On non-Hermitian quantum mechanics

by

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Abstract

The purpose of this dissertation is to review the salient features of non-Hermitian quantum mechanics. An introduction to Hermitian quantum mechanics is included to make this review as accessible as possible. Attempts at formulating a consistent physical theory are introduced, before examining non-Hermitian theories' uses as convenient computational frameworks. Particular emphasis is placed on recent developments in open quantum systems that utilise non-Hermitian Hamiltonians. Chapter four introduces a logic that maps a non-Hermitian Hamiltonian onto a non-Hamiltonian algebra that has a Hermitian Hamiltonian. This was put forward by Sergi, who then goes on to show its application to a two level system. The time evolution is then derived in terms of the density matrix model. This system can then be used to analyse different types of decay such as coherence and population difference. This serves to illustrate the usefulness of the approach.

Preface

The work described by this dissertation was carried out at the University of KwaZulu-Natal, School of Chemistry and Physics, Pietermaritzburg, from **02/02/2011** until **01/03/2013**, under the supervision of **Dr A. Sergi**.

This dissertation is entirely, unless specifically contradicted in the text, the work of the candidate, Jared Peacock, and has not been previously submitted, in whole or in part, to any other tertiary institution. Where use has been made of the work of others, it is duly acknowledged in the text.

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1. The research reported in this dissertation, except where otherwise indicated, is my original research.
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Contents

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Many people have taken time to discuss various aspects of this project. Their assistance has been invaluable.

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Many conversations were had on a range of subjects (ranging) from physics to the more subjective topic of writing styles. In addition to numerous discussions, Professor R Raab also read many of the early drafts, a tedious business. His assistance with these matters is greatly appreciated and valued.

Finally, thanks to D. Uken and N. Dlamini for many discussions, especially when the complexities of non-Hermitian quantum mechanics were becoming bewildering. The rest of the department is also thanked for their input and assistance.

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Chapter 1

Introduction

The Hermitian condition has been the cornerstone of quantum mechanics. However, it seems that while the non-Hermitian condition does not ensure real eigenvalues, attempts are being made to find a more general condition that ensures real eigenvalues and allows non-Hermitian Hamiltonians[1].

Why are non-Hermitian Hamiltonians of interest? It is hoped that previously unexplained or unsolvable systems may now be treated. Research into non-Hermitian Hamiltonians follows two paths. The first involves trying to find a physically reasonable alternative to Hermitian quantum mechanics. The second uses non-Hermitian Hamiltonians to formulate new computational schemes in the hope of making problems more tractable.

Non-Hermitian Hamiltonians have been applied to a wide variety of fields and in some cases are necessary to make the problem tractable. An example of an open quantum system model that gives rise to non-Hermitian Liouville operator can be found in [2].

In particular in reference[2] some simple kinetic models of open quantum systems are studied. The various systems are one-dimensional with particle reservoirs on each side, allowing the systems to be driven far from equilibrium.

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \nu(x), \tag{1.1}$$

where $\nu(x)$ is the interaction potential. The time evolution of the system is given by the Liouville-von Neumann equation[2]. By applying open boundary conditions, dissipative effects on the properties of the various models can be investigated[2].

While this is not directly applicable to the work covered in this thesis it does highlight

the diverse applications that non-Hermitian quantum mechanics can be applied to. It is hoped that current work in non-Hermitian quantum mechanics is presented in an accessible manner.

An example of a more unusual application is the use of a non-Hermitian Hamiltonian applied to the problem of unzipping DNA[3]. Other fields include quantum optics and open quantum systems[4].

The value of a non-Hermitian Hamiltonian comes from the fact that if it provides a physically reasonable and consistent theory, then it will enrich the number of solvable systems available to physicists.

The aim of this dissertation is to provide a review of the field of non-Hermitian quantum mechanics that is accessible to researchers with little experience in the field. In order to achieve this, various approaches are discussed with particular focus on the use of non-Hermitian descriptions of open quantum systems. In addition, the more general and popular non-Hermitian theories of PT-symmetric[1], [5] and pseudo-Hermitian Hamiltonians[6], [7], [8] are introduced.

It is hoped that this review will allow readers to draw their own conclusions on whether non-Hermitian quantum mechanics is likely to form a robust and considered physical theory.

In an attempt to keep this review as accessible as possible, Chapter 2 is written to provide an introduction to the use of Dirac notation in quantum mechanics. Important concepts, particularly if they are of relevance to non-Hermitian theories, are also introduced.

Chapter 3 is a review of the available literature on non-Hermitian quantum mechanics. Non-Hermitian approaches used thus far can be broken into three groups:

1. A non-Hermitian Hamiltonian is used to represent open dynamics and attention is given to the eigenvalue problem.

2. PT-symmetric Hamiltonains are frequently used and utilise a symmetry argument

to ensure a real eigen-spectrum.

3. A more recent approach utilises pseudo-Hermitian Hamiltonians. While not as popular as the PT-symmetric approach, it is a more general theory.

Approach 1 was used first and provides a look at early development in the field. Approaches 2 and 3 are discussed in detail and compared.

The fourth Chapter[9], [10] introduces some recent applications of non-Hermitian theories to open quantum systems. By making use of non-Hermitian theories it is possible to significantly reduce the computational load. This technique can be used to undertake studies to investigate dissipation and coherence in a two-level system.

Chapter 2

Hermitian quantum mechanics

By the end of the 19th century many physicists believed that in principle all major problems in physics had been solved; that is to say, that the physical principles were understood, and with enough information and computational power any problem could in theory be solved. This belief was called into question in the early part of the 20th century by physicists who were investigating the behaviour of black-body radiation.

A black body is one that absorbs all incident radiation and radiates at any temperature greater than absolute zero. The emission of radiation occurs over a range of frequencies, the power distribution of which exhibits a maximum dependent on the temperature of the body. The theory of black-body radiation was initially attempted by Wien in 1896[11]. Wien's law agreed with experiment at high frequencies and as a result enjoyed early success. However, it soon became apparent that it was unable to describe the observed behaviour of black bodies at low frequencies. This failure of Wien's law prompted Planck to formulate an alternative theory of black-body radiation, which was published in 1901[12]. It relates the power R_f radiated at a frequency f to the frequency and absolute temperature T according to

$$R_f = \frac{2\pi h}{c^2} \frac{f^3}{e^{\frac{hf}{kT}} - 1}. \tag{2.1}$$

Here c is the vacuum speed of light, k the Boltzmann constant, and h a new universal constant, named after Planck, and defined as

$$h = \frac{E}{f}, \tag{2.2}$$

where f is the radiation frequency and E the energy.

A startling aspect of Plank's theory is an assumption he made: that a black body modelled as a collection of oscillators absorbs and emits only discrete amounts of energy described by $E = hf$[13]. At the time this was regarded as a mathematical device by Planck and others, in that energy was considered to be continuous.

In 1905 physicists were faced with further evidence of quantization in nature in a landmark paper by Einstein. The quantization of electromagnetic radiation was central to his explanation of the photoelectric effect, which suggested that electromagnetic radiation was discrete, acting in this effect as if it possessed particle properties.

Further evidence for the particle-like nature of electromagnetic radiation was obtained from the experiments of Compton in 1923. He noticed that when a graphite target is bombarded with monochromatic X-rays, there is a decrease Δf in the frequency of the rays emerging from the target, implying that energy has been lost. Based on Einstein's assumption, the energy lost will be $E = h\Delta f$. Compton found that scattered X-rays form two peaks of intensity; the first peak corresponds to the incident X-ray's frequency, while the second peak is shifted by a small amount. Accordingly, the incident X-ray beam can be understood as a stream of particles, each termed a photon, that collide with an electron in the target, losing energy in the process. Compton's experiment also confirmed that in certain effects electromagnetic radiation is discrete in nature[14].

In 1924 de Broglie postulated that wave-particle behaviour applies to matter as well as to electromagnetic radiation. He derived an expression for the wavelength associated with a moving particle. Known as the de Broglie wavelength, it is given by,

$$\lambda = \frac{h}{p}, \tag{2.3}$$

where p is the particle's momentum[14]. Due to a lack of experimental evidence supporting his postulate, it was regarded as not being physically relevant. This changed as a result of an experiment in 1927 by Davisson and Germer which confirmed the de Broglie

postulate.

These two physicists found that, by firing electrons at a nickel target, a diffraction pattern was produced a clear example of wave behaviour. The diffraction pattern was found to obey Bragg's law for X-rays, namely

$$n\lambda = 2d\sin\phi, \tag{2.4}$$

where d is the atom spacing in the lattice, λ the de Broglie wavelength, and ϕ the angle between the incident beam and the scattering plane. Such a clear example of matter exhibiting wavelike behaviour provided confirmation of the de Broglie hypothesis.

Several new insights into the behaviour of energy and matter have occurred as a result of experiment. Planck's explanation of black-body radiation lead to the idea of discrete quantities of energy. Eistein's work on the photoelectric effect confirmed that energy was discrete. The particle like nature of electromagnetic radiation was first revealed by the experiments of Compton. It was postulated by de Broglie that wave particle behaviour applies to both matter and electromagnetic radiation, confirmation was provided by Davisson and Germer. Collectively the work performed in this period lead to a fundamental shift in understanding of the behaviour of electromagnetic radiation and matter. However, as yet, there was no approach that encompassed these profound changes in physics. This void was fulled by two approaches to quantum mechanics that were developed by Schrödinger and Heisenberg respectively.

The two separate approaches to quantum mechanics were formulated by Schrödinger and Heisenberg early in the 20th century[15]. The central feature in Schrödinger's formalism is wavefunctions, which have a probabilistic interpretation. In contrast, Heisenberg's formalism makes use of matrices and is known as matrix mechanics. These formalisms were the first successful attempts to explain quantum mechanics that were not empirical in nature. Heisenberg's and Schrödinger's approaches were unified later by Dirac.

2.1 Quantum mechanics: Dirac's approach

The standard formulation of quantum theory is constructed from a number of postulates. The first states that each quantum state of a physical system is described by a state vector of a Hilbert space[16], which is an inner product linear vector space of orthonormal vectors. In this dissertation, Dirac bra-ket notation will be used throughout. Accordingly, state vectors will be known as kets and written as $|\phi\rangle$. Kets provide a description for all possible physical states, and collectively make up a ket space where all the properties associated with linear algebra apply. Bras are dual vectors of the kets and have a one to one correspondence with kets and are written as $\langle\phi|$[16]. Of importance in our treatment of kets is the principle of superposition.

Any ket of a vector space in quantum mechanics can be written as a superposition of two or more other kets of the space. The fundamental difference between superposition in quantum and classical mechanics, is the indeterminacy present in quantum systems. The superposition of two quantum states forms a new state describing the system. This state gives the probability of obtaining a particular result, making quantum mechanics indeterminate in nature.

1

Consider a state $|\phi\rangle$ that is in a superposition of two states $|\phi_1\rangle$ and $|\phi_2\rangle$, that produce eigenvalues a and b.

$$|\phi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle, \tag{2.5}$$

where c_1 and c_2 are constants that in general are complex.

By making successive measurements of a system in a superposition of states, a series of results will be obtained that will be either a or b. The probability of producing a particular result is dependent on the weight that $|\phi_1\rangle$ and $|\phi_2\rangle$ are present in state $|\phi\rangle$[15]. A dependent state is made up of two or more other states for example, state $|\phi\rangle$. The alternative is an independent state. The set of kets $|\phi_i\rangle$, where i = 1,2,...,n, is linearly independent if

$$\sum_{i=1}^{n} a_i|\phi_i\rangle = 0 \tag{2.6}$$

and all $a_i = 0$.

The ordered product of kets $|\phi_1\rangle$ and $|\phi_2\rangle$ can be written as $(|\phi_1\rangle, |\phi_2\rangle)$, which Dirac denoted as

$$\langle\phi_1|\phi_2\rangle, \tag{2.7}$$

termed the inner product. Inner products have the following properties[16]:

1. $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$, where the complex conjugate is denoted by an asterisk.
2. $\langle\psi|c\phi\rangle = c\langle\psi|\phi\rangle$, where c is a number, possibly complex.
3. $\langle\psi|\phi + \varphi\rangle = \langle\psi|\phi\rangle + \langle\psi|\varphi\rangle$
4. $\langle\phi|\phi\rangle \geq 0$, that is, the inner product is always greater than zero unless $|\phi\rangle$ is the null ket.
5. If $\langle\phi|\phi\rangle = 1$, then $|\phi\rangle$ is a normalised ket.
6. If neither $|\phi\rangle$ or $|\psi\rangle$ is the null ket, then they are orthogonal if $\langle\phi|\psi\rangle = 0$.
7. An orthonormal basis is made up of normalised kets, where all kets in the basis are orthogonal to one another. If $|\phi_i\rangle$ and $|\psi_j\rangle$ are members of such a set, then $\langle\phi_i|\psi_j\rangle = \delta_{ij}$, where δ_{ij} is the Kronecker delta defined by $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$.

An orthonormal set can be produced from a linearly independent set that spans the space by making use of the Gram-Schmidt process.

2.2 Linear operators, observables, and the Hermitian condition

An observable is a linear Hermitian operator whose eigenkets $|\phi_i\rangle$ form a basis in state space. A Hermitian operator A, is defined by

$$\langle\phi_i|A|\phi_j\rangle = \langle\phi_j|A|\phi_i\rangle^*, \tag{2.8}$$

where $|\phi_i\rangle$ and $|\phi_j\rangle$ are arbitrary vectors. In the standard (Hermitian) form of quantum mechanics the Hamiltonian is required to be Hermitian. This ensures that the eigenvalues are real. The reality of the eigenvalues is desirable as non-real eigenvalues are

non-sensical from a physical point of view. In addition, the Hermitian condition is necessary to ensure a positive definite norm.

It is helpful to introduce the closure relation,

$$\sum_{i=1}^{n} |\phi_i\rangle\langle\phi_i| = 1, \tag{2.9}$$

where 1 is the identity operator.

Using the closure relation an arbitrary ket can be written as

$$|\phi\rangle = \sum_{i=1}^{n} |\phi_i\rangle\langle\phi_i|\phi\rangle, \tag{2.10}$$

where n is possibly infinite.

It is postulated that a measurable physical quantity of a physical system is represented by a linear Hermitian operator, termed an observable, that acts on vectors of the Hilbert space representing the physical system. A measurement that is made when the system is in a pure state yields an eigenvalue of the observable operator. This can be expressed as

$$A|\phi_i\rangle = a_i|\phi_i\rangle, \tag{2.11}$$

where A is an operator that operates on the eigenvector $|a_i\rangle$ and a_i is the associated eigenvalue. The equation above is termed the eigenvalue equation of A.

The eigenvectors of an operator on the Hilbert space $\mathcal{H}$ span the space and can be chosen to be an orthonormal basis of $\mathcal{H}$ [17]. The eigenvectors form an orthonormal basis on $\mathcal{H}$ if the eigenvectors are independent. This is a standard result from linear algebra.

It is now proved that the eigenvalues of a Hermitian operator are real.

Proof: Let A be a Hermitian linear operator.

$$A|\phi_i\rangle = a_i|\phi_i\rangle. \tag{2.12}$$

Now introduce the ordered product,

$$\langle\phi_i|A|\phi_i\rangle = a_i\langle\phi_i|\phi_i\rangle \tag{2.13}$$

but $\langle\phi_i|A|\phi_i\rangle$ must be real and non-zero since

$$\langle\phi_i|A|\psi_i\rangle = \langle\psi_i|A|\phi_i\rangle^*. \tag{2.14}$$

Then a_i must be real as $\langle\phi_i|\phi_i\rangle$ is the norm. Therefore if A is a Hermitian linear operator, the associated eigenvalue will be real.

