

Master's thesis

# Non-Hermitian Quantum Mechanics

On the role of  $\mathcal{PT}$ -Symmetry and Exceptional Points

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# Abstract

Since 1998, when Bender & Boettcher demonstrated that non-Hermitian Hamiltonians exhibiting space-time reflection ( $\mathcal{PT}$ ) symmetry can have entirely real spectra the study of non-Hermitian systems has gained increasingly more traction and  $\mathcal{PT}$ -symmetry have been observed in a plethora of physical phenomena with an increasing number of studies being published, especially in the last few years.

In this thesis we give a set of postulates generalising the traditional Dirac-von Neumann postulates of quantum mechanics to non-Hermitian theories. By a direct comparison to the Dirac-von Neumann postulates, only two amendments are needed to generalise them: *observables are represented by para-Hermitian operators* and *the Hilbert space inner product is endowed with a metric operator dynamically determined by the Hamiltonian*. Furthermore, by introducing a generalised  $\mathcal{PT}$  operator – a combination of a linear and anti-linear operator – the basic foundations for quantum mechanics can be derived by requiring  $\mathcal{PT}$ -symmetry. In particular, the requirement of  $\mathcal{PT}$ -symmetry of operators is for finite dimensional Hilbert spaces equivalent to the condition of pseudo-Hermiticity, a generalisation of para-Hermiticity. It is explicitly shown how the condition of pseudo-Hermiticity of the Hamiltonian follows directly from requiring conservation of metric norms – introduced to ensure an orthogonal rather than a biorthogonal eigenbasis.

One of the emergent effects in non-Hermitian systems are points in parameter space, known as exceptional points (EPs), where the Hamiltonian loses dimensionality. In  $\mathcal{PT}$ -symmetric systems the EPs are related to spontaneous breaking of  $\mathcal{PT}$ -symmetry and can be seen as phase transition from a region of real eigenvalues to complex conjugate pairs. Furthermore, near  $n$ -th order EPs non-Hermitian systems exhibit a characteristic  $\sqrt[n]{\epsilon}$  dependence in external perturbations  $\epsilon \ll 1$ , whereas Hermitian systems has a maximally linear dependence. This  $\sqrt[n]{\epsilon}$  dependence could be utilised to construct enhanced sensing experiments. Moreover, we demonstrate the existence of a second order EP in a stochastically driven qubit and show that it is associated with a sudden change in the decoherence rates and oscillation frequencies.



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# Introductory Remarks

Following the seminal paper by Bender & Boettcher [1] on non-Hermitian Hamiltonians with real eigenvalues and parity-time inversion ( $\mathcal{PT}$ ) symmetry has been the topic of much study with a large number of papers published, especially in recent years. The overall aim of this thesis is to review some of this work, condense it and provide some examples. In particular the purpose of the thesis is twofold: it is to

- review the formulation of non-Hermitian quantum mechanics with an emphasis on the role of  $\mathcal{PT}$ -symmetry and how it generalises Hermitian quantum mechanics,
- review some effects of non-Hermiticity, discuss their role in the dynamics of non-Hermitian systems and construct some examples to demonstrate the effects.

Before we begin, some brief comments on the structure of the thesis and some notation are in order. It is assumed that the reader is familiar with basic quantum mechanics, it's origin, some standard methods as well as the mathematics necessary for quantum mechanics. Moreover, some familiarity with other fields in physics, such as quantum field theory, general relativity and statistical mechanics is an advantage. However, this will mostly be relevant to only a few subsections and on topics peripheral to the overall topic of the thesis.

## Outline of Thesis

The thesis is loosely separated into four parts; an introduction & motivation, the fundamentals of non-Hermitian quantum mechanics, some examples and effects of non-Hermiticity &  $\mathcal{PT}$  symmetry, and lastly some brief discussions and applications before giving some final remarks. In particular the general outline of the thesis is as follows:

- Chapter 1: Introduce the notion of symmetries in physics and its role a guide in constructing or extending physical theories. In particular introduce space-time inversion symmetry and some familiar properties from both classical and quantum physics, as well as state some of its mathematical properties.
- Chapter 2: Present normal operators and some key features. Present the main results of the seminal paper by Bender & Boettcher [1] and review some examples of non-Hermiticity in classical and quantum physics to motivate the formal study of non-Hermitian quantum mechanics and especially with respect to  $\mathcal{PT}$ -symmetry.
- Chapter 3: Present the Dirac-von Neumann postulates of quantum mechanics and review their generalisation to non-Hermitian quantum mechanics. In par-

ticular discuss how the non-Hermitian postulates differ from the Hermitian postulates.

Chapter 4: Introduce the generalised notion of  $\mathcal{PT}$ -symmetry and demonstrate how it ensures that operators have real eigenvalues. Moreover, demonstrate how  $\mathcal{PT}$ -symmetry implies a metric inner product structure and ensures unitary evolution of states. Moreover, review some other characteristic features of non-Hermitian operators as well as give a simple example.

Chapter 5: A theorem regarding the realisations of  $\mathcal{PT}$ -symmetric quantum systems by Scheel & Szameit [2], to illustrate the theorem we give a related example on the role of loss and gain in open quantum systems. Moreover, we introduce the notion of exceptional points, review some of the characteristic properties and present a simple example.

Chapter 6: As a demonstration of exceptional points, we derive the master equations for quantum systems under the influence of telegraph noise and solve the equations in for the particular example of qubit systems. The solutions for a qubit system is used to explicitly demonstrate the presence of an exceptional point in the matrix generating the averaged time evolution.

Chapter 7: Lastly, we give some examples of recent developments in physics by utilising  $\mathcal{PT}$ -symmetry and exceptional points. Moreover, we give some brief remarks on current and future applications to physics and technology.

In the final remarks some conclusions and outlooks of the field as well as possible extensions of the example in chapter 6 are given. Appendices A to C contain some calculations relevant to the preceding chapters, however their content is not essential to the discussion.

Lastly, let us give a few remarks on notation used in the thesis.

## Notation

For the most part concepts and notation will be introduced and explained as they appear, however some notation is assumed to be familiar to the reader. For the most part, I have tried to stick to conventions in names and symbols, however some deviations from convention might occur in order to avoid confusion. Whenever multiple conversations exists I have tried to stick to the “physicists convention”, e.g. the definition of the Pauli matrices and naming of angles in spherical coordinates. The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (1)$$

which satisfy the identity

$$\sigma_i \sigma_j = \delta_{i,j} + i \epsilon_{i,j,k} \sigma_k$$

for  $i, j, k$  in the ordered set  $\{x, y, z\}$ .  $\hbar$  denotes the reduced Planck constant,  $i \equiv \sqrt{-1}$  the imaginary unit,  $\mathbb{N}$  the natural numbers,  $\mathbb{R}$  the real numbers and  $\mathbb{C}$  the complex numbers. Complex conjugation will be denoted by  $*$ , that is for a complex number  $\alpha \in \mathbb{C}$  it's complex conjugate is  $\alpha^*$ . The real part of a number  $\alpha$  will be denoted  $\text{Re } \alpha$  and the imaginary part  $\text{Im } \alpha$ .



Similarly to [3], let us define a *Hilbert space* as

**Definition 0.1.** A complex vector space  $\mathcal{H}$ , of finite or infinite dimension with states  $|\psi\rangle, |\varphi\rangle, |\chi\rangle \in \mathcal{H}$ , is a Hilbert space if it satisfies the following requirements:

1. The vector space  $\mathcal{H}$  is endowed with a scalar product between states,  $\langle\psi|\varphi\rangle$ , satisfying the relations

$$\langle\psi|\varphi\rangle = [\langle\varphi|\psi\rangle]^*, \quad (2a)$$

$$\langle\psi|\alpha\varphi + \beta\chi\rangle = \alpha\langle\psi|\varphi\rangle + \beta\langle\psi|\chi\rangle, \quad (2b)$$

$$\langle\psi|\psi\rangle = \|\psi\|^2 = 0 \Leftrightarrow |\psi\rangle = 0, \quad (2c)$$

where  $\alpha, \beta \in \mathbb{C}$  and  $\|\psi\|^2$  denotes the norm of the state  $|\psi\rangle$ .

2.  $\mathcal{H}$  is a space where every Cauchy series has a limit. That is; if there exist a series of vectors  $|\psi^{(l)}\rangle \in \mathcal{H}$  such that  $\|\psi^{(l)} - \psi^{(m)}\| \rightarrow 0$  for  $l, m \rightarrow \infty$ , then there exists a vector  $|\psi\rangle \in \mathcal{H}$  such that  $\|\psi^{(l)} - \psi\| \rightarrow 0$  for  $l \rightarrow \infty$ . The space  $\mathcal{H}$  is a complete space.
3. The dimension of  $\mathcal{H}$  is a unique characteristic, in the sense that all spaces with the same dimension are isomorphic. The dimension of  $\mathcal{H}$  may be finite, i.e.  $d \in \mathbb{N}$ , countably infinite or uncountably infinite.

From definition 0.1 it can be noted that because the limit vectors of Cauchy series may always be added for finite dimensional or separable Hilbert spaces, then requirement 2 is automatically satisfied. Thus requirement 2 of definition 0.1 is usually only mentioned if the Hilbert spaces that will be treated are inseparable and infinite dimensional.

**Corollary 0.2.** The Hilbert space inner product  $\langle\psi|\varphi\rangle$ , for states  $|\psi\rangle, |\varphi\rangle, |\chi\rangle \in \mathcal{H}$  is conjugate linear in the co-vectors  $\langle\psi|, \langle\varphi|$ :

$$\langle\alpha\psi + \beta\chi|\varphi\rangle = \alpha^* \langle\psi|\varphi\rangle + \beta^* \langle\chi|\varphi\rangle$$

For  $\alpha, \beta \in \mathbb{C}$ .

The proof of corollary 0.2 follows directly from eqs. (2a) and (2b). Moreover, a restriction on type of Hilbert spaces necessary for quantum theories can be made:

*Claim 0.3.* All Hilbert spaces associated with Quantum Mechanics are separable [3].

Vectors are generally denoted by boldface letters, e.g. Let  $\mathbf{x}$  be a vector in a general vector space  $\mathcal{V}$ , denoted  $\mathbf{x} \in \mathcal{V}$ . However, when concerned with Hilbert spaces the *Dirac* or *bra-ket* notation will be used. That is  $|\psi\rangle \in \mathcal{H}$  where  $\mathcal{H}$  generally denotes a complex Hilbert space, and  $|\psi\rangle$  is somewhat interchangeably referred to as vector or state in the Hilbert space. Moreover, the covector  $\langle\psi|$  to  $|\psi\rangle$  is a vector in the dual vector space. However, as the dual vector space of a Hilbert space is itself a Hilbert space no distinction will be made and abusing the notation a bit, we will say that  $\langle\psi| \in \mathcal{H}$ . Moreover, unless otherwise stated,  $\langle\cdot|\cdot\rangle$  denotes the *Dirac norm* or *Hilbert-Schmidt inner product*. Expectation values  $\langle\cdot\rangle$  are taken with respect to the Dirac norm, unless otherwise stated. Other expectation values will be denoted with a subscript,  $\langle\cdot\rangle_*$ , for clarity.

Operators are generally written as upper case Latin letters as are matrices, the difference should hopefully be clear from the context. Some operators are denoted by a

hat,  $\hat{O}$ , in order to avoid confusion. This will typically be ladder operators,  $\hat{a}$ , which are conventionally denoted by lower case Latin letters. The symbol  $\mathbf{1}$  refers to the identity element, operator and matrix interchangeably, and will whenever necessary be equipped with a subscript. Furthermore, lower case greek letters are usually used as parameters, and I believe that I have managed to avoid using the letter  $\pi$  for anything other than the mathematical constant.

# Chapter 1

## Symmetry

Symmetry has been an important subject in the natural sciences since Euclid's *Elements* [4], and is to this day one of the guiding principles when exploring new physics [5, 6]. The word *symmetry*, from the ancient greek word *συμμετρία* [7], has typically another meaning to physicists and mathematicians than in the everyday language. According to the Oxford English Dictionary the noun symmetry usually refers to:

*Due or just proportion; harmony of parts with each other and the whole; fitting, regular, or balanced arrangement and relation of parts or elements; the condition or quality of being well-proportioned or well-balanced.* [7]

Although still associated with harmony, balance and beauty, the word takes a much stricter meaning in physics and mathematics. These associations with the word are somewhat historical [4], but remains in the everyday language – often in relation to notions of beauty. The Oxford English Dictionary continues to give a stricter definition with regards to science:

*In stricter use: Exact correspondence in size and position of opposite parts; equable distribution of parts about a dividing line or centre. (As an attribute either of the whole, or of the parts composing it.)* [7]

From a mathematical point of view, this is not a particularly specific nor accurate description. Let us thus begin by introducing the notion of symmetry in physics through a group theoretical definition. Moreover, let us introduce a categorisation of symmetries and briefly discuss some of the famous implications of symmetry in physics. Equipped with the general concept of symmetry in physics, let us briefly introduce and discuss the role of *space-time inversion symmetry*.

### 1.1 Symmetries in Physics

Symmetry is sometimes a loosely used word even in physics. Invariant, covariant and symmetric are all related notions frequently used by physicists, thus in order to be precise let us similarly to [5] define a symmetry in the following manner:

**Definition 1.1.** Let  $O$  be an operator and  $\mathcal{G}$  any group of group elements  $G_a$  with the induced transformations  $T(G_a)$  on the eigenspace of  $O$ . The operator  $O$  is said to *invariant* under the transformations  $T(G_a)$  if

$$T(G_a)OT^{-1}(G_a) = O, \quad (1.1)$$

where  $T^{-1}(G_a)$  denotes the inverse transformation. If the operator  $O$  is left invariant under all group elements  $G_a$ , then  $\mathcal{G}$  is said to be a *symmetry group* of the operator  $O$  and is said to exhibit a  $\mathcal{G}$  symmetry.

Equivalently to eq. (1.1), the operator is said to be symmetric under the group  $\mathcal{G}$  if

$$[T(G_a), O] = 0 \quad \forall G_a \in \mathcal{G}, \quad (1.2)$$

where  $[T(G_a), O] = T(G_a)O - OT(G_a)$  denotes the usual commutator. This definition of symmetry follows directly from eq. (1.1) by multiplying by  $T(G_a)$  from the left and is particularly a useful definition in quantum mechanics. This definition will be revisited in section 4.1. Moreover, we note that if eq. (1.2) holds for one or more group elements but not all,  $O$  will typically be said to be invariant with respect to these group elements and not symmetric.

For those not familiar with group theory, a group is defined as [8]:

**Definition 1.2.** A *group*  $\mathcal{G}$  is a non-empty set of elements equipped with a binary operation,  $\circ$ , such that

$$a \circ b \in \mathcal{G}, \quad \forall a, b \in \mathcal{G}, \quad (\text{closure})$$

$$a \circ (b \circ c) = (a \circ b) \circ c, \quad \forall a, b, c \in \mathcal{G}, \quad (\text{associativity})$$

$$a \circ \mathbf{1} = \mathbf{1} \circ a = a, \quad \forall a \in \mathcal{G} \text{ and } \mathbf{1} \in \mathcal{G}, \quad (\text{identity})$$

and given  $a \in \mathcal{G}$ , there exists an  $a^{-1} \in \mathcal{G}$  such that

$$a \circ a^{-1} = a^{-1} \circ a = \mathbf{1}. \quad (\text{inverse})$$

The group  $\mathcal{G}$  is said to be *commutative* or *Abelian* iff

$$a \circ b = b \circ a, \quad \forall a, b \in \mathcal{G}. \quad (\text{Abelian})$$

### 1.1.1 Continuous Symmetries

If a physical system exhibits a symmetry leaving the system invariant under continuous changes, it is said to exhibit a *continuous symmetry*. That is groups for which any transformation can be achieved through a series of infinitesimal group actions. More formally the groups associated with such symmetries are both infinite and continuous, of which the *Lie groups* are the most studied [8].

Closely connected to continuous symmetries are conservation laws. In particular, Noether's theorem states that every differentiable symmetry of the action,  $\mathcal{S}$ , gives rise to a conservation law [8]. Where the action is a functional of the generalised coordinates,  $\mathbf{q}$

$$\mathcal{S}[\mathbf{q}] = \int dt L(\mathbf{q}, \dot{\mathbf{q}}, t),$$

where  $L$  denotes the Lagrangian of the system. Continuous symmetries thus gives rise to conserved quantities in systems, and as a result symmetries constrains the possible

configurations the system can take. In order for a conserved quantity to change, the associated symmetry must break.

Typical examples of continuous symmetries often appearing in classical physics are time-translations, spatial translations and rotations in Euclidean space. The group of translations in time are the real numbers under addition,  $\mathbb{R}$ , and the associated conserved quantity is energy. The group of spatial translations is the additive group of vectors in  $\mathbb{R}^n$  where  $n$  denotes the dimensionality of the space symmetric under translations, that is systems can exhibit translation symmetry along one or more axes but it need not be along all axes. The conserved quantity associated with spatial translations is momentum, and a partial symmetry of the action gives rise to conservation of only some of the components of the momentum. If the action is invariant under rotations, angular momentum is conserved and the *special orthogonal group*  $SO(n)$  is the associated group. Moreover, for non-Euclidian spacetimes the symmetry groups change. A typical example is the *Poincaré group*, the group of rotations and translations in Minkowski space, an important group in special relativity and quantum field theory [9].

