem

Theorem 4.15. *Let $A : H \mapsto H$ be a quasi-hermitian operator such that it is self-adjoint in the Hilbert space $\mathcal{H}$. Then if there exists a dense subset $\Phi \subset H$ invariant under $A, A^*, \eta,$ and η^{-1} and $E_\lambda\Phi \subset H$, $\forall\lambda \in \Lambda(A)$, where E_λ is the spectral projection in the self-adjoint spectral decomposition of A in $\mathcal{H}$, then the following spectral decompositions hold*

$$\langle\phi|\varphi\rangle_H = \int_{\Lambda(A)} d(\phi, E_\lambda\varphi)_H$$

$$\langle\phi|A\varphi\rangle_H = \int_{\Lambda(A)} \lambda d(\phi, E_\lambda\varphi)_H$$

$$\langle\phi|A^*\varphi\rangle_H = \int_{\Lambda(A)} \lambda d(E_\lambda\phi, \varphi)_H$$

where E_λ is an operator that is an orthogonal projection with respect to the inner product $\langle\cdot, \eta\cdot\rangle_H$. One can show when $E_\lambda : H \mapsto H$ is viewed as a map on H that it is quasi-hermitian so that $E^*_\lambda = \eta^{-1}E_\lambda\eta$.

Proof. See previous construction. □

It is easy to see when A is self-adjoint, so that $\eta = id_H$, that the decompositions correspond with the original spectral theorem for self-adjoint operators.

Interestingly, the above spectral decompositions are defined on essentially the same space as given in theorem 4.14. The only difference is that we don't require any continuity conditions on the operators or finer topology on Φ. It seems that by imposing these conditions, the spectral decomposition with respect to an operator-valued measure can be replaced with a decomposition with respect to a system of eigenkets. A possible extension of this thesis is to see whether the nuclear spectral theorem proof can be altered to account for the quasi-hermitian case by using the above spectral decompositions.

4.4.2 Rigged Hilbert Space of Quantum Systems with both Quasi-Hermitian and Hermitian Observables

In quanum mechanics, we are generally interested in a collection of observables. In the case of a system described by a quasi-hermitian Hamiltonian, the hermitian momentum and position observables are also of interest. As a result, one would generally like to obtain a rigged Hilbert space formulation so that the wavefunctions can be decomposed in terms of the Hamiltonian, position, and momentum eigenkets. Furthermore, we wish all the powers of the operators and their commutation relations to be well defined on the space of wave functions. The extension of the nuclear spectral theorem given in the previous section relies on constructing a rigged Hilbert space using the Hilbert space where the quasi-hermitian operator is self-adjoint. It should be noted that the momentum and position operators are not self-adjoint in this space so that the nuclear spectral theorem cannot be applied to them. In general, it is unclear how to incorporate general quasi-hermitian operators with hermitian operators. This will require further research and is out of the scope of this thesis.

However, we propose a possible method of constructing a rigged Hilbert space that may apply to a number of classes of PT-symmetric(not necessarily qausi-hermitian) quantum systems.

Consider the case where a quantum system is described by a PT-symmetric Hamiltonian that is diagonalizable and has discrete spectrum. In this case the eigenvectors are in the Hilbert space and form a complete basis. We do not need to the nuclear spectral theorem to ensure the existence of a complete set of eigenvectors. We only wish to find a set of wavefunctions and a rigged Hilbert space so that the eigenkets of the momentum and position observables are present. We will propose conditions under which this can be done.

Let H be the Hilbert space where the quasi-hermitian Hamiltonian is defined. Let $h : H \mapsto H$ be the Hamiltonian operator, $P : H \mapsto H$ the momentum operator, and $Q : H \mapsto H$ the position operator. Suppose Φ is a dense subspace of H equipped with a finer topology such that it is a nuclear countably Hilbert space. Furthermore, impose that $h\Phi \subset \Phi$, $P\Phi \subset \Phi$, and $Q\Phi \subset \Phi$ and that the maps are all continuous with respect to the finer topology. In this case, P and Q as self-adjoint operators and the rigged Hilbert space $\Phi \subset H \subset \Phi^\times$ satisfy the conditions of the nuclear spectral theorem. As a result, we have that $|p\rangle$ and $|x\rangle$ form a complete system of eigenkets. Furthermore, since the eigenvectors of h are in the Hilbert space H and form a complete basis, it turns out that h also has a complete set of eigenkets. It should first be noted that even though h has complete set of eigenvectors in H, they are not necessarily in Φ. As a result, one should use the canonical isomorphism into $\Phi^\times$ and consider the eigenvectors of h as elements of $\Phi^\times$. Let the eigenvectors of h be labeled ψ_n and the eigenvectors of h^* be labeled ϕ_n. The $|\psi_n\rangle$ and $|\varphi_n\rangle$ are simply the kets obtained by the canonical injection of these eigenvectors. One can show that for $\varphi \in \Phi$, the ket $|\varphi\rangle \in \Phi^\times$ can be written

$$|\varphi\rangle = \sum_{n=1}^{\infty} \langle \phi_n|\varphi\rangle \, |\psi_n\rangle$$

The above equality simply follwos from the similar equality thats holds in the Hilbert space H. One can similarly obtain a diagonalization for h and h^*.