Now use the closure relation to write down a simplified expression for an observable[16],

$$A = \sum_i a_i|\phi_i\rangle\langle\phi_i|. \tag{2.15}$$

The expectation value of A is

$$\langle\phi|A|\phi\rangle = \langle A\rangle \tag{2.16}$$

which can be thought of as a quantum average. That is, multiple measurements of an observable A, on an identical system, will yield the mean value $\langle A\rangle$.

Consider what happens when a measurement is taken. If we have a completely isolated quantum system, and a measurement is taken, then we have brought a second system into contact with the first, perturbing the system. Although measurements can be taken while trying to minimise the effect of the measurement on the system, crucially, some interference will occur allowing only a single measurement to be taken of an unperturbed system[15].

2.3 Quantum conditions

The peculiar nature of quantum mechanics is represented in large part by the non-commutative multiplication between most operators.

One needs equations called quantum conditions. In order to determine these equations, in Dirac's approach, the method of classical analogy is used. This method exploits the fact that classical mechanics provides a valid description of dynamical systems, provided that the systems are large enough that any disturbance due to observation can be neglected. Dirac concluded that classical mechanics must be a limiting case of quantum mechanics. By making use of the common ground between quantum mechanics and classical mechanics, in the limiting case, the method of classical analogy hopes to determine the laws of quantum mechanics by finding them as generalisation of classical laws[15].

Now consider a system that is made up of a large number (N) of interacting particles. When using canonical coordinates each particle will have position coordinates (q) and momentum coordinates (p) associated with them. If two variables u and v are functions of a set of canonical coordinates, then the classical Poisson Bracket $\{u, v\}$ is

$$\{u, v\} = \sum_k (\frac{\partial u}{\partial q}\frac{\partial v}{\partial p_k} - \frac{\partial u}{\partial p}\frac{\partial v}{\partial q}), \tag{2.17}$$

where $\mathbf{q} = (r_1, r_2, r_3) = (x, y, z)$ and $\mathbf{p} = (p_1, p_2, p_3) = (p_x, p_y, p_z)$.

It follows from equation (17) that[15]:

1. $\{u, v\} = -\{v, u\}$.
2. $\{u, c\} = 0$ where c is a number.
3. $\{u_1 + u_2, v\} = \{u_1, v\} + \{u_2, v\}$.
4. It follows from 3. and 1.
   $\{u, v_1 + v_2\} = \{u, v_1\} + \{u, v_2\}$.
5. $\{u_1 u_2, v\} = \{u_1, v\}u_2 + u_1\{u_2, v\}$.
6. It follows from 5. and 1.
   $\{u, v_1 v_2\} = \{u, v_1\}v_2 + v_1\{u, v_2\}$.

In addition, a useful identity is stated here without proof,

$$\{u, \{v, w\}\} + \{v, \{w, u\}\} + \{w, \{u, v\}\} = 0. \tag{2.18}$$

The quantum analogy of a Poisson Bracket is the commutator,

$$[u, v] = uv - vu. \tag{2.19}$$

The commutator satisfies all the properties (1 to 6), as can be shown from (2.19). Of special significance are the canonical commutation relations, also called the fundamental quantum conditions[16],

$$\begin{aligned} [r_i, r_j] &= 0 \\ [p_i, p_j] &= 0 \\ [r_i, p_j] &= i\hbar\delta_{ij} \end{aligned} \tag{2.20}$$

where i, j = 1,2,3.

If multiple measurements of observables A and B are taken in quick succession and always return the same results, a_n and b_n, then A and B are termed compatible observables and will commute. Non-commuting observables are responsible for much of the unintuitive behaviour present in quantum mechanics.

2.4 The Heisenberg uncertainty principle

Non-commuting observables result in the Heisenberg uncertainty principle which gives the maximum accuracy that can be obtained when they are measured simultaneously[15].

The error ΔA in A, is defined as follows

$$\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle (\delta A)^2 \rangle}, \tag{2.21}$$

where $\delta A = A - \langle A \rangle$.

In order to derive the Heisenberg uncertainty principle let

$$(A + i\lambda B)|\mu\rangle = |\mu\rangle \tag{2.22}$$

where A and B are non-commuting observables and λ is any real number.

Now take the inner-product

$$\langle \mu | (A - i\lambda B)(A + i\lambda B) | \mu \rangle \geq 0. \tag{2.23}$$

Due to the non-negativity of the norm.

$$\langle \mu | A^2 + \lambda^2 B^2 - i\lambda BA + i\lambda AB | \mu \rangle \geq 0, \tag{2.24}$$

$$\langle \mu | A^2 + \lambda^2 B^2 + i\lambda [A, B] | \mu \rangle \geq 0. \tag{2.25}$$

But if A and B are non-commuting observables then $[A, B] = iC$, where $[A, B] = AB - BA$.

Therefore

$$\langle A^2 \rangle - \lambda \langle C \rangle + \lambda^2 \langle B^2 \rangle \geq 0. \tag{2.26}$$

Now the minimum value of the left-hand side can be determined by differentiating with respect to λ,

$$-\langle C \rangle + 2\lambda \langle B^2 \rangle = 0 \tag{2.27}$$

$$\lambda = \frac{\langle C \rangle}{2\langle B^2 \rangle}. \tag{2.28}$$

Substitute equation (2.28) into equation (2.26)

$$\langle A^2\rangle - \frac{\langle C\rangle}{2\langle B^2\rangle}\langle C\rangle + [\frac{\langle C\rangle}{2\langle B^2\rangle}]^2\langle B^2\rangle \geq 0 \tag{2.29}$$

$$\langle A^2\rangle - \frac{\langle C\rangle^2}{2\langle B^2\rangle} + \frac{\langle C\rangle^2}{4\langle B^2\rangle} \geq 0 \tag{2.30}$$

$\langle B^2\rangle$ is non-negative, this can be seen by using the definition of an adjoint

$$\langle\mu|B^\dagger|\phi\rangle = \langle\overline{\phi|B|\mu}\rangle, \tag{2.31}$$

then $\langle B^2\rangle$ can be expressed as

$$\langle\mu|B^2|\mu\rangle = \langle\mu|B^2|\mu\rangle \tag{2.32}$$

$$= \langle\mu|B^\dagger B|\mu\rangle. \tag{2.33}$$

The above equation is the norm of vector $B|\mu\rangle$. Due to the non-negativity of the norm, we can conclude $\langle B^2\rangle$ is positive.

Therefore

$$\langle A^2\rangle\langle B^2\rangle - \frac{\langle C\rangle^2}{2} + \frac{\langle C^2\rangle}{4} \geq 0 \tag{2.34}$$

$$\langle A^2\rangle\langle B^2\rangle \geq \frac{\langle C^2\rangle}{4}. \tag{2.35}$$

A is Hermitian and $\langle A\rangle$ is real. Therefore δA is Hermitian and similarly δB is Hermitian. $\langle A\rangle$ and $\langle B\rangle$ will commute with any operator. Therefore δA and δB must have the same commutator as A and B. Then $[\delta A, \delta B] = C$[16]. If this commutator is now used instead of the commutator of A and B we obtain

$$\langle(\delta A)^2\rangle\langle(\delta B)^2\rangle \geq \frac{\langle C\rangle^2}{4}. \tag{2.36}$$

Now rewrite the above expression using (2.21)

$$(\Delta A)^2(\Delta B)^2 \geq \frac{\langle C\rangle^2}{4}, \tag{2.37}$$

$$\Delta A\Delta B \geq \frac{|\langle C\rangle|}{2}. \tag{2.38}$$

This result is the Heisenberg uncertainty principle. Consider two non-commuting observables A and B. We find that they cannot be measured without a minimum uncertainty

of $\frac{|\langle C \rangle|}{2}$.

For example, if position is measured then measurements can be taken of the momentum but there will be some uncertainty present in these measurements. For the particular case where C is an operator a non-zero real number A and B can have no simultaneous eigenkets. The uncertainty principle is peculiar to quantum mechanics[16].

2.5 The Schrödinger and Heisenberg pictures.

Thus far we have not considered quantum dynamics, only a single instant in time. The expectation value for an observable A when $t = 0$ is

$$\langle A(0) \rangle = \langle \phi(0) | A(0) | \phi(0) \rangle, \tag{2.39}$$

while the expectation value at time t is

$$\langle A(t) \rangle = \langle \phi(t) | A(t) | \phi(t) \rangle, \tag{2.40}$$

where $|\phi(t)\rangle$ is a normalised ket which completely describes the state of the system at time t.

It is useful at this point to introduce the concept of a picture in quantum mechanics. There are two extreme cases. The first is the Heisenberg picture where the operators are dependent on time. The state vectors are time independent. The Heisenberg picture is defined by

$$\frac{d|\phi\rangle}{dt} = 0, \ \frac{dA}{dt} \neq 0. \tag{2.41}$$

The second is the Schrödinger picture. In this picture the state vectors are time-dependent, while the operators are time-independent. Unless an operator is explicitly dependent on time. The Schrödinger picture is defined by

$$\frac{dA}{dt} = \frac{\partial A}{\partial t}. \tag{2.42}$$

The transformation between pictures must be unitary to maintain the invariance of observables. Furthermore, it is required that the normalisation be independent of time[16].

When

$$|\phi(t)\rangle = U(t)|\phi(0)\rangle, \tag{2.43}$$

$$A(t) = U^{\dagger}(t)A(0)U(t), \tag{2.44}$$

the above conditions are satisfied. $U(t)$ is a unitary operator, defined by

$$UU^{\dagger} = U^{\dagger}U = I, \tag{2.45}$$

where I is the identity matrix and the dagger denotes the adjoint. The adjoint operator $A^{\dagger}$ of the operator A is defined by

$$\langle\psi|A^{\dagger}|\phi\rangle = \langle\phi|A|\psi\rangle^{*}. \tag{2.46}$$

It is postulated that the time evolution operator $U(t)$ satisfies the equation[16],

$$i\hbar\frac{dU(t)}{dt} = HU(t). \tag{2.47}$$

If H is assumed to be independent of time the solution to the above equation is

$$U(t) = e^{\frac{-iHt}{\hbar}}. \tag{2.48}$$

A common occurrence when working in the Schrödinger picture is to find a complete set of commuting operators for the system which includes H. Therefore the basis kets $|\phi_i\rangle$ are also eigenkets of H. As a result

$$H|\phi_i\rangle = E_i|\phi_i\rangle, \tag{2.49}$$

where $|\phi_i\rangle$ is the set of energy eigenkets and E_i denotes an energy eigenvalue[16].

When t = 0 the system is in the state $|\phi(0)\rangle$. Now use the closure relation

$$|\phi(0)\rangle = \sum_{i=1}^{n} |\psi_i\rangle\langle\psi_i|\phi(0)\rangle \tag{2.50}$$

and the time evolution operator $U(t) = e^{-\frac{iHt}{\hbar}}$. Combining them we can write down $|\phi(t)\rangle$

$$|\phi(t)\rangle = \sum_{n} |\psi_n\rangle\langle\psi_n|\phi(0)\rangle e^{-\frac{iHt}{\hbar}}. \tag{2.51}$$

If an energy eigenket is an initial state of the system, then $|\psi(t)\rangle$ can be written as

$$|\psi(t)\rangle = |\psi_n\rangle e^{-\frac{iE_nt}{\hbar}}, \tag{2.52}$$

where $|\psi(t)\rangle$ is still in the same eigenstate as $|\psi_n\rangle$[16].

We can now write the expectation value of observable A as

$$\langle\psi(t)|A(0)|\psi(t)\rangle = \langle\psi_n|A(0)|\psi_n\rangle. \tag{2.53}$$

The above equation is independent of time. For this reason the energy eigenkets are known as stationary states.

Now operate equation (2.47) on $|\phi(0)\rangle$

$$i\hbar\frac{dU(t)}{dt}|\phi(0)\rangle = HU(t)|\phi(0)\rangle. \tag{2.54}$$

But $|\phi(t)\rangle = e^{-\frac{iE_nt}{\hbar}}|\phi(0)\rangle$. Therefore

$$i\hbar\frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle, \tag{2.55}$$

giving us the Schrödinger equation for the time evolution.

If H is conservative (independent of time), then the solution to the above equation is

$$U(t) = e^{-iH\frac{t}{\hbar}}. \tag{2.56}$$

Take the time derivative of equation (2.43) and use the above solution

$$\begin{aligned}
\frac{d}{dt}A(t) &= \frac{d}{dt}[U^\dagger(t)A(0)U(t)] && (2.57)\\
&= \frac{d}{dt}[e^{\frac{iHt}{\hbar}}A(0)e^{-\frac{iHt}{\hbar}}] && (2.58)\\
&= \frac{i}{\hbar}(HA(t) - e^{\frac{iHt}{\hbar}}A(0)He^{-\frac{iHt}{\hbar}}). && (2.59)
\end{aligned}$$

Now use equation (2.43). Then

$$\frac{d}{dt}A(t) = \frac{\partial A}{\partial t} + \frac{i}{\hbar}[H, A(t)], \tag{2.60}$$

which is the equation of motion for the Heisenberg picture[16].

2.6 The density matrix

When working with a mixture of several quantum states, it is useful to use the density matrix, as it is then straightforward to describe mixed states[17].

Consider a simple mixed state for a two-level system with pure states $|\psi_1\rangle$ and $|\psi_2\rangle$. The probability of the system being in a particular state is given by γ_1 and γ_2. The density matrix for the system is[17],

$$\rho = \sum_{i}^{n=2} \gamma_i |\psi_i\rangle\langle\psi_i|. \tag{2.61}$$

If there were n possible states this would be generalised as

$$\rho = \sum_{i}^{n} \gamma_i |\psi_i\rangle\langle\psi_i|. \tag{2.62}$$

The density matrix can also be written as an operator. The density operator is a linear operator that has the form of a matrix. The density matrix contains information about the quantum state of a system as well as the uncertainty present[17].

The density operator ρ is said to be in a pure state if

$$Tr(\rho^2) = 1 \tag{2.63}$$

where the trace (Tr) is the sum of the diagonal elements in the density matrix. The density operator is normalised if $Tr(\rho) = 1$. In general, the density operator can be normalised as follows

$$\rho' = \frac{\rho}{Tr(\rho)}, \tag{2.64}$$

where ρ' is the normalised density matrix[17].

Expectation values can also be written in terms of the density matrix. Let O be a linear operator. The expectation value of O can be written as

$$\langle O\rangle = Tr(\rho O). \tag{2.65}$$

The expectation value for a pure state is

$$\langle O\rangle = \langle\psi|O|\psi\rangle. \tag{2.66}$$

The expectation value for a mixed state ρ can be written as

$$\langle O\rangle = Tr(\rho\ O) \tag{2.67}$$

$$= \sum_{j} w_j \langle\psi_j|O|\psi_j\rangle, \tag{2.68}$$

where w_j is the probability of the system being in state $|\psi_j\rangle$.