One of the fundamental symmetries of the universe is Lorentz invariance, which ensures the conservation of four-momentum and gives the energy-momentum relation. That is the invariance under the *Lorentz group*,  $O(1, 3; \mathbb{R})$ , a subgroup of the Poincaré group and it is the group of all isometries of the Minkowski space-time,  $\mathbb{M}^4$ , leaving the origin fixed [9]. The details of the Lorentz group are a bit involved but note that the Lorentz transformations discussed in introductory courses can be found in the *restricted Lorentz group*,  $SO^+(1, 3; \mathbb{R})$ . The restricted Lorentz group contains Lorentz boosts and spatial rotations[10], and is in fact the identity element of the full Lorentz group<sup>1</sup>.

Other prominent examples of continuous symmetries are the symmetries found in particle physics, of which Lorentz invariance is of course one. Moreover the internal symmetry of the *Standard Model of Particle Physics* are that of the unitary product group  $SU(3) \times SU(2) \times U(1)$  [10]. Where  $SU(n)$  is the *special unitary group* of dimension  $n$  and  $U(n)$  is the unitary group. These symmetry groups of the Standard Model are truly fundamental, each associated with a fundamental force on nature and a charge. The  $U(1)$  symmetry of the Standard Model is responsible for the electromagnetic interactions and the electric charge. In deriving Quantum Electrodynamics, the photon enters as a gauge field by requiring that the fermionic Lagrangian density is symmetric under transformations of the  $U(1)$  group [11]. In a similar manner the  $SU(2)$  symmetry gives rise to the  $Z$  and  $W^\pm$  bosons and isospin, whilst the  $SU(3)$  symmetry gives rise to gluons and colour charge [12].

The special unitary group,  $SU(n)$ , also holds a significant role in finite dimensional quantum mechanics. Any linear operator on a complex Hilbert space  $\mathcal{H}$  of dimension  $n$  satisfying the *spectral theorem* [13] or more generally *spectral operators* on a Hilbert space [14] can be represented in terms of a matrix in an orthogonal basis [5]. In fact any operator that admits a tensor representation in an orthogonal basis satisfies the following theorem [15]:

**Theorem 1.3.** *All tensors of order  $f$  can be represented by a  $n^f$ -dimensional representation of the special unitary group,  $SU(n)$ .*

<sup>1</sup>A group with a group as a identity does seem a bit odd, however as will be discussed in section 1.2.3 the full Lorentz group can be constructed from the restricted Lorentz group and the space- and time-inversion operators.

Because  $SU(n)$  is a Lie group, any representation of the group in a vector space gives rise to a representation of its *Lie algebra*,  $\mathfrak{su}(n)$  [6]. A Lie algebra is a vector space equipped with a Lie bracket, i.e. a commutator relation. The theorem thus allows us to perform operator calculations using the properties of the  $\mathfrak{su}(n)$  algebra and in some cases, as will be shown in section 6.2, derive general some properties of quantum systems of general, finite dimension.

### 1.1.2 Discrete Symmetries

*Discrete symmetries* are symmetries based on groups with as discrete set of elements, i.e. eq. (1.1) does not hold under infinitesimal transformations [4]. These symmetries can occur both as internal symmetries and as space or time symmetries. A typical example of a discrete internal symmetry in a system is *permutation symmetry* often appearing in statistical physics [16]. Ensembles made up of indistinguishable particles are insensitive to swapping two or more particles and characteristic quantities of such as the energy is dependent only on the number of possible permutations. The nature permutation symmetry is essential in deriving both the Bose-Einstein and Fermi-Dirac statistics governing the statistics of bosons and fermions, respectively [16].

Moreover, there exists a plethora of systems which exhibit discrete rotation symmetries and/or reflection symmetries along one or more axes. Such systems often appear in crystalline structures, but also in molecules. Taking a crystal as an example, they often exhibit multiple discrete symmetries [17]; The microscopic structure of a crystal can be divided into one or more primitive cells which typically appear in a repetitive structure, such that the configuration of the system remains unchanged after one or more multiples of discrete translations [6]. Within these cells, there might exist one or multiple lines along which the configuration of the cell are indistinguishable under reflections. These are typically known as reflection symmetries and are useful to describe several macroscopic properties of crystals, including their specific heat capacity and electrical conductance through the effect on the electron wave function and phonons propagations [6].

There also exist other reflection symmetries, among which parity,  $\mathcal{P}$ , charge conjugation,  $\mathcal{C}$ , and time-reversal,  $\mathcal{T}$ , symmetry are important examples. Parity and time-reversal will be discussed in some detail in the next section, let us thus briefly discuss some other reflection symmetries. As the name indicates, a system symmetric under charge conjugation is insensitive to the sign of the charges, i.e. the system is unchanged if replacing particles with anti-particles or vice versa. A place where charge conjugation appear are for Dirac fields in Quantum Field Theory, where the operation of charge conjugation is canonically defined as transforming a particle into it's anti-particle without changing the spin [10]. Together with parity and time-reversal symmetry, charge conjugation is a discrete symmetry of three out of four of the fundamental forces of Nature – the strong and electromagnetic interactions, as well as gravity [10]. The accepted theory of weak interactions, the Glashow-Weinberg-Salam theory, breaks both  $\mathcal{C}$  and  $\mathcal{P}$  symmetry, but satisfies  $\mathcal{T}$  symmetry. Violation of the combined action of charge conjugation and parity,  $\mathcal{CP}$ , has experimentally been observed in weak decays but is also expected from exotic strong interactions [12].  $\mathcal{CP}$ -violations has proposed as an explanation for the observed matter-antimatter imbalance in the universe. Although,  $\mathcal{C}$ ,  $\mathcal{P}$  and  $\mathcal{CP}$  are not symmetries, the combination  $\mathcal{CPT}$  is believed be a fundamental symmetry. In particular, the existence of the  $\mathcal{CPT}$  symmetry is stated by the  $\mathcal{CPT}$ -theorem which is believed to hold and is also supported by observations [10].

Lastly, we note that symmetries has been an guiding principle in formulating new physics for a long time, and still is. The early usage of symmetries was largely motivated by geometrical symmetries, whereas the modern use of symmetries are largely motivated from group theory [4]. As noted above, one of the branches in which group theory and symmetry has very prominent is particle physics and attempts at beyond the Standard Model physics has been largely motivated by symmetry. Supersymmetry, including string theory, and minimal extension models of the Standard Model have actively use group theory in extending the Standard Model when trying to include gravity and dark matter [4, 9].

## 1.2 Space-Time Inversion Symmetry

The operation of spatial reflection or inversion often denoted  $\mathcal{P}$ , due to its connection to *parity* in quantum theory, is a reflection of all spatial coordinates about a point, usually taken to be the origin. Unless otherwise explicitly stated, the spatial reflections will be about the origin. By the spatial inversion operator, we refer to an operator  $\mathcal{P}$  transforming coordinates  $\mathbf{x}$  and momenta  $\mathbf{p}$  as

$$\mathcal{P}\mathbf{x}\mathcal{P}^{-1} = -\mathbf{x} \qquad \mathcal{P}\mathbf{p}\mathcal{P}^{-1} = -\mathbf{p}. \quad (1.3)$$

Moreover, the transformation is *linear*, i.e.

$$\mathcal{P}(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha\mathcal{P}\mathbf{x} + \beta\mathcal{P}\mathbf{y} \quad \text{for } \alpha, \beta \in \mathbb{C}, \quad (1.4)$$

such that it leaves non-spatial expressions unchanged.

The operation of time-reversal or temporal reflection often denoted  $\mathcal{T}$ , is the reflection about a point in time, usually take to be the origin. Unless explicitly stated, the operation will be assumed to be about the temporal origin. By the time-reversal operator, we refer to an operator  $\mathcal{T}$  transforming coordinates and momenta as

$$\mathcal{T}\mathbf{x}\mathcal{T}^{-1} = \mathbf{x} \qquad \mathcal{T}\mathbf{p}\mathcal{T}^{-1} = -\mathbf{p}. \quad (1.5)$$

Where the change in sign of the momentum is interpreted as  $\mathcal{T}\frac{d}{dt}\mathcal{T}^{-1} = -\frac{d}{dt}$ , with the coordinate left unchanged. Contrary to  $\mathcal{P}$ ,  $\mathcal{T}$  cannot be a linear transformation, at least not for quantum theories.

From eq. (1.3) it is clear that  $\mathcal{P}$  preserves the canonical commutation relation,

$$[\mathbf{x}, \mathbf{p}] = i\hbar \mathbf{1},$$

given that  $\mathbf{x}$  and  $\mathbf{p}$  are canonical conjugate quantities. However, from eq. (1.5) it is clear that  $\mathcal{T}$  cannot preserve the canonical commutation relation and be a linear operator. Thus if we require that  $\mathcal{T}$  preserves the canonical commutation relation, it is clear that it must satisfy  $\mathcal{T}i\mathcal{T}^{-1} = -i$ . The transformation is thus *anti-linear*,

$$\mathcal{T}(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha^*\mathcal{T}\mathbf{x} + \beta^*\mathcal{T}\mathbf{y} \quad \text{for } \alpha, \beta \in \mathbb{C}. \quad (1.6)$$

Time-reversal thus acts as complex conjugation on scalars. In a related argument, in the Schrödinger picture of quantum mechanics the energy operator is the differential operator  $i\hbar\frac{\partial}{\partial t}$ . Thus in order to prevent the energy becoming negative and possibly un-bounded from below, i.e. no ground state, we require that  $\mathcal{T}$  preserves sign of energy [6]. From the energy operator it is thus clear that  $\mathcal{T}$  must be an anti-linear operator.

Equipped with the space and time reversal operations, we can make the following remark on the operation of space-time inversion:

*Remark 1.4.* The combined operation of spatial and temporal reflection,  $\mathcal{PT}$ , is an anti-linear transformation satisfying

$$\mathcal{PT}\mathbf{x}(\mathcal{PT})^{-1} = -\mathbf{x} \qquad \mathcal{PT}\mathbf{p}(\mathcal{PT})^{-1} = \mathbf{p}. \qquad (1.7)$$

### 1.2.1 In Classical Physics

In classical mechanics, be it Newtonian, Lagrangian or Hamiltonian mechanics, the operators of space and time reversal can be categorised into two classes: quantities that are even or odd under the reversal. Then of course if all quantities in a description are even with respect to reversal, the system is said to be reflection symmetric in time, space or both.

Typical examples of classical quantities that are even under spatial inversion are energy, power, angular momentum, electromagnetic energy density, magnetic field and magnetisation. Conversely, typical examples of quantities odd under spatial inversion are the acceleration, net force, helicity, magnetic flux, electric field and current density, polarisation and the electromagnetic vector potential [18].

Typical examples of classical quantities that are even under time-reversal are the acceleration, net force, energy, electromagnetic energy density, electric field and charge density. Whereas the velocity, angular momentum, electromagnetic vector potential, magnetic field, magnetisation, electric charge density and the power of a particle are odd under time-reversal.

Related to the  $\mathcal{T}$  being an anti-linear operation, we note that energy is even under both space and time reversal. Thus in order for quantum theory to reduce to classical mechanics, energy and the energy operator in quantum mechanics should be even under  $\mathcal{T}$ . Moreover, note that because energy is even under both spatial and temporal reflections, energy should also be even under the combined action of them. We could thus conclude that  $\mathcal{PT}$  is a symmetry of energy, but also energy density, in classical mechanics. However, this is in general not true for non-conservative systems.

### 1.2.2 In Quantum Physics

The symbol  $\mathcal{P}$  used to denote spatial reflection or inversion relates to parity transformations. The parity transformation usually defined as reversing the momentum of a particle without flipping its spin and it is a linear operator, whereas the time-reversal transformation is defined as reversing both the momentum and flipping the spin [10]. In collision processes  $\mathcal{T}$  thus interchanges the roles of incoming and outgoing particles. By assuming that an collision process is  $\mathcal{T}$ -symmetric, one effectively assumes that the probability amplitude of the forward process  $\mathcal{M}_{fi}$  is identical to the backwards process  $\mathcal{M}_{if}$ . Thus requiring  $\mathcal{T}\mathcal{M}_{fi}\mathcal{T}^{-1} = \mathcal{M}_{if}$  effectively implies *the principle of detailed balance* [6]. Moreover, as noted in section 1.1.2,  $\mathcal{T}$  appears to be a symmetry of the fundamental forces of Nature, at least at the microscopic level. However, recent discoveries in exotic superconductors [19] indicate processes that break  $\mathcal{T}$ -symmetry. At the macroscopic level, the irreversibility of thermodynamical processes through the *second law of thermodynamics* explicitly break  $\mathcal{T}$ -symmetry. The Universe is thus not  $\mathcal{T}$ -symmetric although the Laws of Nature seemingly are.

Parity on the other hand is not as perfect a symmetry. Although gravity, both Newtonian and General Relativity, electromagnetism, both Maxwell's equations and Quantum Electrodynamics, and even the strong interaction are  $\mathcal{P}$ -symmetric, weak



interactions have on numerous occasions been shown to break  $\mathcal{P}$ -symmetry. A typical example of this is found in  $\beta$ -decay due to the left-handedness of the neutrino [6, 18].

### 1.2.3 On the Mathematics

For physics in Minkowski spacetimes,  $\mathcal{P}$  and  $\mathcal{T}$  are representations of a larger symmetry group, the Poincaré group. In relativistic physics the most important group is the restricted Lorentz group  $SO^+(1, 3; \mathbb{R})$ , also known as the *proper, orthochronous Lorentz group*, which is the subgroup containing the continuous Lorentz transformations that preserves both orientation and direction in time [9, 10]. The full Lorentz group can be broken up into four disconnected subsets, depending on whether it is proper or improper and/or orthochronous. The four subsets can be related as [10],

$$\begin{array}{ccc}
 L_+^\uparrow = SO^+(1, 3) & \xleftarrow{\mathcal{P}} & L_-^\uparrow = \mathcal{P}L_+^\uparrow \\
 \uparrow \mathcal{T} & & \uparrow \mathcal{T} \\
 L_+^\downarrow = \mathcal{T}L_+^\uparrow & \xleftarrow{\mathcal{P}} & L_-^\downarrow = \mathcal{P}\mathcal{T}L_+^\uparrow
 \end{array}$$

where  $+$  denotes proper and  $\uparrow$  denotes orthochronous. It is thus clear that the full Lorentz group, can be decomposed into the semi-direct product of  $SO^+(1, 3)$  and the discrete group  $\{\mathbb{1}, \mathcal{P}, \mathcal{T}, \mathcal{P}\mathcal{T}\}$ . Then as previously noted, the restricted Lorentz group thus takes the role of the group identity in the full Lorentz group. Spatial and temporal reflections can thus be seen as a part of the relativistic symmetry, although they are not required to be symmetries as symmetry under the restricted Lorentz group is usually the requirement for relativistic theories [10].

Furthermore, since a the operations  $\mathcal{P}$ ,  $\mathcal{T}$  and  $\mathcal{P}\mathcal{T}$  are reflections, then two subsequent reflections must always result in transformations onto it self. That is  $\mathcal{P}$ ,  $\mathcal{T}$  and  $\mathcal{P}\mathcal{T}$  are all involutions, i.e.

$$\mathcal{P}^2 = \mathbb{1}, \quad \mathcal{T}^2 = \mathbb{1}, \quad (\mathcal{P}\mathcal{T})^2 = \mathbb{1}. \quad (1.8)$$

Moreover, because simultaneous reflections in space and time should be independent of the order of reflections,

$$\mathcal{P}\mathcal{T} = \mathcal{T}\mathcal{P}, \quad (1.9)$$

although it is not strictly necessary for  $\mathcal{P}\mathcal{T}$  to be an involution. It is thus clear that along with the identity,  $\mathcal{P}$ ,  $\mathcal{T}$  and  $\mathcal{P}\mathcal{T}$  each form a discrete group of two elements. Moreover, because  $\mathcal{P}$ ,  $\mathcal{T}$  and  $\mathcal{P}\mathcal{T}$  all are involutions they are generators of cyclic groups of order 2 [8]. Because the cyclic groups of order  $n$  are isomorphic to the group of integers,  $\mathbb{Z}$ , under addition mod  $n$  [8], the groups associated with the reflections can be referred to as  $\mathbb{Z}_2$  groups. Consequently  $\mathcal{P}\mathcal{T}$ -symmetry are sometimes referred to as  $\mathbb{Z}_2$ -symmetries, equivalently could also  $\mathcal{P}$  and  $\mathcal{T}$  symmetries be referred to as  $\mathbb{Z}_2$ -symmetries.



## Chapter 2

# Hermiticity

In classical physics, observables are usually represented by real-valued functions on the states of the system. In analogy, observables in quantum theory can be represented as maps from a from the space of states of the system onto the real numbers [20]. These operators are usually taken to be *Hermitian* in order to ensure that they are real-valued but as will be shown in this chapter, they are not the only operators that give real-valued maps and represent observables. However as we will see below, there exists non-Hermitian operators with real eigenspectra. Moreover, several examples of non-Hermitian systems will be given, demonstrating that non-Hermitian systems are a common phenomenon in traditional physics. Some examples of the appearance of  $\mathcal{PT}$ -symmetry in non-Hermitian systems will also be given. However, let us first introduce Hermitian operators as well as the greater class of Normal operators.