Thus, we have constructed a rigged Hilbert space $\Phi \subset H \subset \Phi^\times$ such that all powers of the observables are well defined on Φ and the observables all of a complete set of eigenkets. This space is sufficient to rigorously describe the quantum system. Thus, we see that an extension of the nuclear spectral theorem is not necessarily needed when the quasi-hermitian operator is already diagonalizable.

5 Conclusion

In this thesis, we presented the well-studied rigged Hilbert space formulation of formulation of Quantum Mechanics. We rigorously covered the mathematical theory culminating with the nuclear spectral theorem. We applied the theory to the quantum mechanical system defined by a potential barrier. After illustrating the rigged Hilbert space for self-adjoint operators, non-hermitian operators and their application to quantum mechanics is discussed. Specifically, we introduce the class of PT-symmetric Hamiltonians that have found a wide range of applications. It is known that this class of operators is a subset of pseudo-hermitian operators. A large number of PT-symmetric Hamiltonians of interest happen to be quasi-hermitian. An operator $A : H \mapsto H$ is quasi if it is similar to its adjoint by a bounded positive definite operator η. So that $A^* = \eta^{-1}A\eta$. Currently, little attention has been given to putting such systems in a rigorous framework such as in the rigged Hilbert space formulation. We offer an extension of the nuclear spectral theorem to quasi-hermitian operators.

We show that for a dense subset of the Hilbert space where the quasi-hermitian operator is defined that a resolution of the identity and diagonalization of the operator and its adjoint can be obtained in terms of their eigenkets.

Specifically, we find the following identities for the quasi-hermitian operator $A : H \mapsto H$ where $|E\rangle$ are eigenkets of A and $\eta^{-1\times}|E\rangle$ are eigenkets of A^*. They are defined for a dense subset $\Phi \subset H$. For further details, we refer to theorem 4.14.

$$|A^*\varphi\rangle_H = \int_{\mathbb{R}} E \langle E| \eta^{-1\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$|A\varphi\rangle_H = \int_{\mathbb{R}} E \langle E|\varphi\rangle \eta^{-1\times} |E\rangle \, d\mu(E)$$

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E| \eta^{-1\times} |\varphi\rangle |E\rangle \, d\mu(E)$$

$$|\varphi\rangle_H = \int_{\mathbb{R}} \langle E|\varphi\rangle \eta^{-1\times} |E\rangle \, d\mu(E)$$

The space Φ where the identities are defined must satisfy $A\Phi \subset \Phi$ and $\eta^{-1}\Phi \subset \Phi$. It is possible that for certain operators A that the above space does not exist. Additionally, it is possible that the theorem is only satisfied in the trivial case where A is self-adjoint. If this is the case, there is reason to suspect that there is no such extension for quasi-hermitian operators.

We also obtained a generalization of the traditional spectral decomposition of self-adjoint operators to the quasi-hermitian case. We propose that a better and more natural generalization of the nuclear spectral theorem can be obtained by using the following spectral decompositions. Our approach used the nuclear spectral theorem for self-adjoint operators to gain information about quasi-hermitian operators. It is possible that using the following spectral decompositions to alter the proof itself may lead to an interesting result.

We find that for a subset $\Phi \subset H$ satisfying invariance under $\eta, \eta^{-1}, A,$ and A^* that the following identities hold

$$\langle \phi|\varphi\rangle_H = \int_{\Lambda(A)} d(\phi, E_\lambda\varphi)_H$$

$$\langle \phi|A\varphi\rangle_H = \int_{\Lambda(A)} \lambda d(\phi, E_\lambda\varphi)_H$$

$$\langle \phi|A^*\varphi\rangle_H = \int_{\Lambda(A)} \lambda d(E_\lambda\phi, \varphi)_H$$

where E_λ is an operator that is an orthogonal projection in the Hilbert space obtained by completing H with respect to the inner product $\langle \cdot, \eta \cdot\rangle_H$. One can show when restricted to H and using its inner product, E_λ is quasi-hermitian so that $E_\lambda^* = \eta^{-1}E_\lambda\eta$. One should note that there is no guarantee that $E_\lambda\Phi \subset H$.

We also discuss how to incorporate quasi-hermitian and hermitian operators together in a single rigged Hilbert space framework. We prove necessary conditions for a diagonalizable non-hermitian operator with discrete spectrum and any number of self-adjoint operators to have a complete set of eigenkets in a rigged Hilbert space.

An interesting extension of this thesis would be to see whether a rigged Hilbert space-like framework with a nuclear spectral-like theorem can be found that incorporates both quasi-hermitian and hermitian operators.

Another possible extension of our thesis is to extend the rigged Hilbert space framework and nuclear spectral theorem to the general class of pseudo-hermitian operators. Pseudo-hermitian operators are self-adjoint in Krein spaces so any such theory would likely require studying the spectral theory of self-adjoint operators on such spaces.

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