Then, the scalar product can be written in terms of the density matrix

$$|\langle\phi,\psi\rangle|^2 = \langle\phi|\psi\rangle\langle\psi|\phi\rangle \tag{2.69}$$

$$= \langle\phi|\rho|\phi\rangle. \tag{2.70}$$

The scalar product, $|\langle\phi,\psi\rangle|^2 = Tr(\rho P_\phi)$, where $P_\phi = |\phi\rangle\langle\phi|$. P_ϕ is called the projector operator of the state $|\phi\rangle$.

The time evolution of the density operator for a pure state is defined by

$$[H,\rho] = i\hbar\frac{\partial\rho}{\partial t}. \tag{2.71}$$

This equation is called the von Neuman equation. When the von Neuman equation is satisfied, the pure states evolve under Schrödinger evolution, namely the Schrödinger picture. The time evolution can also be represented in the Heisenberg picture,

$$\rho(t) = U^\dagger\rho_s(t)U. \tag{2.72}$$

Now that time evolution and the scalar product have been defined, it is necessary to consider pure and mixed states in greater detail. A density matrix can be written as a linear combination of pure states. For example, a two-level system can be written as,

$$\rho = w\rho_1 + (1-w)\rho_2, \tag{2.73}$$

where ρ_1 and ρ_2 are pure states and w is the weight (probability) of the system being in the first state. Therefore,

$$\rho_1 + \rho_2 = 1. \tag{2.74}$$

If a state is pure the trace of the density matrix will be one. However, if a state is mixed, the trace of the density matrix will be less than one. A measure of how mixed a state is can be gained using[17]

$$M = Tr(\rho^2). \tag{2.75}$$

By means of a density matrix, quantum states can be broken into pure or mixed states and can then be treated appropriately. In particular, the density matrix is useful for a compound system, one with many subsystems, that is difficult to treat without using the density matrix.

Chapter 3

Non-Hermitian quantum mechanics

In quantum mechanics it is a requirement that the Hamiltonian must be Hermitian. This is to ensure that the eigenvalues associated with the Hamiltonian are real. However, it has been shown that a Hermitian Hamiltonian is not a necessary condition to guarantee real eigenvalues for the Hamiltonian. There are two other approaches that can be taken. The first has been developed primarily by Bender and associates and utilises space-time reflection symmetry[1]. This is known as PT-symmetry. An alternative approach was developed by Mostafazadeh who works with pseudo-Hermitian Hamiltonians[6]. Pseudo-Hermitian Hamiltonians have real and positive eigenvalues[6], [11].

3.1 Historical development of non-Hermitian theories

One of the earliest uses of non-Hermitian Hamiltonians was by Wu in 1959. By making use of a non-Hermitian Hamiltonian, Wu found that the ground state energy of Bose spheres was no longer divergent. Wu made no attempt to justify his use of a non-Hermitian Hamiltonian; he merely used it since it provided the correct results[18].

In 1967 Wong attempted to define a class of physically reasonable Hamiltonians[19]. He had noticed that the Hamiltonian of a closed system is Hermitian, but if the system is perturbed the Hamiltonian is no longer Hermitian. Wong then proceeded by defining

a perturbed Hamiltonian

$$H = H_0 + gH, \tag{3.1}$$

where g varies the influence of H. It is unclear with this class of Hamiltonian whether complex eigenvalues are allowed, yet there is no justification for their admission on physical grounds.

A significant paper in the development of non-Hermitian quantum mechanics was the publication by Haydock and Kelly in 1975[20]. They stated that while the Hermitian condition was sufficient to ensure real eigenvalues, it was not necessary and sufficient. This is very significant in the development of non-Hermitian quantum mechanics, as a necessary and sufficient condition for real eigenvalues is obviously desirable.

While progress was made, for example a probability-conserving algorithm[21], the next big step forward had to wait until 1997. This advance was a justification for the use of complex eigenvalues. Here Hatano and Nelson[22] justified the use of complex eigenvalues to "apply depinned field lines of a non-Hermitian external magnetic field to a type II semiconductor."

The following year Schrödinger operators with complex potentials but real eigenvalues were found[23]. Such potentials with real eigenvalues are of interest, since any physically acceptable non-Hermitian theory must have real eigenvalues or, if not, account for complex eigenvalues in some way.

3.2 Applications

Non-Hermitian quantum mechanics has been applied to a wide variety of fields including: field theory, statistical mechanics, quantum optics, and of particular interest to this review, open quantum systems[24].

Quantum optics, in particular, is a very useful field when considered in conjunction with non-Hermitian quantum mechanics: in large part because theories from non-Hermitian quantum mechanics can be implemented and studied in an environment that

is more easily controlled. An example of this can be seen in[25], which investigates the behaviour of parity-time symmetry.

The two most popular approaches to non-Hermitian quantum mechanics are Mostafazadeh's pseudo-Hermitian Hamiltonians and Bender's PT-symmetric as well as his CPT-symmetric approach. Both approaches have been applied to many fields and are now discussed in more detail.

3.3 PT-symmetry and CPT-symmetry

PT-symmetric quantum mechanics was introduced by Bender and Boettcher. This discussion of PT-symmetry and CPT-symmetry is heavily based on the work of Bender and collaborators.

Interest in PT-symmetric Hamiltonians began after Bessis made the conjecture that the Hamiltonian[5],

$$H = p^2 + x^2 + ix^3, \tag{3.2}$$

has a real and positive spectrum and hence real and positive eigenvalues, where p is the momentum operator and x is the position coordinate[5]. Bender and Boettcher claim that the reality of the spectrum is due to PT-symmetry. There is no rigorous proof of this claim.

These Hamiltonians are called PT-symmetric because they are invariant under a parity and time reversal transformation,

$$[H, PT] = 0. \tag{3.3}$$

However, under a time or a parity transformation the Hamiltonian is not necessarily invariant[1]. The parity operator has the following effect

$$P : x \rightarrow -x \tag{3.4}$$

$$p \rightarrow -p. \tag{3.5}$$

The effect of the time reversal operator is,

$$T : x \rightarrow x, \tag{3.6}$$

$$p \rightarrow -p, \tag{3.7}$$

$$i \rightarrow -i. \tag{3.8}$$

The sign of the complex component changes when the time-reversal operator is applied; as a result, the canonical commutation relation holds[1],

$$[x, p] = i. \tag{3.9}$$

This is relevant as the commutation relation is central to Hermitian quantum mechanics and means that Heisenberg algebra still applies. Bender and associates modified equation (3.2), arriving at a new class of Hamiltonian that is infinite in extent,

$$H = p^2 + x^2(ix)^n, \tag{3.10}$$

where n is real[1]. This class of Hamiltonian is PT-symmetric and hence invariant under a PT-transformation.

Using numerical methods this class of Hamiltonian has been found to have real and positive eigenvalues when $n \geq 0$ [5]. A mixture of real eigenvalues and complex eigenvalues occur when $n < 0$. As n becomes more negative the number of pairs of complex eigenvalues increases until there are only complex pairs of eigenvalues. This was verified by Bender and associates numerically[1].

If the PT-symmetry of the Hamiltonian is unbroken, then the Hamiltonian H has a real spectrum and the PT-operator will commute with H. Then assume that, the PT-operator and the Hamiltonian have simultaneous eigenkets with ϕ (diagonalisable). Using the above, it is possible to prove that the eigenvalues of the Hamiltonian are real[1].

If PT and H commute then,

$$PTH = HPT. \tag{3.11}$$

Now operate from the right-hand side with TP. Then

$$PTHTP = H. \tag{3.12}$$

The above equation is PT invariant since $(TP)^\dagger = PT$ and P and T are unitary. Now we write down the time-independent Schrödinger equation,

$$H|\phi_i\rangle = E_i|\phi_i\rangle. \tag{3.13}$$

Apply the PT transformation to equation (3.13)

$$PTHTP|\phi_i\rangle = PTE_iTP|\phi_i\rangle, \tag{3.14}$$

but $TE_iT = E_i^*$ and $P^2 = I$. Therefore,

$$PTHTP|\phi_i\rangle = E_i^*|\phi_i\rangle. \tag{3.15}$$

Now use equations (3.10) and (3.11) to yield

$$E|\phi_i\rangle = E_i^*|\phi_i\rangle. \tag{3.16}$$

Therefore, $E = E_i^*$ hence the eigenvalues are real, $E_i \; \epsilon \; \Re$.

From this analysis it seems clear that a non-Hermitian Hamiltonian that is PT-symmetric will have real eigenvalues. However, it is not at all clear whether PT-symmetric Hamiltonians define a physical theory. Bender and associates' definition of a physical theory requires two conditions to be satisfied. The first requires a Hilbert space of state vectors. An inner-product with a positive definite norm is the second[1].

The first condition appears to be satisfied on numerical grounds. PT-symmetric Hamiltonians are not positive definite and this is problematic as the inner-product is traditionally viewed as a probability in Hermitian quantum mechanics.

Bender and associates[1] identified an underlying symmetry that is common to all PT-symmetric Hamiltonians with unbroken symmetry. By introducing a new operator C it was found that a new dynamically determined inner-product could be defined. This dynamically determined inner-product begins with the derivation of the new operator C.

Bender and his associates[1] began their derivation of C by examining the Sturm-Liouville differential equation, where the Hamiltonian is

$$H = p^2 + x^2(ix)^\nu, \tag{3.17}$$

where $\nu \geq 0$.

The Sturm-Liouville equation is

$$-\phi_n(x) + x^2(ix)^\nu \phi_n(x) = E_n \phi_n(x). \tag{3.18}$$

In[1] the crucial features of of the Sturm-Liouville equation are summarised, namely that, the eigenfunctions of the Hamiltonian $\phi_n(x)$, are simultaneous eigenstates of the PT-operator

$$PT\phi_n(x) = \lambda_n \phi_n(x). \tag{3.19}$$

Bender incorporates the pure phase λ_n into the eigenvalue ϕ_n, the new eigenvalue can then be made unity using multiplicative rescaling results in,

$$\begin{aligned} PT\phi_n(x) &= \phi_n^*(-x) && (3.20)\\ &= \phi_n(x). && (3.21) \end{aligned}$$

The standard completeness relation is not satisfied by a PT-symmetric non-Hermitian Hamiltonian with real eigenvalues. Therefore, we require a new completeness relation,

$$\sum_n (-1)^n \phi_n(x)\phi_n(y) = \delta(x-y), \tag{3.22}$$

where $x, y \, \epsilon \, \Re$. This result was verified by Bender and associates numerically[1]. However, no information on how it was verified was included.

The validity of the new completeless relation is unclear. It remains an open mathematical question[26].

$$(f, g) = \int dx[PTf(x)]g(x), \tag{3.23}$$

has been proposed where $f(x)$ and $g(x)$ are functions associated with PT-symmetric systems. The inner-product (f, f) seems desirable as it is conserved in time[1].

The inner-product of the Hamiltonian's eigenfunctions, ϕ_m and ϕ_n, is

$$(\phi_m, \phi_n) = (-1)^n \delta_{mn}. \tag{3.24}$$

This inner-product has norms that are ± 1 and there are equal numbers of both, resulting in serious problems as a negative probability has no physical meaning. A consistent physical theory requires a positive definite norm to ensure that the eigenvalues are bounded.

The problem of the negative norm was tackled by looking for an underlying symmetry. Bender claimed that any Hamiltonian with an unbroken PT-symmetry will have an underlying symmetry. The equal numbers of positive and negative norm states connected to the Hamiltonian, form the underlying symmetry.

A new operator C was introduced by Bender and associates to describe this symmetry. This new operator must be linear and can be represented in the position space by writing it as a sum over the energy eigenstates of the Hamiltonian[1]

$$C(x, y) = \sum_n \phi_n(x)\phi_n(y). \tag{3.25}$$

The new operator has eigenvalues of ± 1. In addition it commutes with the Hamiltonian H and the PT-operator and $C^2 = I$. Since C commutes with H the eigenstates of H will have a definite value of C[1]. These properties are similar to the charge conjugation operator, hence both are called C.

The parity operator can be constructed in terms of eigenstates and is[1]

$$PT(x, y) = \sum_n (-1)^n \phi_n(x)\phi_n(-y). \tag{3.26}$$

The parity operator P is real while C is complex. In addition P and C do not commute. This can be expressed in the position representation as[1]

$$(CP)(x,y) = \sum_n \phi_n(x)\phi_n(-y) \tag{3.27}$$

and

$$(PC)(x,y) = \sum_n \phi_n(-x)\phi_n(y). \tag{3.28}$$

If we examine these equations we see that

$$CP = (PC)^*. \tag{3.29}$$

Despite this C commutes with the PT operator.

Now that the new operator C has been defined to explain the underlying symmetry, it is possible to define a new inner-product. The new inner-product is dynamically determined and must be positive definite and is defined by[1]

$$\langle f|g\rangle = \int_c dx[PTf(x)]g(x). \tag{3.30}$$

Dynamically determined inner-products differ from the standard Hermitian inner-product as they depend on the Hamiltonian. The new inner-product is positive definite as the operator C contributes -1 to states with a negative PT-norm[1]. In addition it is phase independent and conserved in time. If the parameter n tends towards zero, then the Hamiltonian equation (3.10) becomes Hermitian, the CPT operator becomes T which has the effect of complex conjugation on the Hamiltonian. However, since the Hamiltonian is now Hermitian there is no change. It is promising that the dynamically determined inner-product reduces to the standard inner-product from Hermitian quantum mechanics.

A new completeness relation is required, this is stated below,

$$\sum_n \phi_n(x)[CPT\phi_n(y)] = \delta(x-y). \tag{3.31}$$

3.4 Pseudo-Hermiticity

In 2002 Mostafazadeh introduced the idea of pseudo-Hermiticity and showed that all Hamiltonains with a real spectrum are in fact pseudo-Hermitian. Before defining pseudo-Hermicity it is necessary to make an assumption. We work in a complex inner-product

space[6], where we will be introducing automorphisms in our discussion of pseudo-Hermiticity. (An automorphism is an invertible operator that maps an inner-product space onto itself)[6]. Let $|\phi\rangle$ and $|\psi\rangle$ be arbitrary kets. Then we define a Hermitian linear automorphism $\hat{\eta}$ which must obey[11]

$$\langle\phi|\eta\psi\rangle = \langle\phi\eta|\psi\rangle, \tag{3.32}$$

where $\hat{\eta}$ is an invertible operator.