### 2.1 Hermiticity & Real Spectra

When considering the hermiticity of a system, we refer to whether the operator generating the dynamics of the system is Hermitian. Similarly to [13], let us define a Hermitian operator as:

**Definition 2.1.** Let  $\mathcal{B}(\mathcal{H})$  denote the set of bounded linear operators on a complex Hilbert space  $\mathcal{H}$  equipped with the Dirac norm  $\langle \cdot | \cdot \rangle$ . Then any operator  $A \in \mathcal{B}(\mathcal{H})$  is *Hermitian* iff

$$A = A^\dagger,$$

where  $A^\dagger$  denotes the adjoint operator.

The definition is formally equivalent to the definition,

$$\langle Ax, y \rangle = \langle x, A^*y \rangle \quad \forall x, y \in \mathcal{H}, \quad (2.1)$$

of Hermitian operators typically given in mathematical textbooks [21], where mathematicians like to use  $*$  rather than  $\dagger$  to denote the adjoint operator. Moreover, the operator  $A$  is said to be *positive definite* if  $\langle x|A|x \rangle > 0$  and *positive semi-definite* or merely *positive* if  $\langle x|A|x \rangle \geq 0$  [13]. Note that operators satisfying definition 2.1 are often referred to as *self-adjoint* or *symmetric*, although usually only in mathematics.

In both classical and quantum mechanics, a system is often referred to as Hermitian if the Hamiltonian  $H$  of the system is Hermitian. Although we often refer to the Hamiltonian

when addressing the hermiticity of a system, it could equally well refer to other operators as long as they generate the dynamics in the system. Other examples are the Liouville superoperator in quantum mechanics but also any other operator satisfy the von-Neumann equation, both of which will be addressed briefly later in this chapter.

From eq. (2.1) it is immediately clear that Hermitian operators have a real set of eigenvalues. More generally, the eigenspectrum of an operator can be defined as [13]:

**Definition 2.2.** For a bounded linear operator  $A \in \mathcal{B}(\mathcal{H})$ , the *spectrum*  $\sigma(A)$  is the set of complex numbers  $\lambda$  for which  $A - \lambda \mathbb{1}$  has no linear bounded inverse where  $\mathbb{1} \in \mathcal{B}(\mathcal{H})$  denotes the identity. And every number  $\mu \in \sigma(A)$  is an *eigenvalue* of  $A$ . Every non-zero vector  $|\psi\rangle \in \mathcal{H}$  for which

$$(A - \mu \mathbb{1}) |\psi\rangle = 0 \text{ for } \mu \in \sigma(A),$$

is an *eigenvector* of  $A$  associated with the eigenvalue  $\mu$ .

Unless otherwise stated, the operators discussed in this thesis will be bounded linear operators, thus definition 2.2 holds not only for Hermitian operators but quite generally.

### 2.1.1 Normal Operators

Hermitian operators belong to a larger class of operators of similar properties known as *normal operators*. Following [13], a normal operator can be defined as

**Definition 2.3.** A bounded linear operator  $A \in \mathcal{B}(\mathcal{H})$  is said to be normal iff

$$AA^\dagger = A^\dagger A.$$

From the definition it is straightforward to verify that the class of normal operators include in addition to Hermitian operators;

- *Unitary* operators:  $UU^\dagger = U^\dagger U = \mathbb{1}$ ,
- *Anti-Hermitian* or *Skew-Hermitian* operators:  $A^\dagger = -A$ ,
- *Positive* operators  $A = BB^\dagger$ ,

for  $U, A, B \in \mathcal{B}(\mathcal{H})$ . The positive operators are of course only a subclass of Hermitian operators. More interestingly are the properties of the spectrum of normal operators.

**Theorem 2.4.** *The spectrum of a compact normal operator  $A \in \mathcal{B}(\mathcal{H})$  lies on the real axis if  $A$  is Hermitian, on the unit circle if  $A$  is unitary, on the imaginary axis if  $A$  is anti-Hermitian and on the real positive axis if  $A$  is positive.*

The theorem is equivalent to [13, Theorem X.4.2].

Most operators encountered in quantum mechanics are thus normal operators, and most of them are either Hermitian or unitary. From a mathematical perspective this is very convenient as normal operators satisfy a range of theorems and identities, amongst which the *spectral theorem* [13]. Calculations with normal operators is thus much simpler. In particular the following theorem follows from the spectral theorem or the eigenprojections of normal operators [22]:

**Theorem 2.5.** *If  $A \in \mathcal{B}(\mathcal{H})$  is a compact normal operator and  $|\psi\rangle \in \mathcal{H}$  is an eigenvector of  $A$  associated with the eigenvalue  $\mu \in \sigma(A)$ , i.e.  $A|\psi\rangle = \mu|\psi\rangle$ . Then  $\langle\psi| = |\psi\rangle^\dagger$  is an eigenvector for  $\mu^*$ . If  $|\phi\rangle \in \mathcal{H}$  is an eigenvector associated with an eigenvalue  $\mu' \in \sigma(A)$  then*

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle = 0 \quad \text{if } \mu \neq \mu'.$$

The eigenvector  $\langle\psi|$  associated with  $\mu^*$  is typically known as the left eigenvector as it satisfies the left eigenvector equation

$$\langle\psi|A = \langle\psi|\mu^*.$$

Then similarly  $|\psi\rangle$  is known as a right eigenvector of  $A$ . However, for non-Normal operators the left and right eigenvectors need not be the same, this will be seen in more detail in chapter 4.

### 2.1.2 The Bender-Boettcher Hamiltonian

In many cases, by theorem 2.4, requiring that an operator is Hermitian has been taken as synonymous with having a real spectrum. However, this is not always the case. Amongst the first realisations that non-Hermitian Hamiltonians might have real eigenvalues appeared during investigations into cubic Hamiltonians on the form

$$H = \hat{p}^2 + \hat{x}^2 + i\hat{x}^3, \quad (2.2)$$

or related forms [1, 23]. Some of the properties of Hamiltonians of this form, including that that its spectrum is real in certain regions of parameter space, was first realised during early studies of Reggeon field theory in the late 1970-ties and early 1980-ties [24–26]. Independently Caliceti *et al.* observed that the spectrum is real during studies of odd anharmonic oscillators that give Hamiltonian relatable to eq. (2.2) [23, 27]. Later, Bessis and Zinn-Justin also observed that the spectrum of a Hamiltonian operator on the form of eq. (2.2) appears to have a real and positive spectrum, an observation originating from the study of Lee-Yang singularities using methods from the realm of renormalisation[1].

Inspired by these initial observations that such non-Hermitian Hamiltonians appeared to have real spectra, Bender & Boettcher [1] launched a more extensive investigation into the spectra of operators on the form

$$H = p^2 - (ix)^{2m}. \quad (2.3)$$

Due to their extensive investigation, Hamiltonians on the form of eq. (2.3) are often referred to as Bender-Boettcher Hamiltonians.

Through a numerical study, Bender & Boettcher arrived at the conjecture that the spectrum of eq. (2.3) is real and bounded from below for  $m \geq 1$  [1]. In particular, the numerical study by Bender & Boettcher found the eigenspectrum of eq. (2.3) to be as shown in fig. 2.1. The Bender & Boettcher full conjecture can be summarised as [1]:

**Conjecture 2.6.** *The eigenvalues  $E_n$  of the Bender-Boettcher Hamiltonian, eq. (2.3) are*

- all real and positive for  $m \geq 1$ ,
- real and positive (finite number of eigenvalues) or form complex conjugate pairs (infinite number of eigenvalues) for  $\frac{1}{2} < m < 1$ ,
- all in complex conjugate pairs for  $m \leq \frac{1}{2}$ .

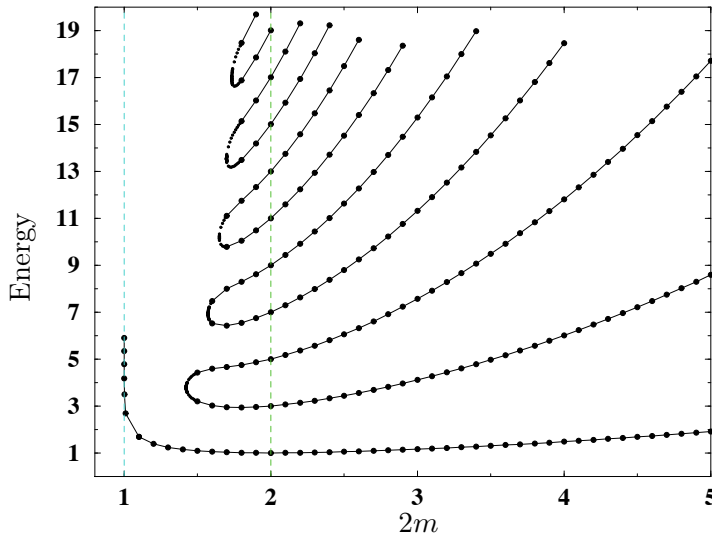


Figure 2.1: The eigenvalues of the Bender-Boettcher Hamiltonian as a function of the parameter  $m$ . Adapted from [23] with permission from Taylor & Francis.

From the numerical analysis by Bender & Boettcher it seems that the spectrum of eq. (2.3) has some quite peculiar properties: the eigenvalues in the spectrum eq. (2.3) seems to be either real or form complex conjugate pairs, a property that has been attributed to the  $\mathcal{PT}$ -symmetry [1]. The connection between spectra of this type and  $\mathcal{PT}$ -symmetry will be the topic of section 4.2. Although [1] was an important paper, a mathematical proof for conjecture 2.6 was not realised until later [28, 29].

It turns out that the so-called Bender-Boettcher Hamiltonian, eq. (2.3), is a part of a larger class of Hamiltonians. Dorey *et al.* [29] generalised eqs. (2.2) and (2.3) to

$$H = p^2 + (ix)^{2m} \pm \alpha(ix)^{m-1} + \frac{l(l+1)}{x^2}, \quad (2.4)$$

where generally  $m, \alpha, l \in \mathbb{R}$ . For Hamiltonians of these types, Dorey *et al.* [28, 29] proved the following theorem:

**Theorem 2.7.** *The eigenspectrum of the Hamiltonians given by eq. (2.3) is entirely real and positive if  $m > 1$ . The eigenspectrum of the Hamiltonians given by eq. (2.4) is entirely real if  $m > 1$  and  $\alpha < m + 1 + |2l + 1|$  and positive if  $\alpha < m + 1 - |2l + 1|$ .*

The properties of spectra such Hamiltonians thus shows that manifestly non-Hermitian operators admits entirely real spectra. Further studies of the spectra of Hamiltonians on the form of eq. (2.4) beyond the condition of a real spectrum has been performed, strengthening conjecture 2.6 [30–32]. This particular observation, Bender has said to inspired his initial investigations into  $\mathcal{PT}$ -symmetry [23], and has inadvertently kick-started the research into the field of non-Hermitian physics.

## 2.2 Non-Hermiticity in Quantum Mechanics

Although the condition of Hermiticity has been dominant in investigating quantum systems since the original formulations of quantum theory, at least since the self-consistent

formulations of quantum mechanics by David Hilbert, Paul A. M. Dirac [33] and John von Neumann [34] by the early 1930-ties. However, considerations of non-Hermiticity are not new. In particular Pauli investigates the extension of Hermitian operators using indefinite metrics in Hilbert spaces as early as the 1940-ties [35]. This extension it turns out is similar to the extension that will be presented in section 4.3, but first let us consider some examples of Non-Hermiticity in quantum mechanics.

### 2.2.1 Complex Potentials

To most physicist systems with non-Hermitian Hamiltonians are not that unfamiliar. Many complicated phenomena in quantum physics are only described by approximations, or more often these approximations are first attempts in describing the phenomena. Such phenomena are typically described using an effective Hamiltonian. However, as the dynamics are only approximate we admit that possibly significant degrees of freedom has been omitted. As a result, the dynamics in such descriptions does often not preserve probabilities, hence the dynamics are *non-unitary*. For the sake of clarity:

*Remark 2.8.* Systems in which probabilities are conserved are referred to as unitary and an evolution that conserves probabilities is referred to as an unitary evolution. Within Hermitian quantum mechanics unitary evolution is taken as synonymous with conservation of the Dirac norm of states.

A typical example of such non-unitary dynamics is decay processes [36]. If one considers the decay of a nuclear particle. Without a full treatment in an exact theory, which for particle decay would be the *Standard Model of Particle Physics*, the description will be only approximate. The decay can thus be treated by an effective Hamiltonian on the form

$$H_{\text{eff}}(x) = \frac{p^2}{2m} + V(x) + i\Gamma(x) \quad (2.5)$$

which has a imaginary potential  $i\Gamma$ . The imaginary potential thus makes these Hamiltonians manifestly non-Hermitian. Effective Hamiltonians can typically be found using the *Feshbach projection approach*, first studied by Feshbach [37, 38] for nuclear nuclear reactions<sup>1</sup> but is also applicable to a larger range of quantum systems including open quantum systems [39]. Moreover, in only considering how the particle decays, the probability of finding the particle decreases in time. However, we do not expect the total probability of finding  $a$  particle to decrease if subject to a full treatment, as the probability of finding the decay products will increase although the effective description is unable to describe it. The non-unitarity of such processes are not thought to be a physical property, rather than an effect of the inability to describe the process in full. More generally, complex potentials in the Hamiltonians can be used to describe problems in which quantum systems which are associated with inelastic scattering [37], classical statistical mechanics or diffusion processes [40].

### 2.2.2 Liouvillian Dynamics

Another familiar example of non-Hermitian dynamics in quantum systems are found in the description open quantum systems – quantum systems coupled to an environment.

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<sup>1</sup>Feshbach introduced complex potentials as early as 1958 in studying a *complex potential model for pure elastic scattering* and *inelastic scattering* processes [37].

Many open quantum systems can be described by the *Lindblad master equation*, typically systems where the coupling to the environment is weak or singular [41]. Following [42] let us state the Lindblad master equation in its most general form, also known as the *Gorini–Kossakowski–Sudarshan–Lindblad master equation*:

**Definition 2.9.** Let  $\rho \in \mathcal{B}(\mathcal{H})$  be the *density operator* of a system described by the Hermitian Hamiltonian  $H$ , the *Gorini–Kossakowski–Sudarshan–Lindblad master equation* of the system is then

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \sum_{i,j} h_{i,j} \left( A_i \rho A_j^\dagger - \frac{1}{2} \{A_j^\dagger A_i, \rho\} \right). \quad (2.6)$$

Where  $A_i, A_j \in \mathcal{B}(\mathcal{H})$  and  $h$  is a positive semi-definite matrix

What is usually referred to as the Lindblad equation is the diagonal form of definition 2.9,

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \sum_i \gamma_i \left( L_i \rho L_i^\dagger - \frac{1}{2} \{L_i^\dagger L_i, \rho\} \right), \quad (2.7)$$

obtained by utilising that  $h$  is diagonalisable due to being positive semi-definite [42]. The  $L_i \in \mathcal{B}(\mathcal{H})$  are thus jump operators that describe the dissipative or non-unitary behaviour of the system and are often referred to as the Lindblad operators. Whereas the Hamiltonian,  $H$ , describes the unitary part of the dynamics as eqs. (2.6) and (2.7) reduce to the *von Neumann equation*,

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho], \quad (2.8)$$

if the jump operators are unital or decouple ( $\gamma_i = 0$ ). Moreover, the dynamics of the density operator can be further generalised, see [42, 43] for a details. Similarly to [42, 43], let us define the generalised Schrödinger type equation for the time-evolution of the density operator.

**Definition 2.10.** Let  $|\rho\rangle\rangle$  be a vector in a complex *Fock-Liouville space*  $\mathcal{F}$  and let  $\mathcal{B}_{\text{FL}}(\mathcal{F})$  denote the set of bounded linear operators on  $\mathcal{F}$ . For a *superoperator*  $\mathcal{L} \in \mathcal{B}_{\text{FL}}(\mathcal{F})$ , the time-evolution of  $|\rho\rangle\rangle$  is given by

$$i\hbar \frac{d}{dt} |\rho(t)\rangle\rangle = \mathcal{L} |\rho(t)\rangle\rangle. \quad (2.9)$$

Represented as Schrödinger type equation, eq. (2.9), the superoperator  $\mathcal{L}$ , often called a *Liouville superoperator*, takes on the same role as the Hamiltonian in the ordinary Schrödinger equation. Moreover, note that some care should be taken when constructing the Fock-Liouville space vector  $|\rho\rangle\rangle$ . Typically,  $|\rho\rangle\rangle$  is for finite dimensional systems constructed by forming an ordered vector of the elements of the density matrix  $\rho$  [42, 43]. However, the matrix representation of  $\mathcal{L}$  is thus dependent of the choice of ordering in  $|\rho\rangle\rangle$ .