Let A be an operator with an adjoint $A^\dagger$. and a pseudo-Hermitian adjoint[6] $A^\#$, where $A^\#$ is defined by

$$A^\# = \eta^{-1}A^\dagger\eta. \tag{3.33}$$

If A is a pseudo-Hermitian operator it satisfies[6]

$$A = A^\#. \tag{3.34}$$

Mostafazdeh introduces several propositions that serve to provide the mathematical framework necessary to work with pseudo-Hermitian Hamiltonians[6]. He first introduces the indefinite inner-product and proposes that it will be invariant under a time translation generated by the Hamiltonian H, if and only if the Hamiltonian is η-pseudo-Hermitian.

$$\langle\langle\phi|\psi\rangle\rangle_\eta = \langle\phi|\eta|\psi\rangle,\ A|\phi\rangle, |\psi\rangle\ \epsilon\ \mathcal{H}. \tag{3.35}$$

In order to prove this result, it should be noted that η-pseudo-Hermiticity of H is equivalent to

$$H^\dagger = \eta H\eta^{-1}. \tag{3.36}$$

Now use the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \tag{3.37}$$

and its inverse

$$i\frac{d}{dt}\langle\phi(t)| = \langle\phi(t)| - H^\dagger. \tag{3.38}$$

Combining these equations

$$i\frac{d}{dt}\langle\langle\phi(t)|\psi(t)\rangle\rangle_\eta = \langle\langle\phi(t)|H - H^\dagger|\psi(t)\rangle\rangle_\eta. \tag{3.39}$$

Now let

$$i\frac{d}{dt}|\psi_1(t)\rangle = H|\psi(t)\rangle \tag{3.40}$$

and

$$i\frac{d}{dt}\langle\phi_1(t)| = \langle\phi(t)| - H^\dagger. \tag{3.41}$$

Then,

$$\langle\phi_1(t)|\eta|\psi_2(t)\rangle = \langle\phi(t)|\eta H - H^\dagger\eta|\psi(t)\rangle. \tag{3.42}$$

Therefore,

$$i\frac{d}{dt}\langle\langle\phi(t)|\psi(t)\rangle\rangle_\eta = \langle\phi(t)|\eta H - H^\dagger\eta|\psi(t)\rangle. \tag{3.43}$$

For the indefinite inner-product to be invariant in time, equation (3.36) must hold. If equation (3.36) holds, then $\langle\langle\phi(t)|\psi(t)\rangle\rangle_\eta$ is a constant. An additional observation made by Mostafazadeh noted that if $\hat{\eta} = \hat{1}$, equation (3.36) reduces to $H^\dagger = H$, which is the condition for Hermiticity of the Hamiltonian[6]. This observation is encouraging and suggests that pseudo-Hermiticity may indeed be a generalisation of Hermitian quantum mechanics.

Now the implications of equation (3.36) can be investigated. The Eigenvalue equation of H and its adjoint are,

$$H|E_i\rangle = E_i|E_i\rangle \tag{3.44}$$

$$\langle E_i|H^\dagger = \langle E_i|E^*. \tag{3.45}$$

Now the indefinite inner products can be formed by making use of the above equations and equation (3.36),

$$\langle\langle E_i|H|E_j\rangle\rangle_\eta = E_j\langle\langle E_i|E_j\rangle\rangle_\eta \tag{3.46}$$

$$\langle\langle E_i|H^\dagger|E_j\rangle\rangle_\eta = E_i^*\langle\langle E_i|E_j\rangle\rangle_\eta. \tag{3.47}$$

Subtract and use $\hat{\eta}H = H^\dagger\hat{\eta}$ then,

$$0 = (E_i^* - E_j)\langle\langle E_i|E_j\rangle\rangle_\eta. \tag{3.48}$$

Equation (3.48) implies that an η-pseudo-Hermitian Hamiltonian will have a vanishing η-semi-norm if the eigenvectors have non-real eigenvalues $E_i \notin \Re$[6]. Then

$$|||E_i\rangle||_\eta^2 = \langle\langle E_i|E_i\rangle\rangle_\eta = 0. \tag{3.49}$$

If any two eigenvalues are not complex conjugates, then the two eigenvectors will be η-orthogonal[6]. If $E_i \neq E_j^*$ then

$$\langle\langle E_i|E_j\rangle\rangle_\eta = 0. \tag{3.50}$$

Thus, eigenvectors with non-degenerate real eigenvalues will be η-orthogonal.

Mostafazadeh made a series of propositions, which are stated here without proof[6]. The first states that if V is an inner-product space with a linear automorphism η and linear operators O_1 and O_2, then[6]

1. $1^\# = 1$,
2. $(O_1^\#)^\# = O_1$,
3. $(z_1O_1 + z_2O_2)^\# = z_1^*O_1^\# + z_2^*O_2^\#$,

where z_1 and z_2 are complex numbers.

Now if we have an inner-product space $V_{(1,2,3)}$ with linear automorphism and $\eta_{(1,2,3)}$ with linear operators $O_1 : V_1 \to V_2$, $O_2 : V_2 \to V_3$ and $\eta_{(1,2,3)}$, then

$(O_2O_1)^\# = O_1^\#O_2^\#$.

A Hermitian linear automorphism η is defined as,

$$\eta = U^\dagger\eta U, \tag{3.51}$$

where U is a unitary operator. If O is a linear operator, then it is η-pseudo-Hermitian if and only if[6]

$$O = U^\dagger OU. \tag{3.52}$$

As a result Mostafazadeh states[6] that pseudo-Hermiticity is unitary invariant.

Now if η_1 and η_2 are linear automorphisms, then

$$O^\# = \eta_1^{-1}O^\dagger\eta_1 = \eta_2^{-1}O^\dagger\eta_2 \tag{3.53}$$

if and only if η_1 and η_2 commute with O.

The propositions introduced above provide the mathematical structure that defines the behaviour of pseudo-Hermitian Hamiltonians. In the next section the necessary condition for a real eigenspectrum is shown.

3.5 The necessary condition for a real eigenspectrum

The linear automorphism is given by

$$\eta = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\phi_{n_0}, a\rangle\langle\phi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n_+}} (|\phi_{n_-}, \alpha\rangle\langle\phi_{n_+}, \alpha| + |\phi_{n_+}, \alpha\rangle\langle\phi_{n_-}, \alpha|). \tag{3.54}$$

The inverse is

$$\eta^{-1} = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\psi_{n_0}, a\rangle\langle\psi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n+}} (|\psi_{n_-}, \alpha\rangle\langle\psi_{n_+}, \alpha| + |\psi_{n_+}, \alpha\rangle\langle\psi_{n_-}, \alpha|). \tag{3.55}$$

The derivation of the linear automorphism can be found in the appendix.

The linear automorphism and its inverse satisfy the condition for pseudo-Hermiticity, $H^\dagger = \eta H \eta^{-1}$, where H is the Hamiltonian[6].

Mostafazadeh introduced an additional theorem[6] which states: "if H is a non-Hermitian Hamiltonian with a discrete spectrum and has a complete biorthonormal eigenbasis, then H is pseudo-Hermitian if and only if one of the following conditions hold":

1. "The spectrum of H is real."

2. "The complex eigenvalues come in complex conjugate pairs and the multiplicity of the eigenvalue pairs is the same."

It has been shown that all pseudo-Hermitian Hamiltonians satisfy the points above. If in addition, the Hamiltonian has a complete biorthonormal eigenbasis, that provides the necessary and sufficient condition for pseudo-Hermiticity. To ensure a real spectrum, pseudo-Hermiticity is required but is not a sufficient condition on its own. Mostafazadeh introduced a necessary and sufficient condition to ensure a real spectrum for pseudo-Hermitian Hamiltonians with a complete set of biorthonormal eigenvectors[7].

Mostafazadeh then introduced another theorem[7]. "Let H:$\mathcal{H} \to \mathcal{H}$ be a Hamiltonian that acts on a Hilbert space $\mathcal{H}$. The Hamiltonian must have a discrete spectrum while allowing a complete set of biorthonormal eigenvectors $\{|\psi_n\rangle, |\phi_n\rangle\}$". The spectrum of H will then be real if and only if there is an invertible linear operator O:$\mathcal{H} \to \mathcal{H}$ picked so

that H is $OO^\dagger$-pseudo-Hermitian.

Proof:

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \tag{3.56}$$

$$H^\dagger|\phi_n\rangle = E_n^*|\phi_n\rangle, \tag{3.57}$$

$$\langle\phi_m|\psi_m\rangle = \delta_{mn}, \tag{3.58}$$

$$\sum_n |\psi_n\rangle\langle\phi_n| = 1. \tag{3.59}$$

Then O:$\mathcal{H} \to \mathcal{H}$ and $H_0 : \mathcal{H} \to \mathcal{H}$ can be defined by

$$O = \sum_n |\psi_n\rangle\langle n| \tag{3.60}$$

and

$$H_0 = \sum_n E_n|n\rangle\langle n|. \tag{3.61}$$

By inspecting equation (3.60) we can see that the inverse will be

$$O^{-1} = \sum_n |n\rangle\langle\phi_n| \tag{3.62}$$

and

$$O^{-1}HO = H_0. \tag{3.63}$$

To prove this result begin with

$$O^{-1}HO = \sum_n (|n\rangle\langle\phi_n|H|\psi_n\rangle\langle n|) \tag{3.64}$$

$$= \sum_n (|n\rangle\langle\phi_n|E_n|\psi_n\rangle\langle n|) \tag{3.65}$$

$$= E_n|n\rangle\hat{1}\langle n| \tag{3.66}$$

$$= \sum_n E_n|n\rangle\langle n| = H_0 \tag{3.67}$$

3.6 A comparison of CPT-symmetry and pseudo-Hermiticity

The most interesting question is whether CPT-symmetry is in fact a subclass of pseudo-Hermiticity. Mostafazadeh claims that it is. He went on to prove that all diagonalisable linear operators with a discrete spectrum will have an anti-linear symmetry, leading him to the following two corollaries[8]:

1. Any diagonalisable linear operator that possesses a discrete spectrum (real eigenvalues) is anti-pseudo-Hermitian.

2. Any diagonalisable pseudo-Hermitian linear operator that posseseses a discrete spectrum will have anti-linear symmetry.

Since all PT-symmetry is an anti-linear symmetry, then PT-symmetric Hamiltonians imply that η-pseudo-Hermiticity is present [27]

$$\eta = \tau PT, \tag{3.68}$$

where $\hat{\tau}$ is an anti-linear operator that obeys the relationship

$$\langle\phi|\tau|\psi\rangle = \langle\psi|\tau|\phi\rangle. \tag{3.69}$$

This goes a long way to backing up Mostafazadeh's claim that pseudo-Hermiticity is the more general of the two frameworks. Mostafazadeh made further motivations asserting that pseudo-Hermiticity is the more general framework. The first involved showing that the PT-symmetric physical quantities can be constructed using the pseudo-Hermitian quantisation scheme.

He further claimed that it is more practical to use the pseudo-Hermitian framework, rather than working in the PT-symmetric framework directly. The fact that a PT-symmetric theory can be constructed in the pseudo-Hermitian framework adds weight to Mostafazdeh's claim that pseudo-Hermitian quantum mechanics is the more general of the two.

3.7 A comparison of PT-symmetry and Hermiticity

Bender and collaborators claimed that PT-symmetry is a more general form of quantum mechanics than Hermitian quantum mechanics[27]. More details on these claims can be found in [1].

Bender asserted that:

1. the PT-symmetric and the CPT-symmetric together form a physically reasonable alternative to Hermitian quantum mechanics.

2. all Hermitian Hamiltonians are PT-symmetric: this was stated but not proved.

3. PT-symmetric Hamiltonians can be used to define real energy eigenvalues for a quantum system. In addition, unitary time evolution can be defined if the CPT-inner product is used to define a Hilbert space.

A critique of PT-symmetric quantum mechanics was published by Mostafazadeh in 2004[27]. He attempted to show that CPT-symmetric quantum mechanics is not an extension of Hermitian quantum mechanics nor an alternative to it.

Mostafazadeh[27] began by making the following point: For an energy eigenvalue to represent the position of a particle it must be associated with a linear operator which in turn must be the observable for position. This is as a direct result of the postulates of quantum mechanics. This has not been adhered to in the formulation of PT-symmetric quantum mechanics (PTSQM).

The problem becomes clear when we consider the Schrödinger equation

$$\left[-\frac{d^2}{d^2x}+x^2(ix)^\nu\right]\phi_n(x)=E_n\phi_n(x). \tag{3.70}$$

Bender and collaborators showed that the Schrödinger equation satisfied the boundary conditions and was orthogonal with respect to PT-symmetric and CPT-symmetric inner products.

The positive definite inner product is defined by

$$\langle\psi|\phi\rangle_+=\int_C dx\,[CPT\psi(x)]\,\phi(x). \tag{3.71}$$

The problem in the PT-symmetric formulation is that x is not necessarily position. While in quantum mechanics x is associated with position, this stems from the postulates. The question is then open as to what physical meaning does x have[27].

If x is to be the position operator in quantum mechanics, then PT-symmetric quantum mechanics must be formulated as a physical theory. Mostafazadeh[27] asked the following questions:

1. “what is the mathematical nature of state vectors?”

2. “what are observables?”

3. “how are observables measured?”

4. how do PT-symmetric theories relate to known theories?

In need of clarification is the definition of Hermiticity. There is some ambiguity in PT-symmetric quantum mechanics. The rigorous definition for Hermicity is

$$\langle\psi|A\phi\rangle = \langle A\psi|\phi\rangle, \tag{3.72}$$

where ϕ and ψ form an orthonormal basis. In Hermitian quantum mechanics

$$A_{ij} = A^*_{ji} \tag{3.73}$$

is equivalent since the Hilbert space has a fixed inner product and orthonormal basis.

In contrast, in PT-symmetric quantum mechanics, the inner product is not fixed, nor are the observables[27]. Equation (3.73) should therefore not be used as a condition for Hermiticity since (3.73) is basis dependent.

If we go on to choose the same measurement theory as quantum mechanics, then observables have to be defined as Hermitian operators acting on the Hilbert space. These differ from Bender and collaborators' CPT-invariant operators [29].

If the above theory of observables is applied, then the operators $\hat{x}$ and $\hat{p}$ in the Schrödinger equation are not physical observables. This is due to the fact that they are not Hermitian when the inner product (3.71) is used.

Mostafazadeh asks the question what are the position and momentum operators in PT-symmetric quantum mechanics?

Mostafazadeh uses a textbook result for a Hilbert space[27]: “up to some isomorphism there is a unique infinite-dimensional separable Hilbert space”, where $L^2(\Re)$ is the Hilbertspace. The significance of this result is in the fact that for some unitary linear transformation U[27],

$$U : \mathcal{H} \to L^2(\Re), \tag{3.74}$$

that satisfies

$$\langle\psi|\phi\rangle = \langle U\psi|U\phi\rangle, \tag{3.75}$$

where ϕ and ψ are arbitrary $\in \mathcal{H}$.

Use the unitary equation (3.75) to construct physical observables for PT-symmetric quantum systems using the Hamiltonian

$$H = p^2 + x^2(ix)^\nu, \tag{3.76}$$

where $\nu \in \Re_+$.

The form of the new operators is [27]

$$O = U^{-1}OU, \tag{3.77}$$

where the Hermitian operator O, acts in $L^2(\Re)$.

The above equation gives the structure for observables in PT-symmetric quantum mechanics. Using this structure Mostafazadeh went on to show that PT-symmetric quantum mechanics reduces to Hermitian quantum mechanics.

If $L^2(\Re)$ is the Hilbert space, then the PT-symmetric system can be described in terms of Hermitian quantum systems. The Hamiltonian is

$$H = UHU^{-1} \tag{3.78}$$

and the observable O is

$$O = UOU^{-1}. \tag{3.79}$$

Since PT-symmetric quantum mechanics reduces to Hermitian quantum mechanics, we can conclude that PT-symmetric quantum mechanics does not serve for a fundamental physical theory.

Mostafazadeh argued that CPTSQM (CPT-symmetric quantum mechanics) can be reduced to ordinary quantum mechanics by using similarity transformations. He then concluded that CPTSQM is equivalent to Hermitian quantum mechanics. While interesting that CPTSQM reduces in this way, it is just as interesting to consider whether

one can transform from non-Hermitian quantum mechanics to PTSQM.

Mostafazadeh attempted to address this problem in his 2004 paper [28]. In it he attempts to show the unitary equivalence between PTSQM and Hermitian quantum mechanics. In addition, he demonstrates that Hermitian Hamiltonians can be recovered from every PT-symmetric Hamiltonian.

Bender and collaborators followed Mostafazadeh's paper with one of their own in 2006. They acknowledged that PT-symmetric systems are equivalent to Hermitian systems. They then went on to examine the efficiency of the two frameworks for calculation[29].

Mosatafazadeh has made compelling arguments against PTSQM being considered a fundamental physical theory and it does seem unlikely that PTSQM will become one. However, this does not mean that PTSQM cannot be used to perform calculations efficiently, even if it does not constitute a new theory[29].

Bender and his collaborators have not provided any convincing counter arguments that CPT-symmetric quantum mechanics should be seen as a fundamental physical theory. Yet, it is of use as a scheme for efficient calculations in certain circumstances.

Chapter 4

Application of non-Hermitian theories to a two-level system

Open quantum systems interact with the environment. This interaction is typically modeled by coupling a subsystem (system of interest) to a heat bath. In numerical models, the heat bath is typically made up of a large number of harmonic oscillators, and thus, has many degrees of freedom. In reality, all systems are open quantum systems, as all systems are coupled to the environment to some degree.

We will make use of a non-Hermitian framework for ease of computation. First the equations of motion will be discussed, before considering a two-level system.

A non-Hermitian Hamiltonian approach is adopted, together with a two-level system that is coupled to a dissipative environment (open quantum system). The population change and the coherence that are then present in the system can be calculated when using an appropriate model that utilises the non-Hermitian approach discussed in the next section. If the phase angles between the components of a quantum system are ordered, then the components are said to be coherent. Population difference is the difference in population between states. For the two-level system, there are only two states: the ground state and the excited.

4.1 Non-Hermitian dynamics

Non-Hermitian quantum mechanics has interesting applications to open quantum systems. In particular, non-Hermitian theories can be used as tools to model the behaviour of open quantum systems.

Previous approaches utilising non-Hermitian theories make use of quantum trajectory jumps to represent the dynamics of the open quantum system[9]. Thus far in this review of non-Hermitian theories, PT-symmetric and pseudo- Hermitian approaches have been examined. An additional approach put forward by Sergi[9] introduces a general structure for non-Hermitian equations of motion. This general structure allows the time evolution, to be defined in terms of a non-Hermitian Hamiltonian. Utilising non-Hermitian evolution allows for a computational advantage: the number of degrees of freedom constituting the bath can be reduced.

Let $\hat{H}$ be a non-Hermitian Hamiltonian, $\hat{H} \neq \hat{H}^{\dagger}$. The time evolution for an arbitrary quantum observable $\hat{\chi}$ is given by

$$-i\hbar\frac{d}{dt}\hat{\rho} = [\hat{\rho}, \hat{H}]. \tag{4.1}$$

Equation (4.1) is a statement of Heisenberg's law of evolution for observables. It can be rewritten in matrix form as[9]

$$-i\hbar\frac{d}{dt}\hat{\rho} = \begin{pmatrix} \hat{\rho} & \hat{H} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \hat{\rho} \\ \hat{H} \end{pmatrix}.$$

Let Ω, the sympletic matrix be defined as[9]

$$\Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

$$-i\hbar\frac{d}{dt}\hat{\rho} = \hat{\rho}^{T}_{\hat{H}}.\Omega.\hat{\rho}_{\hat{H}} \tag{4.2}$$

$$= \left[\hat{\rho}(t), \hat{H}\right]_{\Omega}. \tag{4.3}$$

The column vector is

$$\rho_{\hat{H}} = \begin{pmatrix} \hat{\rho} \\ \hat{H} \end{pmatrix}.$$

The right-hand side of equation (4.2) highlights the underlying anti-symmetric nature of the quantum evolution[9]. Sergi goes on to propose that more general algebras and brackets can be defined by modifying the sympletic matrix Ω.

Now, split the Hamiltonian into its Hermitian and non-Hermitian portions

$$\hat{H} = \hat{H}_+ + \hat{H}_-, \tag{4.4}$$

where $\hat{H}_+ = \frac{1}{2}\left(\hat{H} + \hat{H}^\dagger\right)$ and $\hat{H}_- = \frac{1}{2}\left(\hat{H} - \hat{H}^\dagger\right)$.

Then, the commutator can be split into two parts[9],

$$\left[\hat{\rho}, \hat{H}\right] = \left[\hat{\rho}, \hat{H}_+\right] + \left[\hat{\rho}, \hat{H}_-\right]. \tag{4.5}$$

By exploiting the separation of the commutator, it can be shown that the commutator of an operator with a non-Hermitian Hamiltonian is equivalent to a non-Hamiltonian operator. One begins by defining the anti-symmetric matrix operator[9],

$$\Omega_{-+} \equiv \begin{pmatrix} 0 & 1 + \hat{H}_-(\hat{H}_+)^{-1} \\ -1 - (\hat{H}_+^{-1}\hat{H}_-) & 0 \end{pmatrix}.$$

Then,

$$\begin{aligned} \left[\hat{\rho}, \hat{H}\right]_\Omega &\equiv \hat{\rho}^T_{\hat{H}_+}.\Omega_{-+}.\hat{\rho}_{\hat{H}_+} && (4.6) \\ &= \left[\hat{\rho}(t), \hat{H}_+\right]_{\Omega_{-+}}, && (4.7) \end{aligned}$$

where

$$\rho_{\hat{H}_+} = \begin{pmatrix} \hat{\rho} \\ \hat{H}_+ \end{pmatrix}.$$

Equation (4.7) contains a non-Hamiltonian commutator. Of particular interest are equations (4.6) and (4.7) which show the mapping between the commutator with a non-Hermitian Hamiltonian $\hat{H}$ and also the non-Hamiltonian commutator, which is defined in terms of $\hat{H}_+$[9].

When working with non-Hermitian dynamics, the equivalence between the Heisenberg and Schrödinger picture is lost. From this point onwards, we will work in the

Schrödinger picture. In Schrödinger's picture, starting from the equations of motion for state vectors[9],

$$|\frac{d}{dt}\rho\rangle = -\frac{i}{\hbar}\hat{H}_+|\rho\rangle + \frac{\hat{\Gamma}}{\hbar}|\rho\rangle, \tag{4.8}$$

$$\langle\rho\frac{d}{dt}| = \frac{i}{\hbar}\langle\rho|\hat{H}_+ + \langle\rho|\frac{\hat{\Gamma}}{\hbar}, \tag{4.9}$$

where $\hat{\Gamma}$ is a Hermitian operator defined by $\hat{\Gamma} = -i\hat{H}_-$.

The equation of motion for the density matrix, that contains an anti-commutator $[...,...]_+$ is

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}\left[\hat{H}_+, \hat{\rho}(t)\right] - \frac{i}{\hbar}\left[\hat{\Gamma}, \hat{\rho}(t)\right]_+ \tag{4.10}$$

but since $\hat{\Gamma} = -i\hat{H}_-$,

$$\hat{H}_- = i\hat{\Gamma}. \tag{4.11}$$

Make use of (4.11) and rewrite the equation of motion in matrix form

$$\begin{aligned} -i\hbar\frac{d}{dt}\hat{\rho}(t) &= \rho^T_{\hat{H}_+}.\Lambda.\rho_{\hat{H}_+} && (4.12)\\ &= \left[\hat{\rho}(t), \hat{H}_+\right]_\Lambda, && (4.13) \end{aligned}$$

where Λ is the general matrix operator defined by,

$$\Lambda = \begin{pmatrix} 0 & 1 + i\hat{\Gamma}(\hat{H}_+)^{-1} \\ -1 + i(\hat{H}_+)^{-1}\hat{\Gamma} & 0 \end{pmatrix}.$$

If the inverse of H_+ exists then the logic leading to non-Hamiltonian dynamics equation (4.6) can be reversed and we can get back to non-Hermitian dynamics[9]. It can be shown that from an arbitrary Hermitian Hamiltonian, it is possible to define non-Hermitian dynamics.

Let $\mathcal{H}$ be an arbitrary Hermitian Hamiltonian: since $\mathcal{H}$ is Hermitian it has a real spectrum of eigenvalues. Let $\hat{\zeta}$ be a non-Hermitian operator. Then,

$$\hat{\zeta} \neq \hat{\zeta}^\dagger. \tag{4.14}$$

Now let Ω_ζ be an anti-symmetric non-Hermitian matrix,

$$\Omega_\zeta = \begin{pmatrix} 0 & \hat{\zeta} \\ -\hat{\zeta}^T & 0 \end{pmatrix}.$$

A non-Hermitian evolution can be defined for any observable by using this anti-symmetric matrix[9]. The non-Hermitian evolution is defined in terms of a non-Hermitian commutator.

$$i\hbar\frac{d}{dt}\hat{\rho}(t) = \rho^T_{\hat{H}}.\Omega_\zeta.\rho_{\hat{H}} \tag{4.15}$$

$$= \left[\hat{\rho}(t), \hat{\mathcal{H}}\right]_{\Omega_\zeta}, \tag{4.16}$$

where

$$\rho_{\hat{\mathcal{H}}} = \begin{pmatrix} \hat{\rho} \\ \hat{\mathcal{H}} \end{pmatrix} \tag{4.17}$$

is a two-dimensional column vector.

Equations (4.15) and (4.16) define a way to go from a general Hermitian Hamiltonian to defining non-Hermitian dynamics in terms of the Hermitian Hamiltonian.

4.2 Conserved quantities and mixed states

Conserved quantities are quantities, within the system, that do not change in time. We begin by finding the change-of time-law for the determinant of the density operator[10]. This is done using the evolution equation and the matrix identity $lndet\hat{B} = trln\hat{B}$.

Now applying the identity to the evolution equation produces

$$\frac{\partial}{\partial t}det\hat{\rho}(t) = \frac{2}{i\hbar}det\hat{\rho}(t)tr\hat{H}_-. \tag{4.18}$$

Then integrate,

$$det\hat{\rho}(t) = det\hat{\rho}(0)e^{(\frac{2}{\hbar}t)tr\hat{\Gamma}}. \tag{4.19}$$

Here $\hat{\Gamma}$ is a self-adjoint operator, called the decay-rate operator [10]. If $tr\hat{\Gamma} \leq 0$, then at large times the determinant will in the end have zero determinant state. The behaviour of the trace is particularly significant: if the trace vanishes then the evolution does not lead to a sink dynamics[10].

The rate of evolution of the purity operator is given by[10]

$$\frac{\partial}{\partial t}P\ (\hat{\rho}) = \frac{4}{\hbar}\frac{\Re(\hat{\rho},\hat{\Gamma})}{(tr\hat{\rho})^3}, \tag{4.20}$$

where

$$\Re(\hat{\rho},\hat{\Gamma}) \equiv tr(\hat{\rho}^2\hat{\Gamma})tr\hat{\rho} - tr(\hat{\rho}\hat{\Gamma})tr(\hat{\rho}^2). \tag{4.21}$$

Sergi and Zloshchastiev[10] noted that the purity is conserved under general non-Hermitian evolution if $\Re(\hat{\rho},\hat{\Gamma}) = 0$; this condition depends on the state of the system. They go on to show that for a two-dimensional Hilbert space, purity is conserved for all states that have an initial density matrix with a zero-determinant[10].

If a state is not pure then it is a mixed state. Mixed states are simply the mixture of several states (statistical ensemble) which are described by density matrices

$$\hat{\rho}^{(i)} = |\psi^i\rangle\langle\psi^i|. \tag{4.22}$$

This mixture of states can then be expressed as a linear combination, where the coefficients ρ_i must satisfy the normalisation condition

$$\hat{\rho} = \sum_i p_i\hat{\rho}^{(i)}. \tag{4.23}$$

For time-dependent functions[10]

$$p_i^{'}(t) \equiv p_i\frac{tr(\hat{\rho}^i(t))}{tr(\hat{\rho}(t))},\ 0 \leq p^i(t) \leq 1. \tag{4.24}$$

If at $t = 0$, p_i and $\rho_i^{'}(0)$ have equal traces, then $p_i = \rho_i^{'}(0)$. The normalization condition is then,

$$\sum_i p_i^{'}(t) = 1. \tag{4.25}$$

The expression for a mixed state can now be written as

$$\hat{\rho}'(t) = \sum_i p_i(t)\rho_{(i)}^{'}(t). \tag{4.26}$$

4.3 A two-level non-Hermitian system

A system with two possible states is termed a two-level system. Since there are only two states, the system must be in either the ground state, or the excited state. While a simple system, it is used often to explain physical phenomen. A famous example of a two-level system is spin, spin half particles have only two energy levels and are an example of a

natural two-level system.

The system to be considered is a non-Hermitian two-level system that is used by Sergi and Zloschastiev[10]: where the ground state and the excited state are denoted as $|g\rangle$ and $|e\rangle$ respectively. The Pauli operators keep their standard form[10],

$$\hat{\sigma}_x = |e\rangle\langle g| + |g\rangle\langle e| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\hat{\sigma}_y = i(|e\rangle\langle g| - |g\rangle\langle e|) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\hat{\sigma}_z = |e\rangle\langle e| - |g\rangle\langle g| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In reference[10] emphasis was placed on studying observables; in particular, two observables: the population difference and coherence. In order to determine the exact expression for these observables we make use of

$$\langle\hat{\chi}\rangle = tr\left(\frac{\hat{\rho}(t)\hat{\chi}(t)}{\hat{\rho(t)}}\right), \tag{4.27}$$

where $\langle\hat{\chi}\rangle$ is the observable of interest. For the $\hat{\sigma}_z$ case we substitute the Pauli operator $\hat{\sigma}_z$ and the density matrix into the above equation. This yields the population difference ($\langle\hat{\sigma}_z\rangle_t$) as

$$\langle\hat{\sigma}_z\rangle_t = \frac{\hat{\rho}_{11}(t) - \hat{\rho}_{22}(t)}{\hat{\rho}_{11}(t) + \hat{\rho}_{22}(t)}. \tag{4.28}$$

Similarly, the coherence is given by

$$\langle\hat{\sigma}_x\rangle_t = \frac{\hat{\rho}_{12}(t) + \hat{\rho}_{21}(t)}{\hat{\rho}_{11}(t) + \hat{\rho}_{22}(t)}. \tag{4.29}$$

Notice that the expression for coherence contains off-diagonal density matrix terms.

A convenient check when running simulations is to ensure that the identity

$$\langle\hat{\sigma}_x\rangle_t^2 + \langle\hat{\sigma}_y\rangle_t^2 + \langle\hat{\sigma}_z\rangle_t^2 = 1 - 4\frac{det\hat{\rho}}{(tr\hat{\rho})^2} = 1 - \frac{4det\rho(0)}{(tr\hat{\rho})^2}e^{(\frac{2}{\hbar}t)tr\hat{\Gamma}} \leq 1, \tag{4.30}$$

holds[10].