Furthermore, the superoperator is an operator acting on operators on a Hilbert space. Thus if the dynamics of a system is governed by a Hermitian Hamiltonian,  $H$ , the associated Liouville superoperator is

$$\mathcal{L}\rho \equiv [H, \rho]. \quad (2.10)$$



Thus similarly the *Lindblad superoperator* or *Lindbladian* is

$$\mathcal{L}\rho \equiv [H, \rho] + i\hbar \sum_i \gamma_i \left( L_i \rho L_i^\dagger - \frac{1}{2} \{ L_i^\dagger L_i, \rho \} \right) \quad (2.11)$$

by eq. (2.7).

Note that although the superoperator of eq. (2.10) is Hermitian, the superoperators usually encountered are not [43]. That is of course a by product of the construction of definition 2.10 is typically unnecessarily complicated for constructions involving Hermitian Hamiltonians as it readily reduces to the von Neumann equation, eq. (2.8). The superoperator associated with the Lindblad equation, eq. (2.11), is a typical example of non-Hermitian superoperators.

The above examples of non-Hermiticity show that the phenomenon is not actually new, and is in some cases well-studied. However, there is a class of non-Hermitian quantum systems that up til a few years ago was not as much studied.

### 2.2.3 $\mathcal{PT}$ -Symmetry

After the demonstration of non-Hermitian Hamiltonians with real spectra and the link to  $\mathcal{PT}$ -symmetry by Bender & Boettcher [1], an interest in studying such systems gradually spiked. Apart from Hamiltonians of the types described by eqs. (2.3) and (2.4), the first systems investigated were systems with  $\mathcal{PT}$ -symmetric periodic potentials [44–46]. These potentials can appear in condensed matter physics, and can in its simplest form be given by Hamiltonians of the type

$$H = p^2 - iQ \sin^{2n+1}(x) \text{ for } n \in \mathbb{N}, Q \in \mathbb{R}. \quad (2.12)$$

These Hamiltonians can be used to describe the optical properties of complex crystal lattices and are sometimes referred to as complex diffraction gratings [36]. Although these Hamiltonians are non-Hermitian, they have been shown to exhibit real spectra [44]. Experimentally these systems turned out to be more elusive than anticipated by the early papers such as [44, 45]. However, these systems have in fact been experimentally realised [47]. Later,  $\mathcal{PT}$ -symmetry has also been studied in optics, [48], micro-ring lasers, [49, 50], and diffusive transport, [51], as well. See [52] for a review of non-Hermiticity and  $\mathcal{PT}$ -symmetry in optical systems.

Although significant theoretical endeavours into  $\mathcal{PT}$ -symmetric systems were made, an observation of a fully quantum-physical phenomena displaying  $\mathcal{PT}$  symmetry proved elusive and did not occur until 2019 [53]. Although there were several earlier experimental realisations of  $\mathcal{PT}$ -symmetric systems they were interactions with classical potentials, not interactions between quantum systems. Klauck *et al.* experimentally observed a quantum interference pattern predicted by  $\mathcal{PT}$ -symmetric quantum mechanics [53]. This was obtained by studying a system consisting of two photonic waveguides coupled to a reservoir, inducing an overall energy loss on the system. However, due to an asymmetry in the coupling of the waveguides to the reservoir the Hamiltonian is not Hermitian, but in fact  $\mathcal{PT}$ -symmetric. Through a theoretical calculation a characteristically non-Hermitian behaviour for the waveguide excitations were obtained, and subsequently experimentally observed. The apparent difficulty in realising these systems can be related to the interplay between gain and loss in  $\mathcal{PT}$ -symmetric systems not being well understood until 2018 [2]. The discussion of the interplay between gain and loss as well as the result of Scheel & Szameit [2] will be revisited in section 5.1.

### 2.3 Non-Hermiticity in Classical Mechanics

In classical mechanics the *Laplace operator*  $\nabla^2$  is an important operator appearing in the description of a variety of physical phenomena. Notable examples include diffusion process (diffusion equation), wave dynamics (wave equation) and the Navier-Stokes equation. The eigenvalue problem of the Laplace operator is often known as the *Helmholtz equation*, given by the linear partial differential equation

$$\nabla^2 u = -k^2 u. \quad (2.13)$$

Here  $k^2$  denotes the eigenvalue and  $u$  the eigenfunction of the Laplace operator. The Helmholtz equation appears naturally from more complex equations of motion, typically in using separation of variables. In conventional dynamics  $k$  typically known as the wave number, is a real constant. However, in general it may take a more complicated form.

#### 2.3.1 Optics

Amongst the first investigation of non-Hermitian systems after the seminal paper by Bender & Boettcher appeared in optical systems. Inspired by [1] a number of papers has been published on non-Hermitian optical systems exhibiting  $\mathcal{PT}$ -symmetry [54–57]. These preliminary investigations were largely inspired by the study of periodic  $\mathcal{PT}$ -symmetric potentials [44–46], where [54–56] further studied the theoretical implications complex periodic lattices in optics. Moreover, [57] experimentally demonstrated the breaking of  $\mathcal{PT}$ -symmetry in a complex optical potential. In particular Guo *et al.* demonstrated the symmetry breaking by considering an optical potential originating from a complex refractive index distribution,  $n(x) = n_0 + n_R(x) + in_I(x)$  where  $n_0, n_R, n_I \in \mathbb{R}$  [57]. Then in assuming  $n_0 \gg n_R, n_I$ , the wave equation for the light can be written as the paraxial approximation of the Helmholtz equation also known as the paraxial equation of diffraction [56]. The equation of propagation along the  $z$ -direction thus takes the form

$$i \frac{\partial}{\partial z} u(x, z) = \left( \frac{\lambda_0}{4\pi n_0} \frac{\partial^2}{\partial x^2} + \frac{2\pi}{\lambda_0} [n_R(x) + in_I(x)] \right) u(x, z), \quad (2.14)$$

where  $\lambda_0$  is the wavelength of the light in vacuum and the full light wave is  $E(x, z) = u(x, z) \exp\{i(\omega t - 2\pi \frac{z}{\lambda_0})\}$  [57]. Moreover, eq. (2.14) is algebraically equivalent to the Schrödinger equation such that the right-hand side can be interpreted as the Hamiltonian operator

$$H = \frac{1}{2k} \frac{\partial^2}{\partial x^2} + V(x), \quad (2.15)$$

where  $V(x) = \frac{2\pi}{\lambda_0} [n_R(x) + in_I(x)]$ . As the potential  $V(x)$  is complex it is clear that the Hamiltonian, eq. (2.15), is non-Hermitian. Although slightly more involved, the  $\mathcal{PT}$ -symmetry of eq. (2.15) is obtained if  $n_R(x)$  is an even function in  $x$  and  $n_I(x)$  is odd [56].

Later, several other non-Hermitian phenomena in optics has also been considered and experimentally confirmed. These include unidirectional invisibility, negative refraction, non-trivial band topology and single mode lasers [39]. Other interesting observations of non-Hermitian systems in optics has been found in studying *exceptional points*, see [58] for a recent review. The general notion of exceptional points will be addressed in section 5.2.

### 2.3.2 Non-Equilibrium Statistical Mechanics

Many physical phenomena can be described by the regular formalism of equilibrium statistical mechanics. However, many systems in biological physics and in particular active systems are not in statistical, nor thermodynamical equilibrium. One of the prominent methods for describing non-equilibrium statistical mechanics is using stochastic Markov processes. If  $\mathbf{p}$  is a vector describing the probability distribution of the a finite number of states, then the *Markov master equation* for the system is

$$\frac{d\mathbf{p}}{dt} = W\mathbf{p}, \quad (2.16)$$

where  $W$  is the transition matrix satisfying the conservation of probability condition  $\sum_i W_{i,j} = 0$  [59]. As eq. (2.16) is analogous to definition 2.10, the transition matrix  $W$  is sometimes referred to as a Liouvillian [39]. Note that in general,  $W$  is non-Hermitian, in fact it is only Hermitian if  $W_{i,j} = W_{j,i}$  for real transitions  $W$ . That is,  $W$  is Hermitian only in the transitions from a state  $i$  to a state  $j$  and from a state  $j$  to a state  $i$  are the same, i.e. the transitions between states are reciprocal, which do not generally appear in non-equilibrium dynamics. Moreover, if  $W$  is ergodic then the existence of a steady-state solution,  $W\mathbf{p}_{ss} = 0$ , is ensured by the Perron-Frobenius theorem [39]. This ensures that such systems eventually converges to a solution. A Markovian type master equation for a class of quantum systems will be derived and discussed in chapter 6.

Closely related to the Markovian processes are Langevin processes, combining both stochastic and deterministic forces [60]. If  $p(\mathbf{x}, t)$  is the probability density, where both space  $\mathbf{x}$  and time  $t$  is assumed to be continuous, then it satisfies the *Fokker-Planck equation* [39, 61]

$$\begin{aligned} \frac{\partial}{\partial t} p(\mathbf{x}, t) &= \left( -\nabla \cdot \boldsymbol{\mu}(\mathbf{x}, t) + \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} D_{i,j}(\mathbf{x}, t) \right) p(\mathbf{x}, t) \\ &= \mathcal{L} p(\mathbf{x}, t). \end{aligned} \quad (2.17)$$

Where the vector  $\boldsymbol{\mu}$  denotes the probability drift and  $D$  is a tensor describing the probability diffusion [61]. Then as the diffusion term usually is Hermitian whereas the drift usually is anti-Hermitian, the Liouvillian  $\mathcal{L}$  is generally non-Hermitian [39].

### 2.3.3 Hydrodynamics

The dynamics of systems with a large number of particles are often described by hydrodynamical equations of motion involving only a few classical fields, especially when the relevant dynamics appear at much longer time scales than the microscopic dynamics of the system [39]. If the collection of particles is subject to gain or loss, that could be a non-zero flux of energy, particles, etc. in or out of the system, then the hydrodynamical equations are necessarily non-conservative with respect to one or more metrics. These equations can thus be said to be non-Hermitian.

In acoustics, the study of the propagation of collective longitudinal waves in fluids and solid states, a linear wave equation,

$$\frac{\partial^2 p}{\partial t^2} = \frac{\kappa}{\rho} \nabla^2 p, \quad (2.18)$$

of the acoustic modes can be obtained [39]. Where  $p$  denotes the acoustic pressure,  $\rho$  the mass density and  $\kappa$  the compressional stiffness or bulk modulus. From eq. (2.18) we see that if it can be solved by separation of variables, eq. (2.18) reduces to the Helmholtz equation, eq. (2.13). Although,  $\rho$  and  $\kappa$  are restricted to being positive in conventional solid-state materials, one or both can be negative in *meta-materials* [39] thus inducing complex wave numbers. Moreover, it has been proposed and experimentally realised that through proper manipulation of meta-materials using gain and loss,  $\rho$  and  $\kappa$  can have imaginary components ensuring manifestly non-Hermitian dynamics [62].

Related to non-Hermitian acoustics is the study of *active matter*. The field of active matter studies the dynamics of a large number of self-propelled constituents, that is “fluids” subject to non-zero spontaneous flows rather than externally driven flows [39]. The study of active matter aims to describe the dynamics of living matter, for example animal flocks, molecular motors, microorganisms and other biological systems [63]. The macroscopic dynamics of active matter can be described by the *Toner-Tu equations* [63] which can be linearised around the steady-state solutions of the active matter density field and local mean velocity. Assuming the steady-state mean velocity is small compared to the sound velocity in the matter, the dynamics can be described by [64]:

$$i\frac{\partial \mathbf{j}}{\partial t} = H_{\text{eff}} \mathbf{j}, \quad H_{\text{eff}} = H_0 + iH_D + H_\lambda. \quad (2.19)$$

Where  $\mathbf{j}$  is a vector current and the effective Hamiltonian  $H_{\text{eff}}$  consists of three parts, a Hermitian matrix  $H_0$  similar to a free Hamiltonian, an anti-Hermitian matrix  $iH_D$  incorporating the diffusive motion and  $H_\lambda$ , an intrinsically non-Hermitian matrix [39].

From the above examples of non-hermiticity in classical systems it is clear that similarly to the examples from quantum mechanics, the non-hermiticity typically appears in the Liouvillian operators or effective Hamiltonians. For a more thorough review of non-Hermitian phenomena in classical physics see [39, Section 3]

## Chapter 3

# Postulates of Quantum Mechanics

In order for a theory of Nature to be a good theory there are several criteria it needs to fulfil; It needs to be able to reproduce known results, but more importantly make predictions for formerly unknown results or phenomena. In order to do so theories require a sound theoretical foundation, preferably from a minimal set of assumptions. All the successful theories on Nature has such underlying assumptions. Typical examples are of course the theories of Special and General Relativity, but also Newtonian mechanics, quantum mechanics, etc. In mathematics, the minimal set of assumptions needed to derive all other results are typically known as *axioms*. In physics, this set of assumptions are often referred to as *postulates*, of which notable examples are Einstein's postulates and the postulates of quantum mechanics.

Although the postulates of quantum mechanics, first formulated by P. A. M. Dirac and John von Neumann [33, 34, 1st. Eds.] in the early 1930-ties are usually represented in a quite abstract and mathematical manner, their motivation is physical [33, 65]. This is somewhat contrary to the postulates of Relativity which are stated through more physical invariance principles [66]. Efforts has been made to formulate the postulates of quantum mechanics more directly from physical requirements, see [20, 67, 68]. Among these requirements we find the usual criteria of observables being represented by operators with real spectra. However, as seen in chapter 2 the usual condition of operators being Hermitian is not a necessary condition to fulfil the criteria for observables.

In this chapter, a set of generalised postulates for quantum mechanics will be reviewed with the purpose of establishing the foundations for a  $\mathcal{PT}$ -symmetric formulation of quantum mechanics, chapter 4. In order to properly review the postulates of quantum mechanics generalised to non-Hermitian systems, let us first briefly review the ordinary postulates of quantum mechanics. The postulates will be presented and compared, but otherwise without reference to how to use them for calculations or their origin. Both the following section could warrant entire chapters, if not books of their own, if explained in detail. See for example [33, 69] for books on Hermitian quantum mechanics and [40, 70] on non-Hermitian quantum mechanics

### 3.1 Hermitian Quantum Mechanics

In the ordinary Hermitian quantum mechanics there are various ways of defining a quantum theory, but common to them all is defining a set of axioms or postulates. The first complete mathematical formalisation is known as the Dirac-von Neumann postulates

[33, 34]. Later, alternative formulations has been made such as the path integral [71], phase-space [72], density matrix [73], and  $C^*$ -algebra [74] formalisms. These formulations are equivalent in the sense that they reproduce the same fundamental physics, but they are useful in different contexts.

Following the example of Deutsch, we may construct a quantum theory based on a set of six postulates [20, 75]:

**Hermitian Postulate 1.** Any state of a quantum system at a time,  $t$ , can be represented state vector  $|\psi\rangle$  living in a complex Hilbert space  $\mathcal{H}$ , together with a set of Hermitian operators,  $\hat{O}$ , acting on  $\mathcal{H}$ .

Hermitian postulate 1 ensures that the vectors  $|\psi\rangle$  can represent the quantum system of interest. This is ensured by endowing an additional structure upon vector space, whereupon requiring the vector space to be a Hilbert space. From a practical standpoint, the Hilbert space is defined by what we would require of states representing reality. Furthermore, by postulating the operators are Hermitian ensures that the expectation values of any operator will be purely real and bounded [14]. Moreover, the set of operators on  $\mathcal{H}$  are usually taken to be linear operators. The set of bounded linear operators on  $\mathcal{H}$  will be denoted  $\mathcal{B}(\mathcal{H})$ .

Moreover, the fact that the world appears to be separable into subsystems gives additional structure to the Hilbert space structure of the world:

**Hermitian Postulate 2.** The world may be divided into a set of subsystems, each with a Hilbert space  $\mathcal{H}_i$  of its own. The state space of the world  $\mathcal{H}$  is then a direct product  $\bigotimes_i \mathcal{H}_i$  of the Hilbert spaces of the subsystems.

By postulating that unrelated systems can be separated, the postulates allows for them to be treated independently. Hermitian postulate 2, incorporates the idea that the full evolution of the world can be found by considering the collection of unrelated systems. Moreover, note that the direct product  $\bigotimes$  is sometimes referred to as a *tensor* or *Kronecker product* of Hilbert spaces, or more generally of Banach spaces [21].

Furthermore, in order for the theory to be able to represent the physical world, it needs to relate the theory to observation. The quantities of the theory that relates to physical observations are known as *observables*. Because the results of measurements of the world in general yields real numbers, the theory should incorporate this behaviour. The simplest manner in achieving this is given in Hermitian postulate 3.

**Hermitian Postulate 3.** In a quantum system, the observables  $\mathcal{O}$ , i.e. measurable quantities, are described by a set of bounded self-adjoint operators  $\hat{O}$  in the associated Hilbert space  $\mathcal{H}$ .

Hermitian postulate 3 can alternatively be formulated as: *Observables  $\mathcal{O}$  corresponds to Hermitian operators  $\hat{O}$  on  $\mathcal{H}$ .* That is because the inner product assigned to the Hilbert space, is the usual Hilbert-Schmidt norm, self-adjoint with respect to that particular inner product is equivalent with the operator being Hermitian. By formulating Hermitian postulate 3 in this manner the notion of a Hermitian theory of Quantum Mechanics becomes more apparent, as an effective description of a quantum theory can be obtained from the Hamiltonian  $H$  of a system. That is the Hamiltonian is associated with the energy of the system, such that  $H$  is an observable of the quantum theory and is thus Hermitian.