All pure states lie on the Bloch sphere,

$$\langle\hat{\sigma}_x\rangle_t^2 + \langle\hat{\sigma}_y\rangle_t^2 + \langle\hat{\sigma}_z\rangle_t^2 = 1. \tag{4.31}$$

A Bloch sphere can be thought of as a three-dimensional vector that defines a sphere with a radius that cannot be larger than unity[13]. In ideal conditions where the system is closed, there would be transitions between the two states and the Hamiltonian would be in the standard Hermitian form for a two-level system,

$$\hat{H}_+ = -\hbar\Omega\hat{\sigma}_x. \tag{4.32}$$

Sergi and Zloschastiev added open-system dynamics to the model by introducing an anti-Hermitian Hamiltonian of the form[10],

$$\hat{H}_- = i\hbar\Omega(a_0\hat{I} + a_1\hat{\sigma}_x + a_2\hat{\sigma}_y + a_3\hat{\sigma}_z). \tag{4.33}$$

The total Hamiltonian can be obtained by adding the two portions of the total Hamiltonian together, $\hat{H}_+$ and $\hat{H}_-$

$$\begin{aligned} \hat{H} &= \hat{H}_- + \hat{H}_+ && (4.34)\\ &= \hbar\Omega\left[i(a_0\hat{I} + a_1\sigma_x + a_2\sigma_y + a_3\sigma_z) - \sigma_x\right] && (4.35) \end{aligned}$$

The non-Hermitian Hamiltonian can be written in terms of the decay-rate operator $\hat{\Gamma}$,

$$\hat{\Gamma} = \hbar\Omega(\gamma\beta\hat{\sigma}_x - a_2\hat{\sigma}_y - W\hat{\sigma}_z - \gamma\hat{I}). \tag{4.36}$$

Then,

$$\begin{aligned} \hat{H} &= \hat{H}_+ + i\hat{\Gamma} && (4.37)\\ &= -\hbar\Omega\left[\hat{\sigma}_x + i(\gamma\hat{I} - \gamma\beta\hat{\sigma}_x + a_2\hat{\sigma}_y + W\hat{\sigma}_z)\right]. && (4.38) \end{aligned}$$

Now choose

$$\begin{aligned} a_0 &= -\gamma, && (4.39)\\ a_1 &= \gamma\beta, && (4.40)\\ a_3 &= W = \sqrt{(1+\gamma^2)(1-\beta^2) - a_2^2}. && (4.41) \end{aligned}$$

We ensure that the density matrix is always finite[10] through our choice of γ.

The coefficients $a_i (i = 0, ..., 3)$ are assumed to be real. Consider the expression for W. It is clear that,

$$(1 + \gamma^2)(1 - \beta^2) \geq a_2^2. \tag{4.42}$$

We adopt the same initial condition used in [10]

$$\hat{\rho}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

the simplicity of this condition is convinient.

Below is the equation of motion

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar}[\hat{H}_+, \hat{\rho}(t)] - \frac{i}{\hbar}[\hat{H}_-, \hat{\rho}(t)], \tag{4.43}$$

the diagonal terms are

$$\hat{\rho}_{11}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2 + \gamma^2}[A_1 \cos(\omega t)] + B_1 \sin(\omega t) + C_1 \cosh(\Gamma t) + D_1 \sinh(\Gamma t)] \tag{4.44}$$

and

$$\hat{\rho}_{22}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2 + \gamma^2}[A_4 \cos(\omega t)] + B_4 \sin(\omega t) + C_4 \cosh(\Gamma t) + D_4 \sinh(\Gamma t)]. \tag{4.45}$$

Similarly, the off-diagonal terms are

$$\hat{\rho}_{12}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2 + \gamma^2}[A_2 \cos(\omega t)] + B_2 \sin(\omega t) + C_2 \cosh(\Gamma t) + D_2 \sinh(\Gamma t)] \tag{4.46}$$

and

$$\hat{\rho}_{21}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2 + \gamma^2}[A_3 \cos(\omega t)] + B_3 \sin(\omega t) + C_3 \cosh(\Gamma t) + D_3 \sinh(\Gamma t)], \tag{4.47}$$

where $\Gamma = 2\gamma\Omega > 0$ and $\omega = 2\beta\Omega$. The decay-rate coefficient is Γ and the tunneling frequency is ω. The decay rate Γ specifies the rate that decay from the excited state to the ground state happens. The tunneling frequency is the frequency with which tunneling can occur either from the ground to the excited state or in the opposite direction.

The new coefficients are[10]

$$A_1 = \beta^2 + \gamma^2 - W^2,\ B_1 = 2\beta W,\ C_1 = \beta^2 + \gamma^2 + W^2,\ D_1 = 2\gamma W, \tag{4.48}$$

$$A_2 = -C_2 = iW(1 - a_2 + i\gamma\beta),\ B_2 = -(\gamma + i\beta),\ D_2 = iB_2, \tag{4.49}$$

$$A_3 = -C_3 = A_2^*,\ B_3 = B_2^*,\ D_3 = D_2^*, \tag{4.50}$$

$$A_4 = -C_4 = -(1 - a_2)^2 - \gamma^2\beta^2,\ B_4 = D_4 = 0. \tag{4.51}$$

The density matrix remains Hermitian since $\rho_{21} = \rho_{12}$. However, the trace is no longer conserved. We expect the non-conservation of the trace when the Hermitian system is coupled to the environment. This coupling is described by the anti-Hermitian portion of the Hamiltonian, which allows probability to be gained or lost by the system[10].

Sergi and Zloschastiev[10] found that the exact evolution of the trace is given by

$$tr(\hat{\rho}(t)) = \frac{e^{-\Gamma t}}{\beta^2 + \gamma^2}\hat{\Gamma}(t), \tag{4.52}$$

where $T(t) = A_5\cos(\omega t) + \frac{1}{2}B_1\sin(\omega t) + C_5\cosh(\Gamma t) + \frac{1}{2}D_1\sinh(\Gamma t)$. Here two new coefficients have been introduced, $A_5 = A_2 - 1 + \beta^2$ and $C_5 = 1 - a_2 + \gamma^2$.

By using the definition for observables and the solution for the density operator, the exact time-dependence of the average Pauli operators can be determined[10].

$$\langle\hat{\sigma}_x\rangle_t = \frac{1}{T(t)}[A_6(\cos(\omega t) - \cosh(\Gamma t)) - \gamma A_5\sin(\omega t) + \beta C_5\sinh(\Gamma t)], \tag{4.53}$$

$$\langle\hat{\sigma}_y\rangle_t = \frac{1}{T(t)}[W(a_2 - 1)(\cos(\omega t) - \cosh(\Gamma t)) + \beta C_5\sin(\omega t) - \gamma A_5\sinh(\Gamma t)], \tag{4.54}$$

$$\langle\hat{\sigma}_z\rangle_t = \frac{2}{T}[A_7\cos(\omega t) + \frac{1}{2}B_1\sin(\omega t) + C_7\cosh(\Gamma t) + \frac{1}{2}D_1\sinh(\Gamma t)], \tag{4.55}$$

where $A_6 = -\gamma\beta W$, $A_7 = C_5 - W^2$ and $C_7 = A_5 + W^2$.

4.4 Observables and their asymptotic limits

The asymptotic values were also determined in [10] and found to be,

$$\lim_{t\to+\infty}\langle\hat{\sigma}_x\rangle_t = -(\hbar\Omega)^{-1}\lim_{t\to+\infty}\langle\hat{H}_+\rangle_t = \beta, \tag{4.56}$$

$$\lim_{t\to+\infty}\langle\hat{\sigma}_y\rangle_t = \frac{(a_2 - 1)(\gamma + W) + \gamma\beta^2}{a_2 - 1 - \gamma(\gamma + W)}, \tag{4.57}$$

$$\lim_{t\to+\infty}\langle\hat{\sigma}_z\rangle_t = \frac{a_2+\gamma W}{\gamma^2+1}. \tag{4.58}$$

Fig 4.1, Fig 4.2 and Fig 4.3 show analytical plots of the profiles $\langle\hat{\sigma_z}\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$.

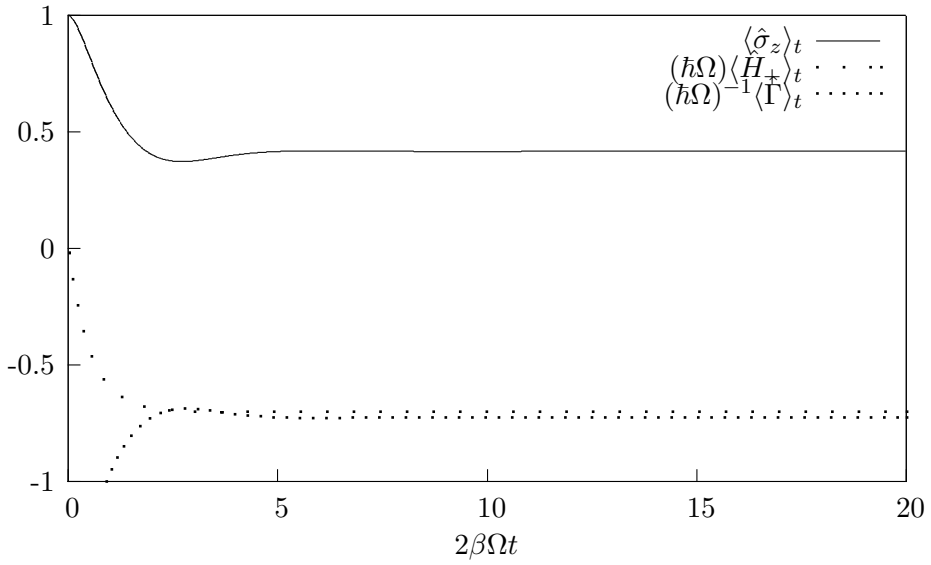

Figure 4.1: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.7$ and $\frac{\gamma}{\beta} = 1$.

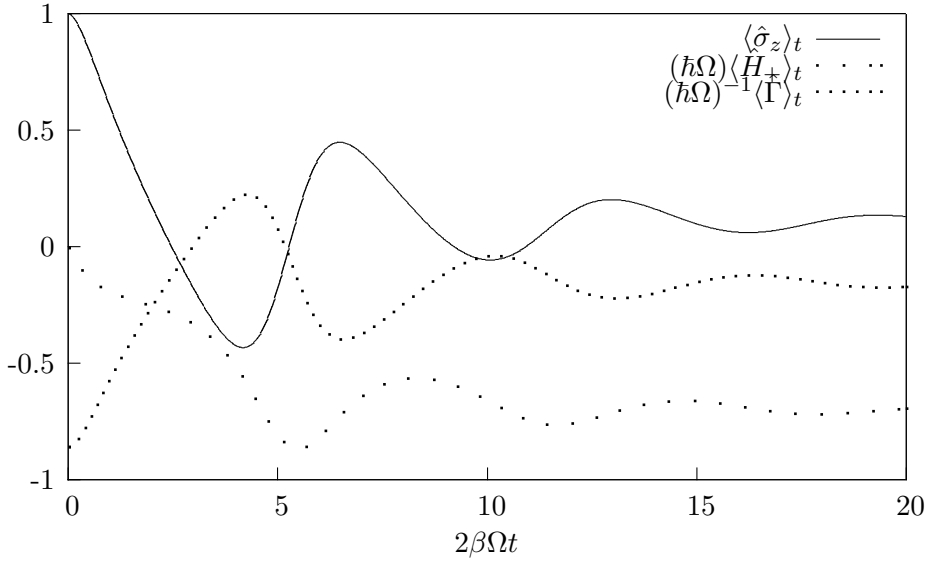

Figure 4.2: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.7$ and $\frac{\gamma}{\beta} = 0.5$.

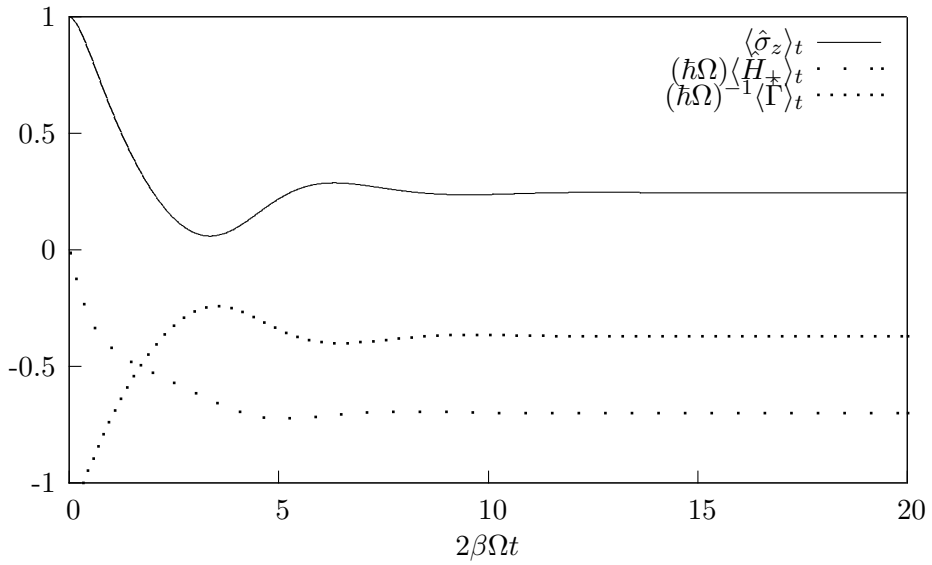

Figure 4.3: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where, $\beta = 0.7$ and $\frac{\gamma}{\beta} = 0.2$.

As t tends towards infinity in an open quantum system, it is expected that the population difference will go to zero as the system reaches equilibrium:

$$\lim_{t\to+\infty}\langle\hat{\sigma}_z\rangle_t = 0. \tag{4.59}$$

Sergi and Zloshchastiev[10] determined that this is equivalent to the following conditions

$$a_2 - \gamma\sqrt{1-\beta^2} = 0,\ W = \sqrt{1-\beta^2}, \tag{4.60}$$

which allows the anti-Hermitian Hamiltonian to be simplified to[12]

$$\hat{\Gamma}^{\mu\rho} = \hbar\gamma\Omega[\beta\hat{\sigma}_x - \sqrt{1-\beta^2}(\hat{\sigma}_y + \gamma^{-1}\hat{\sigma}_z) - \hat{I}]. \tag{4.61}$$

We now make use of these new constraints and determine the new analytical solutions,

$$\hat{\rho}_{11}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2+\gamma^2}\left[A_8\cos(\omega t) + \tilde{\gamma}^2\cosh(\Gamma t) - 2W((\beta\sin(\omega t) + \gamma\sinh(\Gamma t))\right], \tag{4.62}$$

$$\hat{\rho}_{12}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2+\gamma^2}\left[A_9(\cos(\omega t) - \cosh(\Gamma t)) + B_5(\sinh(\Gamma t) - i\sin(\omega t))\right], \tag{4.63}$$

$$\hat{\rho}_{22}(t) = \frac{1}{2}\frac{e^{-\Gamma t}}{\beta^2+\gamma^2}\left[(2\gamma W - \tilde{\gamma}^2)(\cos(\omega t)) - \cosh(\Gamma t)\right], \tag{4.64}$$

where $\tilde{\gamma} = \sqrt{1+\gamma^2}$, $A_8 = \tilde{\gamma}^2 - 2W^2$, $A_9 = W(\gamma\beta + i(\gamma W - 1))$ and $B_5 = \beta(\tilde{\gamma}^2 - \gamma W) + i\gamma W(\gamma - W)$.

Consider Fig 4.4, Fig 4.5 and Fig 4.6, these three figures show the profiles for three averages. The constraints change for the different graphs. It can be seen from the graphs that as t tends towards infinity the graphs are tending towards some limiting factor.

In reference [10] these limiting values have been calculated and are as follows;

$$\lim_{t\to+\infty}\langle\hat{\sigma}_x\rangle_t = -(\hbar\Omega)^{-1},\ \lim_{t\to+\infty}\langle\hat{H}_+(t)\rangle = \beta \tag{4.65}$$

and

$$\lim_{t\to+\infty}\langle\hat{\sigma}_y\rangle_t = -\sqrt{1-\beta^2}. \tag{4.66}$$

The critical frequency w_c is defined by

$$w_c = \beta_c w_+, \tag{4.67}$$

where $w_+ = 2\Omega$ and $\beta_c^2 = 1 - \left(\frac{a_2^2}{\gamma^2+1}\right)$. The critical frequency is bounded by $w \leq w_c \leq w_+$.

These relations were summarized by Sergi and Zloshchastiev[10] by noting that a_2 measures the difference between the system's critical frequency and the tunneling frequency for the system that has been introduced above.

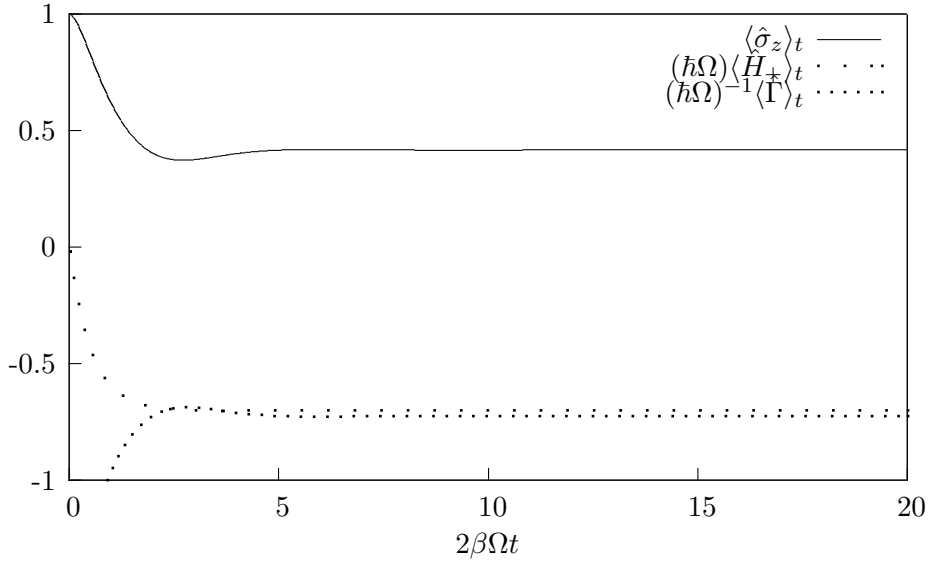

Figure 4.4: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.8$ and $\frac{\gamma}{\beta} = 1.0$.

One of the properties that is well suited to investigation using a non-Hermitian Hamiltonian is dephasing. Dephasing is the process that takes an initial non-diagonal density matrix and causes it to become a diagonal matrix at large times. It is of interest to see what effect non-Hermitian dynamics has on dephasing (see [10] for details).

In order to investigate dephasing it is necessary to choose an initial density matrix that has off-diagonal terms[10]

$$\hat{\rho}(0) = \frac{1}{2}\sum_{k,m=g,e} |k\rangle\langle m| = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2}, \end{pmatrix},$$

and then choose the anti-Hermitian portion of the Hamiltonian to be[10]

$$\hat{\Gamma}^{dph} = \hbar\Omega\left[\hat{\sigma}_y - \gamma(\sigma_z + \hat{I})\right]. \tag{4.68}$$

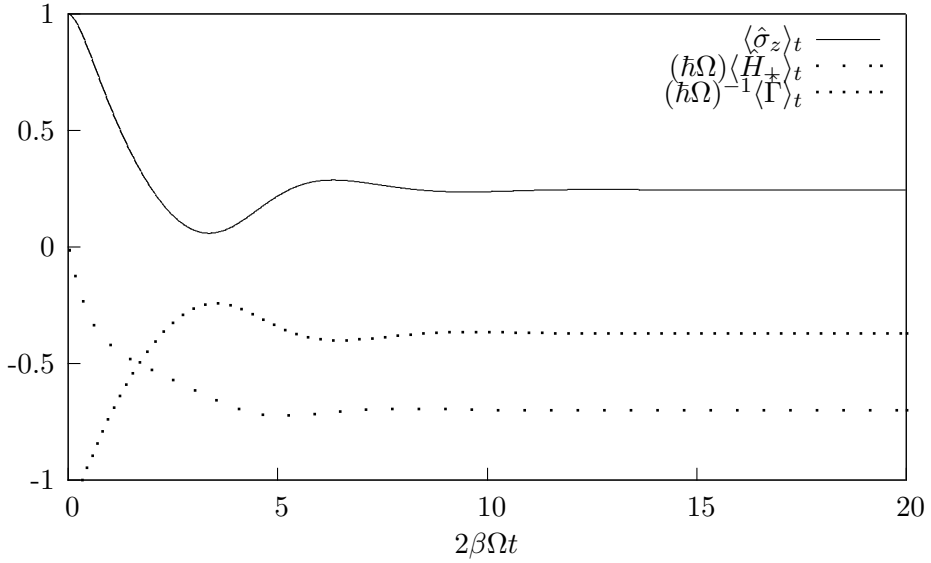

Figure 4.5: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.9$ and $\frac{\gamma}{\beta} = 0.5$.

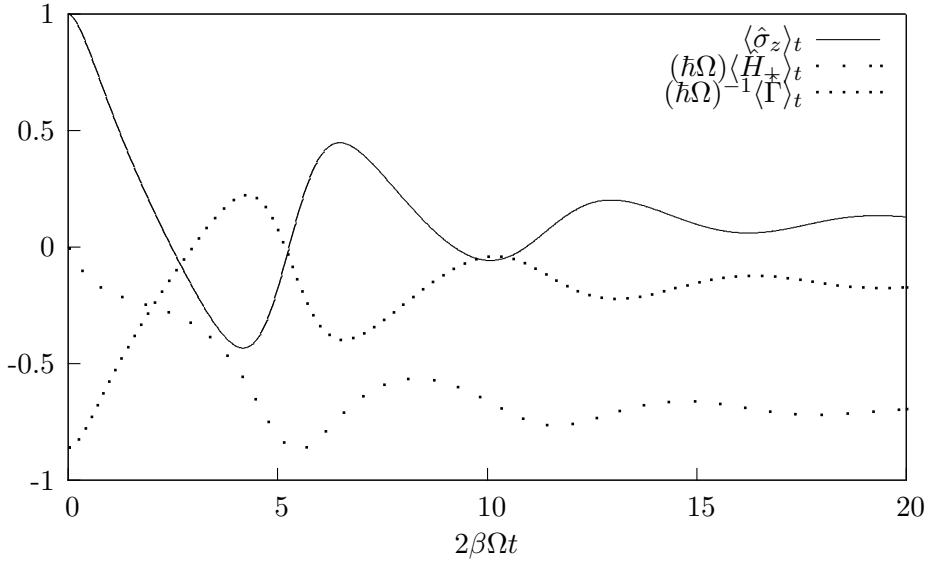

Figure 4.6: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.9$ and $\frac{\gamma}{\beta} = 0.2$.

This choice means that the evolution equation produces

$$\hat{\rho}_{11}(t) = \frac{1}{2}e^{-2\Gamma t}, \tag{4.69}$$

$$\hat{\rho}_{12}(t) = \hat{\rho}^*_{21}(t) = \frac{1}{2\gamma}e^{-2\Gamma t}\left[(\gamma - i)e^{\Gamma t} + i\right], \tag{4.70}$$

and

$$\hat{\rho}_{22}(t) = \frac{1}{2\gamma^2}\left[(e^{-\Gamma t} - 1)^2 + \gamma^2\right]. \tag{4.71}$$

Now the averages are

$$\langle\hat{\sigma}_x\rangle_t = \frac{\gamma^2}{\tilde{\gamma}^2\cosh(\Gamma t) - 1}, \tag{4.72}$$

$$\langle\hat{\sigma}_y\rangle_t = \frac{\gamma(1 - e^{-\Gamma t})}{\tilde{\gamma}^2\cosh(\Gamma t) - 1}. \tag{4.73}$$

The definition of average defined in Eq (2.27) is being used.

Now we consider Fig 4.7, Fig 4.8 and Fig 4.9. From the graphs we can see that as t tends towards infinity

$$\langle\hat{\sigma}_x\rangle_t = \langle\hat{\sigma}_y\rangle_t \tag{4.74}$$

in the limit t approaching infinity.

Similarly we can see that $\langle\hat{\sigma}_z\rangle_t$ is approaching negative one. Where

$$\langle\sigma_z\rangle_t = \frac{1 - \cosh(\Gamma t) - \gamma^2\sinh(\Gamma t)}{\hat{\gamma}^2\cosh(\Gamma t) - 1} \tag{4.75}$$

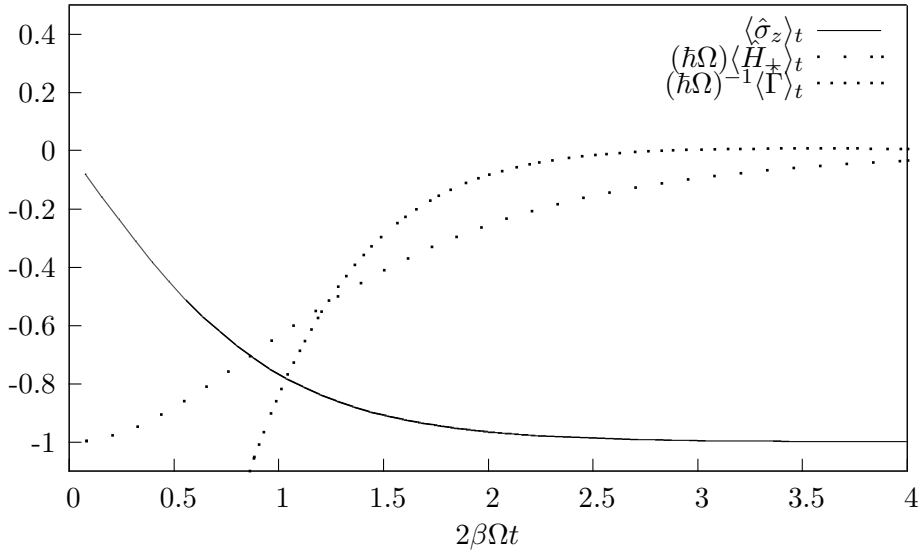

Figure 4.7: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.8$ and $\gamma = 4$.

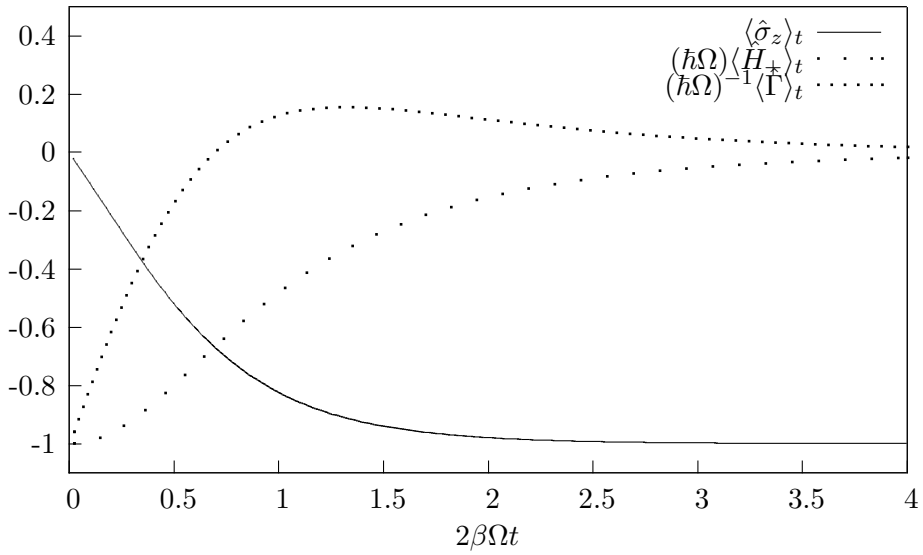

Figure 4.8: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.8$ and $\gamma = 1$.

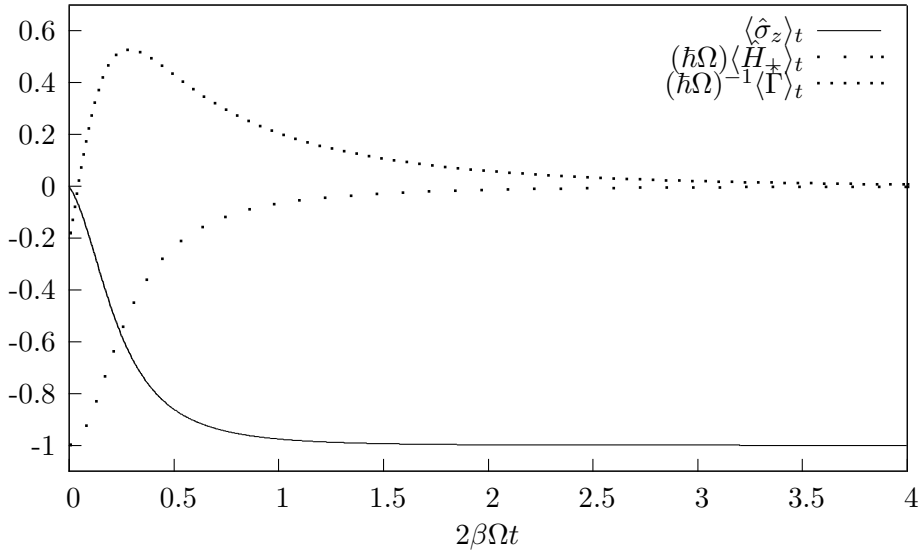

Figure 4.9: Analytical plots showing the profiles of $\langle\hat{\sigma}_z\rangle_t$, $\frac{\langle\hat{H}_+\rangle_t}{\hbar\Omega}$ and $\frac{\langle\hat{\Gamma}\rangle_t}{\hbar\Omega}$, where $\beta = 0.8$ and $\gamma = 0.2$.

Chapter 5

Conclusion

Non-Hermitian quantum mechanics can be used as a computational framework. Attempts are also being made to formulate a fundamental non-Hermitian physical theory. Attempts at formulating a physically reasonable theory are put forward but neither of the two mathematical frameworks, PT-symmetric and pseudo-Hermitian, appear to be a fundamental theory at the moment.

The major complication with both frameworks is the exotic inner products that they utilise, that vary with basis.

A comparison of the two frameworks is extremely interesting. The first point of interest concerns the relationship between PT-symmetric and pseudo-Hermitian quantum mechanics. The PT-symmetric framework is a special case of the pseudo-Hermitian framework, implying that the latter is the more general of the two. The second concerns the ability to transform between Hermitian and non-Hermitian Hamiltonians.

It is the opinion of the author at the time of writing that, it is extremely unlikely that the PT-symmetric framework will form a fundamental theory. However, the fact that it is possible to transform from Hermitian to non-Hermitian Hamiltonians provides an opportunity to exploit these frameworks to ease the computational burden for certain problems.

Both frameworks have been applied to a wide variety of different problems, in partic-

ular, the PT-symmetric formalism has been widely used. Some examples of these fields include: quantum optics, open quantum systems and nuclear physics amongst others.

Recent applications of non-Hermitian theories to open quantum systems have been discussed. These applications are an example of non-Hermitian Hamiltonians' uses in formulating a convenient numerical scheme. By exploiting the ability to transform between Hermitian and non-Hermitian Hamiltonians, a more efficient numerical scheme can be formulated. Using a non-Hermitian Hamiltonian for the calculations allows a significant reduction in the number of degrees of freedom, resulting in more efficient computations. This has been covered in more detail in Chapter four.