Furthermore, a consistent way of assigning numbers to the operators  $\hat{\mathcal{O}}$  is needed in order for the observables  $\mathcal{O}$  to be constructed.

**Hermitian Postulate 4.** If the state  $|\psi\rangle$  is an eigenvector of an operator  $\hat{\mathcal{O}}$  associated with an observable with an eigenvalue  $\lambda$ . Then the eigenvalue is given as  $\lambda = \langle\psi|\hat{\mathcal{O}}|\psi\rangle$ . If a perfect measurement of the observable were made, the measurement would yield  $\lambda$ .

Thus as the eigenvalues of  $\hat{\mathcal{O}}$  dictates the value of  $\mathcal{O}$ , then the eigenvalues must be real numbers. This is ensured by Hermitian postulate 3 as bounded self-adjoint operators have a purely real spectrum [13], as briefly discussed in section 2.1.1. Furthermore, we note that if the state  $|\Psi\rangle$  of a system can be represented by a weighted sum of eigenvectors  $|\psi_i\rangle$  of  $\hat{\mathcal{O}}$ , that is  $|\Psi\rangle = \sum_i c_i |\psi_i\rangle$  where the weights  $c_i \in \mathbb{C}$  satisfy  $\sum_i |c_i|^2 = 1$ . Then the value of  $\mathcal{O}$  is given by a weighted sum of the eigenvalues  $\lambda_i$  of  $\hat{\mathcal{O}}$ :

$$\mathcal{O} = \langle\Psi|\hat{\mathcal{O}}|\Psi\rangle = \sum_i |c_i|^2 \langle\psi_i|\hat{\mathcal{O}}|\psi_i\rangle = \sum_i |c_i|^2 \lambda_i$$

For consistency, let us point out that the inner product  $\langle\cdot|\cdot\rangle$  denotes the regular Hilbert space inner product, sometimes referred to as a Hilbert-Schmidt inner product or a Dirac norm.

Moreover, in order to describe dynamics not only statics, states at one time must be relatable to states at another time.

**Hermitian Postulate 5.** The evolution of the state vector in time  $t$ ,  $|\psi(t)\rangle \in \mathcal{H}$  is given by the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle, \quad (3.1)$$

where the  $\hat{H}$  denotes the Hamiltonian operator which is generally time-dependent.

From Hermitian postulate 5 it follows that the Hamiltonian operator is both the generator of time-translations. However, from Hermitian postulate 1  $\hat{H} \in \mathcal{B}(\mathcal{H})$  it thus satisfies Hermitian postulate 3 and is therefore associated with an observable. The Hamiltonian is thus both the generator of time-translations and an observable. Moreover, if the state  $|\psi\rangle$  is invariant under time-translations, eq. (3.1) implies the time-independent Schrödinger equation. Thus because invariance under time-translations implies that the eigenvalue of  $\hat{H}$  is conserved in time, which through Noether's theorem identifies  $\hat{H}$  as the energy operator. Thus in Hermitian quantum mechanics,  $\hat{H}$  takes the both the roles of generator of time-translations and energy operator. Hence the name Hamiltonian, in reference to the Hamiltonian in classical mechanics.

Note that the appearance of the Schrödinger equation as the equation describing the time-evolution is largely due to the choice of presenting a set of postulates similar to that of Dirac [33] and von Neumann [34]. Other mathematically equivalent equations could be given in the alternate formulations, such as the von Neumann equation for the density matrix formulation [73]. This would also require some or all of the other postulates to be reformulated. Moreover, the postulates could be formulated in a more general manner without assigning a special role to the Hamiltonian and time, see [20].

## 3.2 Non-Hermitian Quantum Mechanics

Contrary to Hermitian quantum mechanics, the Hilbert space inner products of non-Hermitian systems is in the simplest manner dependent on the Hamiltonian or the chosen basis [76]. An example of this is the  $\mathcal{PT}$ -symmetric quantum theory described by Bender [23] in which the inner product, the so-called  $\mathcal{CPT}$ -inner product, depends on an operator  $\mathcal{C}$  constructed from the eigenfunctions of the Hamiltonian. Ordinary Hermitian quantum mechanics on the other hand, that is in the Dirac-von Neumann formalism, is dependent on neither, as seen from the Hermitian postulates 1 to 5. The goal for a non-Hermitian quantum mechanics is thus a mathematical formalism in which the Hilbert space inner product of a non-Hermitian system is neither Hamiltonian- nor basis-dependent and that reduces to the Dirac-von Neumann formalism in the case of a Hermitian system.

Similarly to the postulates of Hermitian quantum mechanics, Hermitian postulates 1 to 5 described above, a set of postulates generating non-Hermitian quantum mechanics may be formulated. Following the work of Chen [76], based on the traditional Dirac-von Neumann formalism [33, 34], a set of mathematical postulates can be given:

**Non-Hermitian Postulate 1.** Associated with a non-Hermitian quantum system there is a complex separable Hilbert space  $\mathcal{H}$ , the state space. For any given time  $t$  the system is described by a non-zero state vector  $|\psi\rangle \in \mathcal{H}$ .

We recognise that this postulate is essentially the same as the first Dirac-von Neumann postulate, Hermitian postulate 1. From the discussion on examples of non-Hermitian systems in chapter 2 this should not be surprising as the non-Hermitian systems in many cases can be seen as extensions of ordinary quantum systems. The motivation for choosing the state space to be Hilbert spaces remains unchanged from that of Hermitian postulate 1.

Moreover, it is still assumed that the world may be divided into subsystems, some of which may be treated as independent. The postulate of composite systems, or to some extent separability, of non-Hermitian systems can be stated as:

**Non-Hermitian Postulate 2.** The world may be divided into a set of subsystems, each with a Hilbert space  $\mathcal{H}_i$  associated with each component system. The Hilbert space  $\mathcal{H}$  associated with the composite non-Hermitian system is then a direct product  $\bigotimes_i \mathcal{H}_i$  of the Hilbert spaces of the subsystems.

Also this postulate takes essentially the same form as its regular Dirac-von Neumann counterpart, Hermitian postulate 2. From an argumentative point, the notion of Hermiticity of the operators associated with a system does not appear to be connected to the separability of the system into composite system. At least not in general as the property of Hermiticity is a property of operators with respect to inner products, not vice versa. The parts of the non-Hermitian postulates concerned with Hilbert spaces should thus be unaffected by the Hermiticity. Note however, that non-Hermitian systems might allow for connections prevented by Hermiticity which prevent the separation of subsystem. Although, in general, truly unconnected systems are postulated to form component systems, which can be described in a Hilbert subspace of the full Hilbert space.

After Hermitian postulate 2, the next postulate concerns observables. The observables hold a slightly particular role as they can be seen as postulation of the connection between



theory and reality, as the observables should relate to *observations* or *measurements*. Of course, the what an *observation* or *measurement* of a quantum theory actually means is directly linked to the interpretation of quantum mechanics [65]. In philosophical sense the exact nature of the relation between theory and observation is thus highly disputed, and no general census exists [77, 78]. Unfortunately, it is not time for a lengthy discussion of this problem – it could be the topic on an entire master’s thesis in it self.

Sticking to the traditional way of postulating observables, the non-Hermitian postulation takes on a slightly generalised form compared to the corresponding Hermitian postulate.

**Non-Hermitian Postulate 3.** In a non-Hermitian quantum system associated with a complex separable Hilbert space  $\mathcal{H}$ , each observable is represented by a para-Hermitian operator in  $\mathcal{H}$ .

By comparison to Hermitian postulate 3, the only major difference in non-Hermitian postulate 3 is the hitherto undefined notion of *para-Hermitian* operator. Following again [76], let a para-Hermitian operator be defined as:

**Definition 3.1.** A densely defined operator  $\hat{O}$  in a Hilbert space  $\mathcal{H}$  is called a para-Hermitian operator, if it is a spectral operator of scalar type with a real spectrum. That is  $\sigma(\hat{O}) \subset \mathbb{R}$ .

Where a *densely definded operator* is an operator from one topological vector space to another, defined on a dense domain of the subspace of the initial vector space and takes values in the other. Where the subspace domain is said to be dense if every point in the topological space either belongs to the subspace or is arbitrarily “close” to it [14].

Furthermore, a spectral operator is a bounded linear operator that maps element of complete normed vector space onto itself, in this case Hilbert spaces. Furthermore, all linear operators acting on a finite-dimensional space as well as all self-adjoint operators on a Hilbert space are spectral operators [14] A simple example of such an operator is a finite-dimensional Hermitian operator, that is it acts on states in a Hilbert space giving scalar multiples of states in the same Hilbert space. Spectral operators of scalar type thus form the class of operators that are of interest for describing quantum mechanics as they act as maps from the space of states to the real numbers. It should of course be noted that Hermitian operators does in fact satisfy definition 3.1, indicating that non-Hermitian postulate 3 readily reduces to Hermitian postulate 3 for Hermitian systems.

Although non-Hermitian postulate 3 is a mathematical postulate, it is clear that it is a generalisation of Hermitian postulate 3. However, as become apparent in section 4.3 the requirement of pseudo-Hermiticity ensures that many of the constraints imposed by Hermiticity in non-Hermitian postulate 3 generalises to similar non-Hermitian constraints. Non-Hermitian postulate 3 is thus the first of the non-Hermitian postulates that is fundamentally different than the Hermitian postulates.

Having established the connection between observables and the operators of theory, similarly to Hermitian postulate 4, let us now establish the connection between the operators and outcome of measurements.

**Non-Hermitian Postulate 4.** For an observable  $\hat{O}$  in  $\mathcal{H}$ , if  $\hat{g}$  is a metric operator associated with  $\hat{O}$ , then  $\hat{g}$  induces a measurement context for the operator  $\hat{O}$  such that the expectation value of  $\hat{O}$  is determined by a non-zero vector  $|\psi\rangle$  with  $\hat{g}^{-1/2}|\psi\rangle \in \mathcal{D}(\hat{O})$  is given by

$$\langle \hat{O} \rangle_{\hat{g}} = \frac{\langle \psi | \hat{g}^{\frac{1}{2}} \hat{O} \hat{g}^{-\frac{1}{2}} | \psi \rangle}{\|\psi\|^2}, \quad (3.2)$$

where  $\mathcal{D}(\hat{O})$  denotes the domain of the operator  $\hat{O}$ .

Non-Hermitian postulate 4 is a bit compact and mathematical, so a few remarks are in order. For the sake of clarity, the expectation value has been given a subscript in order to distinguish it from its counterpart in Hermitian quantum mechanics.

By the notion of *metric operator*,  $\hat{g}$ , we refer to an operator inducing an additional metric structure on the Hilbert space. Non-Hermitian postulate 4 could equally well be formulated in a similar manner to Hermitian postulate 4 through postulating that the state-space is a complex vector space equipped with the inner product

$$\langle \psi, \phi \rangle_{\hat{g}} \equiv \langle \psi, \hat{g}\phi \rangle \text{ for any } \psi, \phi \in \mathcal{H},$$

where  $\langle \cdot, \cdot \rangle$  is a bilinear map that is linear in its second argument and anti-linear in the first [76]. However, as  $\hat{g}$  is dependent on the operator  $\hat{O}$  a formulation in terms of this new metric space would obscure some of the properties of non-Hermiticity. We thus stick to the present representation, in which the operator  $\hat{g}$  defines the notion of distances between states in the Hilbert space. In this sense  $\hat{g}$  can be said to be a *measurement context* for  $\hat{O}$  with respect to the Hilbert-Schmidt inner product. This is in some sense analogous to the metric tensor in relativity, as it assigns a distance measure on vector spaces [66].

In comparing non-Hermitian postulate 4 to Hermitian postulate 4, one major difference jumps out. Recall that although not explicitly specified in Hermitian postulate 4, it implies the Hilbert-Schmidt inner product with a trivial metric, i.e. the identity. Non-Hermitian postulate 4 however, postulates a non-trivial metric upon the inner product in order for the expectation value of operators to yield the desired properties, e.g. real and bounded from below. As will be shown in section 4.4.1 this type of inner product structure will ensure that the inner product space remains positive semi-definite for non-Hermitian systems, i.e. non-negative norms of state vectors.

From non-Hermitian postulate 4 it is clear that the vectors  $|\psi\rangle$  are not related to observables in the manner familiar from Hermitian Quantum Mechanics. In fact, if we define a new operator

$$\hat{O} = \hat{g}^{\frac{1}{2}} \hat{O} \hat{g}^{-\frac{1}{2}},$$

it follows from non-Hermitian postulate 4 that

$$\langle \hat{O} \rangle_{\hat{g}} = \frac{\langle \psi | \hat{O} | \psi \rangle}{\|\psi\|^2} = \langle \hat{O} \rangle.$$

Thus indicating that so long as the map  $\hat{g}^{\frac{1}{2}}$  exists such that this new operator may be constructed, non-Hermitian postulate 4 seems to imply some connection to a Hilbert-Schmidt inner product with a trivial metric. In fact, as will be shown in section 4.4.1 it

implies that under certain conditions there exists Hermitian operators associated that are associated with non-Hermitian operators through such a map. In such cases, care should be taken to ensure that it is clear from which operator any given set of state vectors are defined, e.g. is the state  $|\psi\rangle$  an eigenstate of  $\hat{O}$  or  $\hat{O}^\dagger$ .

Furthermore, similarly to Hermitian postulate 4 let us specify the what is meant by a perfect measurement:

**Non-Hermitian Postulate 5.** If the state  $|\psi\rangle$  is an eigenvector of an operator  $\hat{O}$  associated with an observable with an eigenvalue  $\lambda$ . Then the eigenvalue is given as  $\hat{O}|\psi\rangle = \lambda|\psi\rangle$ . If a perfect measurement of the observable were made, the measurement would yield  $\lambda$ .

At first glance non-Hermitian postulate 5 appears almost identical to Hermitian postulate 4, however there is an important difference. Because the operator  $\hat{O}$  is not Hermitian,  $\hat{O} \neq \hat{O}^\dagger$ , the eigenvectors of  $\hat{O}$  and  $\hat{O}^\dagger$  are generally no longer the same. Thus non-Hermitian postulate 5 cannot be stated in the same manner as Hermitian postulate 4, unless the metric-inner product is used, eq. (3.2). Note also that the eigenvector in non-Hermitian postulate 5 is generally not the non-zero vector in non-Hermitian postulate 4.

Having covered the state space, states and operators of a non-Hermitian system, only specifying the evolution remains. Similarly Hermitian postulate 5 the evolution of states is given by the Schrödinger equation.

**Non-Hermitian Postulate 6.** The evolution of the state-vector representation of the system is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle, \quad (3.3)$$

here  $H$  is a para-Hermitian operator associated with the energy of the system.

It is perhaps a bit surprisingly, non-Hermitian postulate 6 gives the evolution in terms of the usual Schrödinger equation. However, as already noted, because the left and right eigenstates of the Hamiltonian generally no longer are the same, unitary evolution does no longer follow trivially. However, as will be shown in section 4.7 the above postulates still ensures unitary evolution under certain constraints.

From comparing non-Hermitian postulates 1 to 6 to Hermitian postulates 1 to 5, it is clear that the only fundamental difference between the postulates is the notion of para-Hermitian operators rather than Hermitian along with a redefinition of the inner product structure. At the level of the postulates we can thus make the following remark:

*Remark 3.2.* In generalising the Dirac-von Neumann postulates of quantum mechanics to non-Hermitian operators, it is sufficient to require that;

- observables are represented by para-Hermitian operators,
- the inner product structure of the Hilbert space is dynamically determined the operators associated with observables.

Thus at the level of the postulates, the generalisation of quantum mechanics to non-Hermitian operators does not appear to be that extensive. However, as we shall see in chapter 4, the mathematics changes quite drastically at the level of calculations. Moreover, the introduction of the above generalised postulates lacks a motivation aside

from the fact that para-Hermitian operators are a class of non-Hermitian operators guaranteed to have real spectra. Hopefully, the motivation for the use of para-Hermitian operators will become clear by the end of chapter 4.

## Chapter 4

# $\mathcal{PT}$ -Symmetric Quantum Mechanics

In chapter 3 the generalisation from Hermitian to non-Hermitian quantum mechanics was shown at the level of the postulates. However, apart from some technical remarks on the extension of Hermitian operators to para-Hermitian operators and an additional metric structure on inner products, the discussion was void of any examples of what the generalisation entails in practise. The goal of the present chapter is to illustrate how the generalisation changes the mathematics familiar from Hermitian quantum mechanics. In particular the characteristic features of the eigenspectra and eigenvalues of non-Hermitian operators satisfying non-Hermitian postulates 1 to 6, how to construct the inner product metric and the implications on unitary evolution of states. Most of the present chapter will be purely technical, without reference to either calculations or physical applications. In the last section, section 4.8, a calculational example will be given to demonstrate the mathematics presented in this chapter. A discussion of direct physical applications will be postponed to chapter 7, whereas some manifestly non-hermitian features will be addressed in chapter 5

From non-Hermitian postulates 1 to 6 it is clear that not all non-Hermitian operators imaginable will satisfy the postulates. In fact many non-Hermitian operators will not satisfy definition 3.1, i.e. they are not para-Hermitian. Moreover, the metric map  $\hat{g}^{-1/2}$  guaranteed to exist if the operator does not satisfy definition 3.1. The class of non-Hermitian operators satisfying the non-Hermitian postulates is thus severely constrained by the requirement of them being para-Hermitian. However, the constraint of being para-Hermitian is physically ambiguous and not well motivated other than being a natural generalisation of Hermitian operators.

From the examples of non-Hermiticity given in chapter 2, especially the discussion of the Bender-Boettcher Hamiltonian, section 2.1.2, complex periodic potentials, section 2.2.1, and classical optics, section 2.3.1, space-time inversion symmetry is a recurring similarity in these systems. From the discussion of symmetries in physics, chapter 1, we saw that space-time inversion symmetry is a fundamental symmetry in much of physics<sup>1</sup>. On the basis of the conjecture by Bender & Boettcher, conjecture 2.6, Hamiltonians symmetric under space-time inversion are thus good candidate for non-Hermitian quantum systems satisfying non-Hermitian postulates 1 to 6. Since paper by Bender & Boettcher in 1998, [1], several various, equivalent formulations of quantum mechanics for systems exhibiting

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<sup>1</sup>In section 1.2, we saw that space-time reflection symmetry is a fundamental symmetry of gravitational and electromagnetic interaction. Combined with charge conjugation, space-time reflection appears to be a fundamental symmetry of the interactions in Nature.

$\mathcal{PT}$ -symmetry has been made [23, 36, 70, 76, 79, 80]. The following presentation will to a large extent follow Fring, [80].

## 4.1 The $\mathcal{PT}$ operator

In order to construct a quantum mechanical theory from a system exhibiting  $\mathcal{PT}$ -symmetry, certain requirements must be fulfilled. Due to the special role of the Hamiltonian from non-Hermitian postulate 6, we let the  $\mathcal{PT}$  operator defined with respect to the Hamiltonian. Following Fring [80] let us define the  $\mathcal{PT}$ -operators as:

**Definition 4.1.** Given a Hamiltonian operator  $\hat{H}$  acting on states in a Hilbert space  $\mathcal{H}$ , let us assume that there exists some operator  $\mathcal{PT}$ . If the operator  $\mathcal{PT}$

- i) commutes with the operator  $\hat{H}$ ,

$$[\hat{H}, \mathcal{PT}] = 0, \quad (4.1a)$$

- ii) shares eigenstates  $|\psi\rangle \in \mathcal{H}$  with  $\hat{H}$ ,

$$\mathcal{PT}|\psi\rangle = e^{i\varphi}|\psi\rangle, \quad (4.1b)$$

- iii) and is antilinear,

$$\mathcal{PT}\lambda|\psi\rangle = \lambda^*\mathcal{PT}|\psi\rangle, \quad (4.1c)$$

then the Hamiltonian is said to exhibit an unbroken  $\mathcal{PT}$ -symmetry.

We thus see that eq. (4.1a) is equivalent to the definition of symmetry given in section 1.1, in particular eq. (1.2), as the  $\mathcal{PT}$ -operator along with the identity  $\mathbb{1} \in \mathcal{B}(\mathcal{H})^2$  form a cyclic group of order two<sup>3</sup>. Moreover, by eq. (4.1c) it is clear that operation space-time inversion can be represented by an operator  $\mathcal{PT}$  defined by definition 4.1, hence the name. It should be noted that definition 4.1 bears no reference to the physical operation of space-time inversion, such that it forms a larger set of operations incorporating the essential behaviour of space-time inversion. Thus any reference to  $\mathcal{PT}$  operators or symmetry in this thesis, except in chapter 1, should be interpreted in this generalised sense, rather than a physical space-time property. It should also be noted that it does not follow directly definition 4.1 that the  $\mathcal{PT}$  operator can be decomposed into two operators  $\mathcal{P}$  and  $\mathcal{T}$  that are also symmetries of  $\hat{H}$ . However, the  $\mathcal{PT}$  operator can always be represented as a product of a linear and an anti-linear operator[81].

From eqs. (4.1a) to (4.1c) it is clear that the operator  $\hat{H}$  in definition 4.1 need not be a Hamiltonian operator as none of makes use of properties specific of Hamiltonian operators. Definition 4.1 may thus be generalised by theorem 4.2 to operators beyond Hamiltonians.

**Theorem 4.2.** Any operator  $\hat{O}$  acting on states in a Hilbert space associated which satisfies all properties i-iii in definition 4.1 is said to exhibit an unbroken  $\mathcal{PT}$ -symmetry.

<sup>2</sup>Note that by eq. (4.1c),  $\mathcal{PT} \notin \mathcal{B}(\mathcal{H})$  as  $\mathcal{B}$  is the set of linear operators whereas the  $\mathcal{PT}$  operator is explicitly non-linear.

<sup>3</sup>This statement is not technically accurate before the establishment of corollary 4.3 as it ensures that the group has only two elements.

Furthermore, it is possible that the  $\mathcal{PT}$  operator only satisfies some of the properties in definition 4.1.

- If the Hamiltonian does not commute with the  $\mathcal{PT}$  operator, it cannot be said to be  $\mathcal{PT}$ -symmetric. (property i) not satisfied)
- If the operators does not share eigenstates (property ii)) but the other properties are satisfied, then the operator is said to exhibit a *broken  $\mathcal{PT}$ -symmetry*.
- If the operator  $\mathcal{PT}$  is not anti-linear (property iii)), it cannot be associated with a time-reversal symmetry operation and is thus a different operation than intended.

As will be discussed in at a later point, a violation of property ii will be of interest and could give rise to interesting physics. However, if one or more of the other properties are not satisfied, the theory will not posses the desired structure for the current investigation.

**Corollary 4.3.** *The operation of  $\mathcal{PT}$ -inversion is an involution, that is  $(\mathcal{PT})^2 = \mathbb{1}$ .*

*Proof.* It follows from properties ii and iii of definition 4.1 that

$$\mathcal{PTPT}|\psi\rangle = \mathcal{PT}e^{i\varphi}|\psi\rangle = e^{-i\varphi}\mathcal{PT}|\psi\rangle = e^{-i\varphi}e^{i\varphi}|\psi\rangle = |\psi\rangle,$$

thus implying that  $(\mathcal{PT})^2 = \mathbb{1}$ . □

Moreover, form the discussion of the origin of the  $\mathcal{PT}$  operator in symmetry, section 1.2.3,  $\mathcal{PT}$  operator should be a involution even when condition ii is not satisfied. The  $\mathcal{PT}$  operator is thus unitary as corollary 4.3 implies that

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

given that the inverse exists. At the moment, the properties of the parity and time-inversion operators individually are not required but can in some cases be useful. The properties of the  $\mathcal{P}$  operator will be relevant in section 4.4.2 and will thus be presented in that context, in particular in theorem 4.18. The specific properties of the  $\mathcal{T}$  operator , are will not be included in section 4.4.2. Thus, let us for consistency include a brief theorem:

**Theorem 4.4.** *The time-inversion operator,  $\mathcal{T}$ , is an anti-linear and unitary operator , i.e.*

$$\mathcal{T}\alpha|\psi\rangle = \alpha^*\mathcal{T}|\psi\rangle \text{ and } \mathcal{T}^\dagger = \mathcal{T}^{-1},$$

*which has an inverse. The operator  $\mathcal{T}$  is also an involution, i.e.  $\mathcal{T}^2 = \mathbb{1}$ .*

This theorem is a generalisation of the properties of the time-reversal operator discussed in section 1.2.3. Further comments and a brief proof, can be found in appendix A.2.

Having established the nature of the  $\mathcal{PT}$ -symmetry, let us now move on to some immediate consequences. Starting with the eigenspectrum of  $\mathcal{PT}$ -symmetric operators.

## 4.2 The Eigenspectrum

Having established the basic mathematical structure of  $\mathcal{PT}$ , a condition for the Hamiltonian having real eigenvalues can be given.

**Theorem 4.5.** *The eigen spectrum, i.e. the set of all eigenvalues, of an operator exhibiting an unbroken  $\mathcal{PT}$ -symmetry is real.*

*Proof.* It follows from the properties of definition 4.1 together with theorem 4.2 that for an operator with an eigenspectrum  $\lambda$  and eigenvectors  $|\psi\rangle$ , i.e.  $\hat{O}|\psi\rangle = \lambda|\psi\rangle$ :

$$e^{i\varphi}\lambda|\psi\rangle = e^{i\varphi}\hat{O}|\psi\rangle = \hat{O}\mathcal{PT}|\psi\rangle = \mathcal{PT}\hat{O}|\psi\rangle = \mathcal{PT}\lambda|\psi\rangle = \lambda^*\mathcal{PT}|\psi\rangle = \lambda^*e^{i\varphi}|\psi\rangle.$$

Then as  $e^{i\varphi}$ ,  $\lambda$  and  $\lambda^*$  merely are numbers, then it follows that  $\lambda = \lambda^*$  implying that  $\lambda \in \mathbb{R}$ .  $\square$

Theorem 4.5 is not actually a new result, in fact it follows from a more general result on the properties of operators invariant under *anti-unitary* operators by Wigner from 1960 [81]. Where notion of anti-unitary refers to an operator that is both anti-linear and unitary. The more general result by Wigner will be revisited in section 4.3.

Moreover theorem 4.5,  $\mathcal{PT}$ -symmetry ensures that operators satisfying the symmetry have real spectra, thus implying that these operators can represent observables. That is, the expectation values of such operators are bound to be real. However, what does not follow is that the expectation values of such operators are bounded, e.g. the spectra of Hamiltonians is bounded from below guaranteeing the existence of ground states. In order for the expectation values to be bounded additional structure is needed, structure which will become more apparent in section 4.5.

Furthermore, it follows from the proof of theorem 4.5 that if the eigenvalue  $\lambda_i$  of an operator  $\hat{O}$  is complex, then the associated eigenvector  $|\psi_i\rangle$  cannot be shared by  $\hat{O}$  and  $\mathcal{PT}$ . Thus showing that when at least one eigenvalue is complex, then  $\hat{O}$  exhibits a broken  $\mathcal{PT}$ -symmetry. Following [80], it is clear that in the event that the  $\mathcal{PT}$ -operator transform one eigenvector to another, i.e.  $\mathcal{PT}|\psi_1\rangle = |\psi_2\rangle$ , then the eigenvalues of these states will form a complex conjugate pair because

$$E_1|\psi_1\rangle = H|\psi_1\rangle = H\mathcal{PT}|\psi_2\rangle = \mathcal{P}TH|\psi_2\rangle = \mathcal{P}TE_2|\psi_2\rangle = E_2^*\mathcal{PT}|\psi_2\rangle = E_2^*|\psi_1\rangle.$$

Thus implying that  $E_1 = E_2^*$ . As we will see below, this pairing of eigenvalues in complex conjugate pairs is a general result for operators exhibiting broken  $\mathcal{PT}$ -symmetry. A general condition for their appearance will be given in theorem 4.9.

Having seen some of the implications of definition 4.1 on the properties of the eigenspectra of  $\mathcal{PT}$ -symmetric operators, let us revisit non-Hermitian postulate 3. Recall that non-Hermitian postulate 3 is given with reference to *para-Hermitian* operators. However, in the following section we will, similarly to [80], introduce the notion of *pseudo-Hermitian* operators. Towards the end of section 4.3, the an exact link between *para-Hermiticity* and *pseudo-Hermiticity* will be given. A few brief comment on both their similarities and their differences will also be given.

### 4.3 Pseudo-Hermiticity

The notion of *pseudo-Hermitian* operators was largely introduced to quantum mechanics through a series of papers by Mostafazadeh in 2002 [82–84]. In a series of later papers, [85–89], Mostafazadeh further clarified and extended the notion of pseudo-Hermitian operators in the context of quantum mechanics and provided some applications to theoretical systems. Similarly to [76], let us define pseudo-Hermitian operators as:



**Definition 4.6.** Any operator  $\hat{O}$  is *pseudo-Hermitian* if there exists a bounded, invertible similarity transformation  $V$  such that

$$\hat{O}^\dagger = V\hat{O}V^{-1}. \quad (4.2)$$

Where eq. (4.2) will typically be known as a *pseudo-Hermiticity relation*. Furthermore, we can similarly to [83, 84] give an example of a subclass of pseudo-Hermitian operators.

**Theorem 4.7.** If  $\mathcal{A}(\mathcal{H})$  is the set of pseudo-Hermitian operators on a Hilbert space  $\mathcal{H}$ , there exists a subset  $\mathcal{C}(\mathcal{H}) \subseteq \mathcal{A}(\mathcal{H})$  for which there exists a map  $\eta$  such that  $\forall \hat{O} \in \mathcal{C}(\mathcal{H})$

$$\hat{O} = \eta\hat{O}\eta^{-1} \text{ and } \hat{O} = \hat{O}^\dagger.$$

From definition 3.1 we remember that a para-Hermitian operator is a spectral operator with a real spectrum. By the definition of the spectral properties of operators, definition 2.2, it thus follows that any linear operator satisfying theorem 4.7 is para-Hermitian. The notions of para- and pseudo-Hermitian operators are thus be closely related, and the map  $\eta$  is in fact para-Hermitian map. Following [76], let us make the following remark.

*Remark 4.8.* Any pseudo-Hermitian operator is para-Hermitian if the similarity transformation  $V$ , eq. (4.2), is a positive operator.

Furthermore, the transformation maps are often referred to as Dyson maps[80], especially when referring to theorem 4.7. Note, that theorem 4.7 is not exactly the definition given in [83] but as we will see from theorem 4.12, the definition given by [83] follows from theorem 4.7. It should also be noted that in an earlier paper, Mostafazadeh gives the definition of pseudo-Hermiticity in terms of new inner product space rather than the operator definition given above[82]. A similar definition of an inner product will be given in section 4.4.1.

Furthermore, Mostafazadeh gives two equivalent conditions on a special class of non-Hermitian operators being pseudo-Hermitian [82, Theorem II]. For clarity the, these conditions are stated in theorem 4.9.

**Theorem 4.9.** Any operator  $\hat{O}$  with a complete biorthonormal basis of eigenvectors and discrete spectrum is pseudo-Hermitian iff the following conditions are satisfied:

1. The spectrum of  $\hat{O}$  is real.
2. The complex eigenvalues in the spectrum of  $\hat{O}$  come in pairs of complex conjugates and the multiplicity of complex conjugate eigenvalues are the same.

The notion of a biorthonormal basis of eigenvectors will be discussed further in theorem 4.17 below. At this point, it should probably be noted that non-Hermitian operators does not in general have a complete biorthonormal eigenbasis. Thus theorem 4.9 does not apply in general, and no analogue to arbitrary non-Hermitian operators seems to exist[82–84]. It is also immediately clear from theorem 4.7 that pseudo-Hermitian operators that as a similarity transformation to a Hermitian operator has a purely real spectrum.

Furthermore, it follows from theorem 4.9 that there exist a constraint on  $\mathcal{PT}$ -symmetric operators being pseudo-Hermitian.

**Theorem 4.10.** *Operators that satisfy conditions i) and iii) of definition 4.1 are pseudo-Hermitian if they possess a complete biorthonormal basis of eigenvectors and a discrete spectrum.*

Where theorem 4.10 follows directly from [82, Corollary II.3] but also from [81]. Theorem 4.10 also clarifies Theorem 4.9 in that it immediately follows that the spectrum of a pseudo-Hermitian operator that admits a complete biorthonormal basis is entirely real, or appears in complex conjugated pairs. It also follows from theorem 4.10 that both Hamiltonians with broken and unbroken  $\mathcal{PT}$ -symmetries can in principle be described by a pseudo-Hermitian operator.

Moreover, from our discussion of normal operators, section 2.1.1, we can make the following statement on some familiar operators.