Chapter 6

Appendix

6.1 Derivation of Hermitian linear automorphism with degeneracy

The derivation of the Hermitian linear automorphism makes use of Mostafazadeh's approach. It is included due to the importance of the Hermitian linear automorphism in the formulation of pseudo-Hermitian quantum mechanics.

If H is an η-pseudo-Hermitian Hamiltonian with a complete biorthonormal eigenbasis $\{|\psi_n, a\rangle, |\phi_n, a\rangle\}$ and a discrete spectrum[6], then, by definition,

$$H|\psi_n, a\rangle = E_n|\psi_n, a\rangle, \tag{6.1}$$

$$H^\dagger|\phi_n, a\rangle = E_n^*|\phi_n, a\rangle, \tag{6.2}$$

$$\langle\phi_m, b|\psi_n, a\rangle = \delta_{mn}\delta_{ab}, \tag{6.3}$$

$$\sum_n \sum_{a=1}^{d_n} |\phi_n, a\rangle\langle\psi_n, a| = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle\langle\phi_n, a| = 1, \tag{6.4}$$

where d_n is the degree of degeneracy (multiplicity) of the eigenvalue E_n, and a and b are the degeneracy labels.

In order to derive an expression for the Hermitian linear automorphism, an extra result is required, called proposition seven by Mostafazadeh. Proposition seven can be

derived by making use of equations (6.1) and (6.2) and then using equation (3.36),

$$\eta H \eta^{-1} |\phi_n, a\rangle = E_n^* |\phi_n, a\rangle. \tag{6.5}$$

We now operate from the left with η^{-1},

$$\begin{aligned} H\eta^{-1}|\phi_n, a\rangle &= \eta^{-1} E_n^* |\phi_n, a\rangle & (6.6)\\ &= E_n^* (\eta^{-1}|\phi_n, a\rangle). & (6.7) \end{aligned}$$

Now

$$E_n^* |\phi_n, a\rangle = H^\dagger |\phi_n, a\rangle. \tag{6.8}$$

Operate from the left with η^{-1},

$$\begin{aligned} \eta^{-1} E_n^* |\phi_n, a\rangle &= \eta^{-1} H^\dagger |\phi_n, a\rangle & (6.9)\\ &= H\eta^{-1}|\phi_n, a\rangle. & (6.10) \end{aligned}$$

Therefore,

$$\eta^{-1} H^\dagger |\phi_n, a\rangle = H\eta^{-1}|\phi_n, a\rangle. \tag{6.11}$$

Then proposition seven can be written as,

$$H(\eta^{-1}|\phi_n), a\rangle = E_n^*(\eta^{-1}|\phi_n, a\rangle) = \eta^{-1} H^\dagger |\phi_n, a\rangle. \tag{6.12}$$

Mostafazadeh's notation is now adopted; the subscript "0" denotes real eigenvalues and the corresponding basis eigenvectors. The subscript "$\pm$" denotes complex eigenvalues that have "$\pm$" imaginary parts and their corresponding basis eigenvectors[6].

Now using the new notation and equation (6.4),

$$I = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\psi_{n_0}, a\rangle\langle\phi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n_+}} (|\psi_{n_+}, \alpha\rangle\langle\phi_{n_+}, \alpha| + |\psi_{n_-}, \alpha\rangle\langle\phi_{n_-}, \alpha|), \tag{6.13}$$

where a is an index for the real components and α applies to the complex components.

Now use equation (6.4) to write the Hamiltonian as

$$H = \sum_{n_0} \sum_{a=1}^{d_{n_0}} H|\psi_{n_0}, a\rangle\langle\phi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n_+}} H(|\psi_{n_+}, \alpha\rangle\langle\phi_{n_+}, \alpha| + |\psi_{n_-}, \alpha\rangle\langle\phi_{n_-}, \alpha|). \tag{6.14}$$

Use equation (6.14) and proposition 7 to write the Hamiltonian as

$$H = \sum_{n_0} \sum_{a=1}^{d_{n_0}} E_{n_0} |\psi_{n_0}, a\rangle\langle\phi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n_+}} (E_{n_+} |\psi_{n_+}, \alpha\rangle\langle\phi_{n_+}, \alpha| + E^*_{n_+} |\psi_{n_-}, \alpha\rangle\langle\phi_{n_-}, \alpha|). \tag{6.15}$$

Any linear combination of degenerate eigenvectors belonging to the same eigenvalue is also an eigenket of that eigenvalue, so

$$|\psi_{n_0}\rangle = \sum_{a=1}^{d_{n_0}} C_a |\psi_{n_0}, a\rangle. \tag{6.16}$$

To find a given C_a, let $\bar{a}$ be a particular a. Multiply (6.16) on the left-hand side with $\langle\phi_{n_0}, \bar{a}|$,

$$\begin{aligned} \langle\phi_{n_0}, \bar{a}|\psi_{n_0}\rangle &= \sum_{a=1}^{d_{n_0}} C_a \langle\phi_{n_0}, \bar{a}|\psi_{n_0}, a\rangle \\ &= \sum_{a=1^{d_{n_0}}} C_a \delta_{n_0 n_0} \delta_{\bar{a}a} \\ &= C_{\bar{a}}. \end{aligned} \tag{6.17}$$

Substitute equation (6.17) into (6.16),

$$|\psi_{n_0}\rangle = \sum_{a=1}^{d_{n_0}} \langle\phi_{n_0}, a|\psi_{n_0}\rangle |\psi_{n_0}, a\rangle. \tag{6.18}$$

Since an inner product is a number we can write

$$|\psi_{n_0}\rangle = \sum_{a=1}^{d_{n_0}} |\psi_{n_0}, a\rangle\langle\phi_{n_0}, a|\psi_{n_0}\rangle. \tag{6.19}$$

Therefore

$$I = \sum_{a=1}^{d_{n_0}} |\psi_{n_0}, a\rangle\langle\phi_{n_0}, a|, \tag{6.20}$$

is the closure relation for the degenerate state. Now,

$$\begin{aligned} \eta^{-1} |\phi_{n_0}, a\rangle &= I \eta^{-1} |\phi_{n_0}, a\rangle \\ &= \sum_{b=1}^{d_{n_0}} |\psi n0, b\rangle\langle\phi_{n_0}, b|\eta^{-1}|\phi_{n_0}, a\rangle \\ &= \sum_{b=1}^{d_{n_0}} \langle\phi_{n_0}, b|\eta^{-1}|\phi_{n_0}, a\rangle |\psi_{n_0}, b\rangle. \end{aligned} \tag{6.21}$$

Similarly for the first complex case,

$$|\psi_{n_+}\rangle = \sum_{\alpha=1}^{d_{n_+}} C_\alpha |\psi_{n_+}, \alpha\rangle. \tag{6.22}$$

Let $\bar{\alpha}$ be a particular α. Now multiply equation (6.22) on the left-hand side with $\langle \phi_{n_+}, \bar{\alpha}|$. Then

$$\begin{aligned} \langle \phi_{n_+}, \bar{\alpha}|\psi_{n_+}\rangle &= \sum_{\alpha=1}^{d_{n_+}} C_\alpha \langle \phi_{n_+}, \bar{\alpha}|\psi_{n_+}, \alpha\rangle \\ &= \sum_{\alpha=1}^{d_{n_+}} C_\alpha \delta_{n_+ n_+} \delta_{\bar{\alpha}\alpha} \\ &= C_{\bar{\alpha}}. \end{aligned}$$

Therefore

$$C_\alpha = \langle \phi_{n_+}, \alpha|\psi_{n_+}\rangle. \tag{6.23}$$

Substitute equation (6.23) into (6.22),

$$\begin{aligned} |\psi_{n_+}\rangle &= \sum_{\alpha=1}^{d_{n_+}} \langle \phi_{n_+}, \alpha|\psi_{n_+}\rangle |\psi_{n_+}\alpha\rangle \\ &= \sum_{\alpha=1}^{d_{n_+}} |\psi_{n_+}, \alpha\rangle\langle \phi_{n_+}, \alpha|\psi_{n_+}\rangle. \end{aligned} \tag{6.24}$$

Therefore,

$$I = \sum_{\alpha=1}^{d_{n_+}} |\psi_{n_+}, \alpha\rangle\langle \phi_{n_+}, \alpha| \tag{6.25}$$

is the closure relation for the degenerate state. Now,

$$\begin{aligned} \eta^{-1}|\phi_{n_-}, \alpha\rangle &= I\eta^{-1}|\phi_{n_-}, \alpha\rangle \\ &= \sum_{\beta=1}^{d_{n_+}} |\psi_{n_+}, \beta\rangle\langle \phi_{n_+}, \beta|\eta^{-1}|\phi_{n_-}, \alpha\rangle. \end{aligned} \tag{6.26}$$

Then

$$\eta^{-1}|\phi_{n_-}, \alpha\rangle = \sum_{\beta=1}^{d_{n_+}} \langle \phi_{n_+}, \beta|\eta^{-1}|\phi_{n_-}, \alpha\rangle |\psi_{n_+}, \beta\rangle. \tag{6.27}$$

Now for the other case,

$$|\psi_{n_-}\rangle = \sum_{\alpha=1}^{d_{n_+}} C_\alpha |\psi_{n_-}, \alpha\rangle. \tag{6.28}$$

To find a given C_α let $\bar{\alpha}$ be a particular α. Multiply the above equation on the left-hand side with $\langle \phi_{n_-}, \bar{\alpha}|$. Then

$$\begin{aligned}\langle \phi_{n_-}, \bar{\alpha}|\psi_{n_-}\rangle &= \sum_{\alpha=1}^{d_{n_+}} C_\alpha \langle \phi_{n_-}, \bar{\alpha}|\psi_{n_-}, \alpha\rangle \\ &= \sum_{\alpha=1}^{d_{n_+}} C_\alpha \delta_{n_- n_-}\delta_{\bar{\alpha}\alpha}. \\ &= C_{\bar{\alpha}}\end{aligned}$$

Therefore,

$$C_\alpha = \langle \phi_{n_-}, \alpha|\psi_{n_-}\rangle. \tag{6.29}$$

Substitute equation (6.29) into (6.23),

$$|\psi_{n_+}\rangle = \sum_{\alpha=1}^{d_{n_+}} |\psi_{n_-}, \alpha\rangle\langle \phi_{n_-}, \alpha|\psi_{n_-}\rangle. \tag{6.30}$$

Therefore

$$I = |\psi_{n_-}, \alpha\rangle\langle \phi_{n_-}, \alpha|. \tag{6.31}$$

But

$$\begin{aligned}\eta^{-1}|\phi_{n_+}, \alpha\rangle &= I\eta^{-1}|\phi_{n_+}, \alpha\rangle \\ &= \sum_{\beta=1}^{d_{n_+}} |\psi_{n_-}, \beta\rangle\langle \phi_{n_-}, \beta|\phi_{n_+}, \alpha\rangle \\ &= \sum_{\beta=1}^{d_{n_+}} \langle \phi_{n_-}, \beta|\phi_{n_+}, \alpha\rangle|\psi_{n_-}, \beta\rangle. \end{aligned}\tag{6.32}$$

$$\eta^{-1}|\phi_{n_0}, a\rangle = \sum_{b=1}^{d_{n_0}} C_{ba}^{(n_0)}|\psi_{n_0}, b\rangle, \tag{6.33}$$

where $C_{ab}^{(n_0)} = \langle \phi_{n_0}, a|\eta^{-1}|\phi_{n_0}, b\rangle$.

$$\eta^{-1}|\phi_{n_+}, \alpha\rangle = \sum_{\beta=1}^{d_{n_+}} C_{\beta\alpha}^{(n_+)}|\psi_{n_-}, \beta\rangle, \tag{6.34}$$

where $C_{\alpha\beta}^{(n_+)} = \langle \phi_{n_-}, \alpha|\eta^{-1}|\phi_{n_+}, \beta\rangle$.

$$\eta^{-1}|\phi_{n_-}, \alpha\rangle = \sum_{\beta=1}^{d_{n_+}} C_{\beta\alpha}^{(n_-)}|\psi_{n_+}, \beta\rangle, \tag{6.35}$$

where $C^{(n_-)}_{\alpha\beta} = \langle \phi_{n_+}, \alpha | \eta^{-1} | \phi_{n_-}, \beta \rangle$.

$C^{(n_0)}_{ab}$ and $C^{(n_\pm)}_{ab}$ are complex coefficients. These complex coefficients can be thought of as matrices since η and η^{-1} are Hermitian operators. It is possible to make a unitary transformation of the Hilbert space to map the biorthonormal system of eigenbasis vectors of the Hamiltonian to a new system, in which these matrices are diagonal. If the basis vectors are further rescaled, then $C^{(n_0)}_{ab}$ and $C^{(n_\pm)}_{ab}$ will become the identity matrix. It is assumed that such a transformation has been performed without loss of generality.

Then

$$|\phi_{n_0}, a\rangle = \eta |\psi_{n_0}, a\rangle, \tag{6.36}$$

and

$$|\phi_{n_\pm}, \alpha\rangle = \eta |\psi_{n_\mp}, \alpha\rangle. \tag{6.37}$$

Now by making use of the above result and the definitions it is possible to obtain the pseudo-Hermitian orthonormality relations

$$\langle\langle \psi_{n_0}, a | \psi_{m_0}, b \rangle\rangle_{\hat{\eta}} = \delta_{n_0 m_0} \delta_{ab}, \tag{6.38}$$

$$\langle\langle \psi_{n_\pm}, \alpha | \psi_{m_\mp}, \beta \rangle\rangle_{\hat{\eta}} = \delta_{n_\pm m_\mp} \delta_{\alpha\beta}. \tag{6.39}$$

From equation(6.33), (6.34) and (6.35)

$$|\psi_{n_0}, a\rangle = \eta^{-1} |\phi_{n_0}, a\rangle, \tag{6.40}$$

$$|\psi_{n_\mp}, \alpha\rangle = \eta^{-1} |\phi_{n_\pm}, \alpha\rangle. \tag{6.41}$$

Now substitute equation (6.40) and (6.41) into equation (6.13)

$$I = \sum_{n_0} \sum_{a=1}^{d_{n_0}} \eta^{-1} |\phi_{n_0}, a\rangle\langle\phi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n_+}} (\eta^{-1} |\phi_{n_-}, \alpha\rangle\langle\phi_{n_+}, \alpha| + \eta^{-1} |\phi_{n_+}, \alpha\rangle\langle\phi_{n_-}, \alpha|). \tag{6.42}$$

Then operate η from the left-hand side

$$\eta = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\phi_{n_0}, a\rangle\langle\phi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n_+}} (|\phi_{n_-}, \alpha\rangle\langle\phi_{n_+}, \alpha| + |\phi_{n_+}, \alpha\rangle\langle\phi_{n_-}, \alpha|). \tag{6.43}$$

By substituting equation (6.40) and (6.41) into equation (6.13) we obtain,

$$\eta^{-1} = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\psi_{n_0}, a\rangle\langle\psi_{n_0}, a| + \sum_{n_+} \sum_{\alpha=1}^{d_{n+}} (|\psi_{n_-}, \alpha\rangle\langle\psi_{n_+}, \alpha| + |\psi_{n_+}, \alpha\rangle\langle\psi_{n_-}, \alpha|). \quad (6.44)$$

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