**Theorem 4.11.** *Linear operators  $\hat{O} \in \mathcal{B}(\mathcal{H})$  with discrete spectra are pseudo-Hermitian if one of the following statements are true. The operator  $\hat{O}$*

- *is Hermitian,  $\hat{O} = \hat{O}^\dagger$ ,*
- *anti-Hermitian,  $\hat{O} = -\hat{O}^\dagger$ ,*
- *positive,  $\|\hat{O}\| \geq 0$ ,*
- *unitary,  $\hat{O}\hat{O}^\dagger = \hat{O}^\dagger\hat{O} = \mathbf{1}$ .*

*Proof.* Hermitian operators satisfies both definition 4.6 and theorem 4.7 trivially, where both transformation maps are necessarily identity maps. The pseudo-Hermiticity of positive operators follows from that of Hermitian operators as any positive operator is Hermitian. By the spectral properties of anti-Hermitian operators, theorem 2.4, their eigenvalues are all complex. However, the eigenvalues anti-Hermitian operators discrete spectra all appear in complex conjugate pairs. Anti-Hermitian operators are thus pseudo-Hermitian by theorem 4.9. And lastly by the condition that the eigenvalues of unitary operators all have norm one,  $|\lambda| = 1$ , both  $\lambda$  and  $\lambda^*$  are eigenvalues. Hence unitary operators are pseudo-Hermitian by theorem 2.4.  $\square$

We thus remark that the set of Hermitian operators on  $\mathcal{H}$  form a subset of the pseudo-Hermitian operators. Thus any condition ensuring pseudo-Hermitian operators is also a condition on Hermitian operators. Moreover the subset of Hermitian operators will always satisfy theorem 4.7. That being said, pseudo-Hermitian operators does not in general behave as Hermitian operators. For example, let  $\hat{O}$  be a pseudo-Hermitian operator. It then follows from theorem 4.7 that  $\hat{O} = \eta\hat{O}\eta^{-1}$  where  $\hat{O}$  is a Hermitian operator given that  $\eta$  is well defined. Furthermore, if  $\hat{O}$  has a spectrum  $\lambda$  and eigenvectors  $|\phi\rangle$ , it follows that

$$\hat{O}|\phi\rangle = \hat{O}|\phi\rangle = \eta\hat{O}\eta^{-1}|\phi\rangle \Rightarrow \lambda\eta^{-1}|\phi\rangle = \hat{O}\eta^{-1}|\phi\rangle.$$

However, this is simply the eigenvalue equation

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle \text{ where } |\psi\rangle \equiv \eta^{-1}|\phi\rangle,$$

thus implying that the operators  $\hat{O}$  and  $\hat{O}$  share the eigenvalues  $\lambda$ , i.e.  $\sigma(\hat{O}) = \sigma(\hat{O})$ . Because  $\hat{O}$  is a Hermitian operator, the spectrum  $\sigma(\hat{O})$  is guaranteed to be real.

Furthermore, from the pseudo-Hermitian maps we can similarly to non-Hermitian postulate 4 define a metric operator.

**Theorem 4.12.** *For every well defined transformation map  $\eta$  associated with pseudo-Hermitian operators there exists a metric operator*

$$\rho \equiv \eta^\dagger \eta,$$

*which is a Hermitian,  $\rho = \rho^\dagger$ , and positive operator. Then a pseudo-Hermitian operator equipped with such a map satisfies the pseudo-Hermiticity relation*

$$\hat{O}^\dagger = \rho \hat{O} \rho^{-1}. \quad (4.3)$$

*Proof.* From theorem 4.7 and the Hermiticity of  $\hat{O}$  it follows that

$$\eta \hat{O} \eta^{-1} = (\eta^{-1})^\dagger \hat{O}^\dagger \eta^\dagger \Leftrightarrow \eta^\dagger \eta \hat{O} = \hat{O}^\dagger \eta^\dagger \eta \Rightarrow \rho \hat{O} = \hat{O}^\dagger \rho,$$

because  $(\eta^{-1})^\dagger = (\eta^\dagger)^{-1}$  as  $\eta$  is an invertible bounded operator. It thus follows that

$$\rho^\dagger = \eta^\dagger (\eta^\dagger)^\dagger = \eta^\dagger \eta = \rho,$$

proving that  $\rho$  is Hermitian. And because  $\eta$  is invertible,  $\rho$  is invertible by construction. Thus showing that  $\rho$  satisfies definition 4.6.

Furthermore, following [90], it follows from  $\rho$  being Hermitian that  $\rho$  can be diagonalised by a unitary transformation. Specifically, an unitary operator  $\hat{U}$  that diagonalises  $\rho$  as  $\hat{U} \rho \hat{U}^\dagger = \rho_D$ . Then by construction the unitary transformation ensures that

$$\hat{U} \rho \hat{U}^\dagger = \hat{U} \eta^\dagger \hat{U}^\dagger \hat{U} \eta \hat{U}^\dagger = \eta_D^\dagger \eta_D,$$

such that in a given basis any diagonal element of  $\rho_D$  is given by

$$\rho_{i,i}^D = \sum_j (\eta_{i,j}^D)^\dagger \eta_{i,j}^D = \sum_j (\eta_{i,j}^D)^* \eta_{i,j}^D.$$

Thus as every  $(\eta_{i,j}^D)^* \eta_{i,j}^D$  are real positive numbers,  $\rho$  is a positive operator.  $\square$

This pseudo-Hermiticity relation will prove useful as it allows the eigenvectors of  $\hat{O}^\dagger$  to be connected to the eigenvectors of  $\hat{O}$ . Although not immediately clear from explicit form of theorem 4.12, the eigenvectors of  $\hat{O}^\dagger$  are not necessarily eigenvectors of  $\hat{O}$  and vice versa. That is, if  $|\phi\rangle$  is an eigenvector of  $\hat{O}^\dagger$ , i.e.  $\hat{O}^\dagger |\phi\rangle = \lambda |\phi\rangle$ , then

$$\hat{O}^\dagger |\phi\rangle = \rho \hat{O} \rho^{-1} |\phi\rangle \neq \hat{O} |\phi\rangle.$$

In general an eigenvector of  $\hat{O}^\dagger$  will only be an eigenvector of  $\hat{O}$  if  $\rho \simeq \mathbb{1}$ . The fact that the left and right eigenvectors of non-Hermitian operators are not the same and what this implies will be discussed further in section 4.4.2 and section 4.8.

Having defined what is meant by pseudo-Hermiticity and seen some necessary conditions of being pseudo-Hermitian, let us now briefly discuss some of the benefits of having pseudo-Hermiticity. Especially what having a mapping between Hermitian and non-Hermitian systems entails.

### 4.3.1 From Non-Hermitian to Hermitian

The pseudo-Hermiticity ensures that a transformation between non-Hermitian and Hermitian descriptions of a system exist. Although the pseudo-Hermiticity maps might be complicated in practice, they constrain the dynamics of non-Hermitian systems. Through their link to  $\mathcal{PT}$ -symmetry they act as symmetries imposing conservations but also allows us to make calculations using either Hermitian or pseudo-Hermitian operators, depending on which gives simpler or more convenient calculations. From the point of view of efficiency, it provides another framework for doing calculations which usually is beneficial. Furthermore, because Hermitian quantum mechanics have unitary time evolution, we would expect that pseudo-Hermitian systems also exhibit unitary evolution. As will be shown in section 4.7, pseudo-Hermiticity of the Hamiltonian ensures unitary time evolution and  $\mathcal{PT}$ -symmetry is in fact a necessary and sufficient condition for unitary evolution [90].

Furthermore, the connection between non-Hermitian and Hermitian operators, theorem 4.7, shows that this formulation of  $\mathcal{PT}$ -symmetric quantum mechanics is not a fundamentally new formulation. Instead the  $\mathcal{PT}$ -symmetric formulation is rather a generalisation of Hermitian quantum mechanics, which shows that in some cases physical systems thought to be non-Hermitian due to a naive construction are in fact Hermitian systems in disguise. The  $\mathcal{PT}$ -symmetric formulation allows us write down descriptions of system that are only Hermitian in some obscure or new configurational space in which the usual physical intuition does not apply. The pseudo-Hermiticity thus allows for an entire new class of systems to be considered in a consistently using Hermitian quantum mechanics.

Although powerful, the connection to Hermitian operators is critically dependent on the existence of the Dyson map,  $\eta$ . If this map breaks down, the connection to the Hermitian description will be lost. This can however, give new physics in terms of manifestly non-Hermitian effects which will be discussed further in section 5.2 and chapter 7. The break down is often associated with singularities in the parameter space of the system and close to these, examples of non-Hermitian behaviour can be found [91]. An example of the breakdown of the Dyson map and the metric will be given in section 4.8.

Lastly, it should be noted that although pseudo-Hermiticity allows the Dyson map to be found it is necessarily a trivial task. It does thus seem to be both necessary and beneficial to obtain a consistent procedure for treating non-Hermitian systems even though they in principle could be transformed into its Hermitian counterparts. Thus, having established the need for the metric operator and the associated Dyson map in order to obtain the pseudo-Hermiticity relations. Let us now briefly look at how the Dyson map may be obtained and some of the difficulties involved.

### 4.3.2 Constructing a Dyson Map

There are several ways of obtaining or constructing a Dyson map, of which an educated guess is always a possibility. However, it is in general difficult constructing these maps exactly without knowing the Hermitian counterpart, additionally these maps are in general not unique[82]. Starting from a non-Hermitian operator  $\hat{O}$ , one will typically attempt to solve the pseudo-Hermiticity relation, theorem 4.7, in order to obtain the Dyson map, or equivalently the metric using the relation of theorem 4.12[80]. Whether  $\eta$  or  $\rho$  are more easily obtained, will depend on the specifics of the particular system. It

should however be noted that obtaining the Dyson map from the metric,  $\eta = \sqrt{\rho}$ , is in general an awkward procedure. However awkward, it is in principle always possible to do so because the metric is a positive operator, theorem 4.12.

In order to simplify, let us, similarly to [80], make the *ansatz* that the operator,  $\hat{O}$ , can be expressed in terms of the generators  $T_a$  of a Lie algebra  $\mathfrak{g}$ . Then the Dyson map is given by the exponential map of the Lie algebra, that is  $\eta = \exp\{\alpha^a T_a\}$  where the Einstein summation notation indicates a sum over the rank of the algebra  $\mathfrak{g}$  for all coefficients  $\alpha^a \in \mathbb{C}$ , where  $a \in \text{Rank } \mathfrak{g}$ . Similarly, the metric would take the form  $\rho = \exp\{\beta^a T_a\}$  with  $\beta^a \in \mathbb{C}$  and  $a \in \text{Rank } \mathfrak{g}$ . The action of the Dyson map, or metric, on the operator,  $\hat{O}$ , along with the adjoint action will produce expressions expanded in the generators of  $\mathfrak{g}$ . Given that such an expansion exists, it gives a well defined set of equations for the coefficients  $\alpha^a$  or  $\beta^a$ , which in principle can be solved. Thus solving these, one obtains an exact representation of the Dyson map or metric operator. However, as the number of equations will scale as the rank of  $\mathfrak{g}$  it is clear that this would become difficult or almost impossible in practise for systems with Hilbert spaces of large or infinite dimension. Furthermore, it is not guaranteed that the operator can be represented in terms of the generators of a closed algebra,  $\mathfrak{g}$ .

In the cases where, the aforementioned procedure is inefficient or does not work, one can usually turn to perturbation theory. Following, once again, [80], let us look at one perturbative procedure. As an example, let us consider a non-Hermitian Hamiltonian operator  $H$ . However this procedure would be equally valid for any operator with the same mathematical properties. Let us assume that the Hamiltonian  $H$  can be written, or approximately written, as the perturbative expansion

$$H = h_0 + i\epsilon h_1, \quad (4.4)$$

in terms of the Hermitian Hamiltonians  $h_0$  and  $h_1$ , where dimensionless parameter  $\epsilon$  is in the perturbative regime, i.e.  $\epsilon \ll 1$ . Then instead of having to find the Hermitian counterpart of  $H$ , let us use the pseudo-Hermiticity relation of the metric, theorem 4.12, and the Baker-Campbell-Hausdorff (BCH) formula, [92], we find that

$$\begin{aligned} H^\dagger &= \rho H \rho^{-1} \\ &= H + \beta^a [T_a, H] + \frac{1}{2!} \beta^a \beta^b [T_a, [T_b, H]] + \frac{1}{3!} \beta^a \beta^b \beta^c [T_a, [T_b, [T_c, H]]] + \dots \end{aligned} \quad (4.5)$$

Where the previously mentioned exponential map of the metric has been assumed.. It thus becomes clear that by rewriting eq. (4.5) in terms of the perturbative Hamiltonian, eq. (4.4), we obtain the expansion

$$\begin{aligned} &\beta^a [T_a, h_0] + \frac{1}{2!} \beta^a \beta^b [T_a, [T_b, h_0]] + \frac{1}{3!} \beta^a \beta^b \beta^c [T_a, [T_b, [T_c, h_0]]] + \dots \\ &= -i\epsilon \left( 2h_1 + \beta^a [T_a, h_1] + \frac{1}{2!} \beta^a \beta^b [T_a, [T_b, h_1]] + \frac{1}{3!} \beta^a \beta^b \beta^c [T_a, [T_b, [T_c, h_1]]] + \dots \right). \end{aligned}$$

If we now make the *ansatz*  $\beta^a T_a = \sum_{i=0}^{\infty} \epsilon^i q_i$  for some unknown operators  $q_i$ , the terms in the above expansion can be expressed order by order in  $\epsilon$ . The real treat procedure is

that order by order expressions admits the recursive solutions [80]:

$$\begin{aligned}\mathcal{O}(\epsilon) &\rightarrow [h_0, q_1] = 2ih_1 \\ \mathcal{O}(\epsilon^3) &\rightarrow [h_0, q_3] = \frac{i}{3!}[q_1, [q_1, h_1]] \\ \mathcal{O}(\epsilon^5) &\rightarrow [h_0, q_5] = \frac{i}{3!} \left( [q_1, [q_3, h_1]] + [q_3, [q_1, h_1]] - \frac{1}{60}[q_1, [q_1, [q_1, h_1]]] \right).\end{aligned}$$

The unknown operators,  $q_i$ , may thus be determined by solving these recursive equations, up to the ambiguities of commutators. Thus solving these equations will give an expression of the metric, from which one could attempt to obtain the Dyson map. However, as will become clear below, the metric will turn out to be the object of interest moving forward.

Having established some key properties of the Dyson map and associated metric, let us continue the development of the formalism needed for doing calculations in  $\mathcal{PT}$ -symmetric quantum mechanics.

## 4.4 The Inner Product

As noted in section 3.2, contrary to Hermitian quantum mechanics the inner product is no longer implicitly defined and thus requires a bit of delicate care. Thus in the following, two separate definitions will be made and lastly a brief discussion of their equivalence will be made.

### 4.4.1 The Metric-Inner Product

One way of defining the inner product is to do it in a manner such that it closely resembles the usual Hilbert space inner product used in Hermitian quantum mechanics. This can be done through introducing a metric for the inner product, not too dissimilar from non-Hermitian postulate 5 for generic non-Hermitian quantum mechanics.

**Definition 4.13.** For two eigenstates  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$  of a non-Hermitian Hamiltonian, let the metric-inner product or  $\rho$ -inner product be defined as

$$\langle \psi | \phi \rangle_\rho \equiv \langle \psi | \rho \phi \rangle.$$

Where  $\langle \cdot | \cdot \rangle$  denotes the regular Hilbert space inner product.

Note that inner product  $\langle \psi | \rho \phi \rangle$  is a shorthand for the inner product of the vectors  $|\psi\rangle$  and  $\rho|\phi\rangle$ , where the operator has been written inside the ket in order to make it explicit on which vector it acts. This is analogue to the inner product notations found in many mathematical texts, although typeset using the Dirac-notation. Comparing definition 4.13 to non-Hermitian postulate 4, it is clear that the metric-inner product satisfies non-Hermitian postulate 4 as long as the pseudo-Hermitian satisfies non-Hermitian postulate 3. That is non-Hermitian postulate 3 implies that the spectrum of the Hamiltonian is real, it thus from remark 4.8 that Hamiltonian is para-Hermitian. This follows from theorem 4.7 when realising that  $\hat{g}^{1/2} = \eta$  and that  $\hat{g}^{-1/2}|\psi\rangle$  in non-Hermitian postulate 4 is in the domain of the pseudo-Hermitian operator.

Furthermore, the inner product is constructed in this particular manner in order for the inner product to mimic the behaviour of the usual Hilbert space inner product associated with Hermitian constructions.

**Theorem 4.14.** *Any non-Hermitian operator of finite dimension with an unbroken  $\mathcal{PT}$ -symmetry is self-adjoint and symmetric with respect to the metric-inner product for metrics associated with the operator.*

*Proof.* Given two eigenstates  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$  of a non-Hermitian operator  $\hat{O}$  with an unbroken  $\mathcal{PT}$ -symmetry and an associated metric operator  $\rho$  defined by theorem 4.12 it follows that

$$\langle \psi | \hat{O} \phi \rangle_{\rho} = \langle \psi | \eta^{\dagger} \eta \hat{O} \phi \rangle = \langle \eta^{-1} \chi | \eta^{\dagger} \eta \hat{O} \eta^{-1} \xi \rangle,$$

where  $|\psi\rangle = \eta^{-1} |\chi\rangle = |\eta^{-1} \chi\rangle$ ,  $|\phi\rangle = \eta^{-1} |\xi\rangle = |\eta^{-1} \xi\rangle$  and  $|\chi\rangle, |\xi\rangle$  are eigenstates of the Hermitian operator  $\hat{O}$  associated to  $\hat{O}$  by theorem 4.7. Then

$$\langle \eta^{-1} \chi | \eta^{\dagger} \eta \hat{O} \eta^{-1} \xi \rangle = \langle \chi | (\eta^{\dagger})^{-1} \eta^{\dagger} \eta \hat{O} \eta^{-1} \xi \rangle = \langle \chi | \hat{O} \xi \rangle = \langle \chi \hat{O}^{\dagger} | \xi \rangle,$$

such that by reinserting

$$\langle \chi \hat{O} | \xi \rangle = \langle \eta \hat{O} \eta^{-1} \chi | \xi \rangle = \langle \eta \hat{O} \psi | \eta \phi \rangle = \langle \hat{O} \psi | \eta^{\dagger} \eta \phi \rangle.$$

This thus proves that

$$\langle \psi | \hat{O} \phi \rangle_{\rho} = \langle \hat{O} \psi | \phi \rangle_{\rho}.$$

It should be noted that the above steps ignores all domain issues of the included operators. However, the result follows immediately from [88] as long as the operator  $\hat{O}$  is diagonalisable and has a discrete spectrum. It can also be taken to hold from the definition of pseudo-Hermiticity given in [82] in terms of inner product spaces. However, if the operator is not diagonalisable, it is a more difficult procedure. A general proof for non-diagonalisable operators can be found in [93]  $\square$

The metric operator  $\rho$  can thus be seen to play the same role in non-Hermitian quantum mechanics as the metric tensor in General Relativity [88]. If the operator  $\hat{O}$  were Hermitian, then the metric reduces to the identity operator. Definition 4.13, thus reduces to the ordinary Hilbert-Schmidt inner product for Hermitian. In other words, definition 4.13 can be seen as a generalisation of the implied inner product of Hermitian quantum mechanics. It can be easily verified that definition 4.13 satisfies the relations of corollary 0.2 and is a valid inner product of definition 0.1.

#### 4.4.2 The $\mathcal{CPT}$ -Inner Product

Another inner product could be constructed through the symmetry operator  $\mathcal{PT}$  of the system, as demonstrated by [36]. Based on the Hilbert-Schmidt inner product  $\langle \psi | \phi \rangle = \text{Tr} [\psi^* \phi]$ , the naive definition would be

$$\langle \psi | \phi \rangle_{\mathcal{PT}} \equiv \text{Tr} [\psi^{\mathcal{PT}} \phi]$$

where the trace can be promoted to the integral  $\int dx [\psi(-x)]^* \phi(x)$  if the basis is continuous.  $\psi^{\mathcal{PT}}$  refers to the  $\mathcal{PT}$ -conjugate of  $\psi$ , that is  $\mathcal{PT}\psi$ . However, this definition will not suffice as it is not necessarily positive definite, thus the inner product is not required to have a positive norm [36]. Instead, suppose a similar construction with an additional linear operator commuting with both the Hamiltonian and  $\mathcal{PT}$  operators.

**Definition 4.15.** For two eigenstates  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$  of a non-Hermitian Hamiltonian  $\hat{H}$ , if there exists a linear operator  $\mathcal{C}$  acting on states in  $\mathcal{H}$  that commutes with both  $\hat{H}$  and  $\mathcal{PT}$ . Then the  $\mathcal{CPT}$ -inner product is

$$\langle \psi | \phi \rangle_{\mathcal{CPT}} \equiv \text{Tr} [\psi^{\mathcal{CPT}} \phi],$$

where the trace can be promoted to the integral  $\int dx dy \mathcal{C}(x, y) \psi^*(-y) \phi(x)$  if the basis is continuous.

For calculational purposes the inner product is more easily related to the usual product of two vectors,

$$\langle \psi | \phi \rangle_{\mathcal{CPT}} = [\mathcal{CPT} |\psi\rangle]^{\text{T}} \cdot |\phi\rangle.$$

Where by the anti-linear property of the time-inversion operator  $\mathcal{T}$ , then  $[\mathcal{T} |\psi\rangle]^{\text{T}} = |\psi\rangle^{\dagger}$ . Thus  $[\mathcal{T} |\psi\rangle]^{\text{T}} = \langle \psi |$  forms a vector in the usual co-vector space associated with the usual Hilbert space inner product.

In fact, it can be shown [36] that definition 4.15 is consistent the inner product being positive definite and having an unitary time evolution. However, contrary to definition 4.13, the eigenvectors described in definition 4.15 requires some extra care in relating to the usual Hilbert space inner product.

**Corollary 4.16.** Let  $\hat{O}$  be an operator associated with a non-Hermitian system, then the left and right eigenvectors  $|\psi\rangle$  and  $|\phi\rangle$ , respectively, are not identical. Where

$$\hat{O} |\phi\rangle = \lambda |\phi\rangle \quad \text{and} \quad \hat{O}^{\dagger} |\psi\rangle = \lambda |\psi\rangle.$$

That is in general for non-normal operators the eigenvectors of  $\hat{O}$  and  $\hat{O}^{\dagger}$  are generally not the same, even though they share eigenvalues [21]. Moreover, when the left and right eigenvectors are different, they are generally no longer orthogonal either.

**Theorem 4.17.** Given a set of normalised left eigenvectors  $|\psi\rangle$  and a set of normalised right eigenvectors  $|\phi\rangle$  of an operator associated with a non-Hermitian system. Then, in general, these are not orthonormal  $\langle \psi_m | \psi_n \rangle \neq \delta_{m,n}$  and  $\langle \phi_m | \phi_n \rangle \neq \delta_{m,n}$  under the Hilbert-Schmidt inner product. These sets forms a biorthogonal and normalised basis

$$\langle \psi_m | \phi_n \rangle = \langle \phi_m | \psi_n \rangle = \delta_{m,n} \quad \text{and} \quad \sum_n |\psi_n\rangle \langle \phi_n| = \sum_n |\phi_n\rangle \langle \psi_n| = \mathbb{1}$$

For the proof of theorem 4.17 see appendix A.1.

Having defined the biorthogonal basis and the  $\mathcal{CPT}$ -inner product, some key properties of the composite operators of  $\mathcal{CPT}$  can be deduced. And contrary to the metric-inner product, the independent properties of the constituent operators associated with the  $\mathcal{CPT}$ -inner product are of importance.

**Theorem 4.18.** The parity operator  $\mathcal{P}$  associated with a non-Hermitian system transforms right eigenvectors  $|\phi\rangle$  into left eigenvectors  $|\psi\rangle$ ,

$$\mathcal{P} |\phi\rangle = s |\psi\rangle \quad \text{with} \quad s = \pm 1.$$

Furthermore, it is an involution and Dirac-conjugates the Hamiltonian  $\hat{H}$ , i.e.

$$\mathcal{P}^2 = \mathbb{1} \quad \text{and} \quad \hat{H}^{\dagger} = \mathcal{P} \hat{H} \mathcal{P}.$$



For the proof of theorem 4.18 see appendix A.2.2, but note also that these properties are generalisations of the properties of the space-time reflection operator discussed in chapter 1. Theorem 4.18 is thus a generalisation of the physical parity operator. Moreover, from theorem 4.18 it is clear that the parity operator is not necessarily positive. Thus it follows from the naive inner product definition, the  $\mathcal{PT}$ -inner product discussed above, that

$$\langle \psi | \phi \rangle_{\mathcal{PT}} = \left[ \mathcal{P} | \phi \rangle^\dagger \right] \cdot | \phi \rangle = s \langle \phi | \phi \rangle.$$

Which is positive definite iff  $s = +1$ . However in general  $s = \pm 1$ , such that the  $\mathcal{PT}$ -inner product is not guaranteed to be positive definite. Thus showing that another definition, definition 4.15, is required.

Having established the parity operator in some detail, the operator  $\mathcal{C}$  may also be constructed, completing the composition of the  $\mathcal{CPT}$ -operator. Contrary to the charge conjugation operator in Hermitian quantum mechanics and Quantum Field Theory, the  $\mathcal{C}$  operator is not generally associated with some physical symmetry. At least not in the usual sense of transforming charges into opposite charges. Instead the  $\mathcal{C}$  operator should primarily be interpreted as a constituent operator of  $\mathcal{CPT}$ , ensuring that the  $\mathcal{CPT}$ -inner product is positive definite.

**Theorem 4.19.** *Given a complete biorthogonal basis  $\{|\psi\rangle, |\phi\rangle\} \in \mathcal{H}$  associated with a Hamiltonian, there exists an operator*

$$\mathcal{C} \equiv \sum_n s_n |\psi_n\rangle \langle \phi_n|,$$

*which commutes with the  $\mathcal{PT}$  and the Hamiltonian operators. Where the set  $\{s_1, \dots, s_n\}$  defines the signature of the operator, and  $\mathcal{C}^2 = \mathbb{1}$ .*

Given a biorthogonal basis, it is clear that such an operator exists. Furthermore, the proof of the remaining properties may be found in appendix A.2.3. Thus by generalising the discussion of the positive definiteness of the supposed  $\mathcal{PT}$ -inner product above by including the  $\mathcal{C}$  operator, it follows from theorem 4.19 that

$$\langle \psi | \phi \rangle_{\mathcal{CPT}} = \left[ \mathcal{CP} | \psi \rangle^\dagger \right] \cdot | \phi \rangle = s \left[ \mathcal{C} | \psi \rangle^\dagger \right] \cdot | \phi \rangle = s^2 \langle \psi | \phi \rangle.$$

The  $\mathcal{CPT}$ -inner product is thus positive definite independently of the signature of the parity symmetry, and consequently forms a desired inner product.

Equipped with two independently formulated inner products, they must yield the same results. That is, the expectation value of an observable,  $\hat{O}$ , must be independent of the inner product, i.e.

$$\langle \hat{O} \rangle_{\mathcal{CPT}} = \langle \hat{O} \rangle_\rho = \langle \hat{O} \rangle.$$

Note that the last equality follows from the fact that  $\hat{O}$  must be para-Hermitian in order to guarantee the existence of the metric root,  $\rho^{1/2} = \eta$ . This equivalence thus follows from non-Hermitian postulates 3 and 4, showing that the choice of inner product is not unique. A fact which can also be seen from definition 4.6 as the choice of transformation map is not unique either. However, an even stronger equivalence exists between the inner product structures.

### 4.4.3 The Equivalence of the Metric- & $\mathcal{CPT}$ -Inner Products

**Theorem 4.20.** *Given that the spectrum of the Hamiltonian is real, there exists a metric*

$$\rho = \mathcal{PC},$$

*associated with the  $\mathcal{CPT}$ -inner product, definition 4.15, such that it is equivalent with the metric inner product.*

*Proof.* From definition 4.15, the dual vector  $\langle\psi| = [\mathcal{T}|\psi\rangle]^\dagger = |\psi\rangle^\dagger$  is constructed by the action of the time inversion operator. That is given two vectors  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ ,

$$\langle\psi|\phi\rangle_{\mathcal{CPT}} = [\mathcal{CPT}|\psi\rangle]^\dagger \cdot |\phi\rangle = |\psi\rangle^\dagger \mathcal{PC}|\phi\rangle = \langle\psi|\rho\phi\rangle = \langle\psi|\phi\rangle_\rho,$$

as both the operators  $\mathcal{C}$  and  $\mathcal{P}$  are involutions and  $\mathcal{T}$  is an antilinear operator such that  $\langle\psi|\mathcal{T} = |\psi\rangle^\dagger$ . Thus, as the involutionarity of the operators ensures that the action on the bras and kets is the same, the equivalence of definitions 4.13 and 4.15 follows [80].

Furthermore, it follows that

$$\rho^\dagger = \mathcal{C}^\dagger \mathcal{P}^\dagger = \mathcal{CP} = \mathcal{PC} = \rho,$$

by the operators being involutions and thus commuting. Thus showing that the operator  $\rho = \mathcal{PC}$  is a metric operator in the sense of theorem 4.12, and proving theorem 4.20.  $\square$

Note that as both  $\mathcal{P}$  and  $\mathcal{C}$  cannot generally be represented by real matrixes or functions, Moreover, it does not in general follow that  $\eta = \mathcal{C} = \mathcal{P}^\dagger$ . In general, let instead Dyson map be  $\eta = \sqrt{\mathcal{PC}}$ .

## 4.5 Orthogonality and Normalisation of Eigenstates

As previously noted, non-normal operators are not required to have an orthogonal set of eigenvectors. Generally the eigenvector form a biorthogonal set. Now equipped with a definition of the inner product, some more formal statements about orthogonality and normalisation of states can be made. Two states that are said to be orthonormal if they satisfy definition 4.21.

**Definition 4.21.** Let  $|\psi_m\rangle, |\psi_n\rangle \in \mathcal{H}$  be eigenstates of a non-Hermitian Hamiltonian with a discrete spectrum. The eigenstates are said to be orthonormal with respect to the  $\rho$ -inner product iff

$$\langle\psi_m|\psi_n\rangle_\rho = \delta_{m,n}.$$

Then if  $\hat{O}$  is pseudo-Hermitian operator with discrete spectrum  $\lambda$  eigenstates  $|\psi\rangle$ , then the definition of the inner product gives the expectation values

$$\langle\psi_m|\hat{O}\psi_n\rangle_\rho = \lambda_n \langle\psi_m|\psi_n\rangle_\rho \quad \text{and} \quad \langle\hat{O}\psi_m|\psi_n\rangle_\rho = \lambda_m^* \langle\psi_m|\psi_n\rangle_\rho.$$

Thus implying that

$$(\lambda_n - \lambda_m^*) \langle\psi_m|\psi_n\rangle_\rho = 0.$$

Moreover,  $\lambda_n = \lambda_m^*$  can be true in two cases –  $\lambda_n = \lambda_n^*$  for all eigenvalues of  $\hat{O}$  or there exists pairs of eigenvalues which are complex conjugates of each other. For any

other combination of , this implies that  $\langle \psi_n | \psi_m \rangle = 0$ . However, this conditions on the eigenvalues is simply the condition for pseudo-Hermitian operators and should the eigenvalues all be real, then the operator  $\hat{O}$  will be self-adjoint<sup>4</sup> with respect to the  $\rho$ -inner product. With this in mind theorem 4.22 provides a natural way of normalising states orthogonal by definition 4.21.

**Theorem 4.22.** *The eigenstates  $|\psi_n\rangle$  of an operator  $\hat{O}$  with a discrete spectrum  $\lambda_n$  can be normalised, i.e. redefined with respect to the  $\rho$ -inner product, as*

$$\frac{\lambda_n^*}{|\lambda_n|^2} |\psi_n\rangle \rightarrow |\psi_n\rangle \Rightarrow \langle \psi_n | \psi_m \rangle_\rho = \delta_{n,m}$$

Lastly, let us note that although the  $\rho$ -inner product appears explicitly in the above considerations. This would equally hold for any similar inner product defined from  $\mathcal{PT}$ -symmetry or subsequently pseudo-Hermitian operators. It should also be immediately clear from theorem 4.20, that both definition 4.21 and theorem 4.22 holds equally well for the  $\mathcal{CPT}$ -inner product.

Having spent a significant amount of effort on the properties of operators, inner products and the associated eigenstates, let us now consider how this links to reality. That is, remembering back to non-Hermitian postulates 3 and 5 let us make some comments on the observables in  $\mathcal{PT}$ -symmetric quantum mechanics.

## 4.6 Observables

In order for a physical theory to make any sense, it needs an unique and constructive procedure for linking the mathematics to observables in the real world. Similarly to non-Hermitian postulates 3 to 5 and the standard Dirac-von Neumann axioms [33, 34] the notion of observables in this non-Hermitian formulation may be defined in terms of a particular type of operators. As seen in sections 4.2 and 4.3, several constraints on operators having a real spectrum have been formulated.

Then let us clarify the notion of an observable from non-Hermitian postulates 3 to 5:

**Definition 4.23.** Non-Hermitian operators  $\hat{O}$  associated with observables of a quantum theory, are self-adjoint operators with respect to a positive definite inner product  $\langle \cdot | \cdot \rangle_*$ . E.g. the operators  $\hat{O} \in \mathcal{B}(\mathcal{H})$  satisfies

$$\langle \psi | \hat{O} \phi \rangle_* = \langle \hat{O} \psi | \phi \rangle_*,$$

for all states  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ .

Note that the inner product described in definition 4.23 is a generalised inner product similarly to non-Hermitian postulate 4. However, if the operators are  $\mathcal{PT}$ -symmetric, a more concrete statement can be made.

<sup>4</sup>The operator  $\hat{O}$  is said to be self-adjoint with respect to the  $\rho$ -inner product in the same sense that Hermitian operators are said to be self-adjoint with respect to the Hilbert-Schmidt inner product, i.e. an operator is said to be self-adjoint with respect to some inner product  $\langle \cdot | \cdot \rangle_*$  if

$$\langle \psi | \hat{O} \phi \rangle = \langle \psi \hat{O} | \phi \rangle, \quad \forall \psi, \phi \in \mathcal{H} \text{ and } \hat{O} \in \mathcal{B}(\mathcal{H}).$$

**Corollary 4.24.**  $\mathcal{PT}$ -symmetric operators,  $\hat{O}$ , associated with observables,  $\mathcal{O}$ , in a non-Hermitian theory are pseudo-Hermitian operators associated with Hermitian operators,  $\hat{O}$ . The pseudo-Hermitian operators are related to the Hermitian operators through the pseudo-Hermiticity relations

$$\hat{O} = \eta^{-1} \hat{O} \eta \quad \text{and} \quad \hat{O}^\dagger = \rho \hat{O} \rho^{-1},$$

where  $\rho = \eta^\dagger \eta$ .

Because definition 4.23 ensures that the eigenspectra of operators associated with observables are real, then their pseudo-Hermiticity follows directly from theorem 4.9. Moreover, the existence of the maps  $\rho$  and  $\eta$  thus follows from definition 4.6 and remark 4.8 respectively. Furthermore, let  $|\tilde{\psi}\rangle, |\tilde{\phi}\rangle \in \mathcal{H}$  be eigenstates of the Hermitian operator  $\hat{O}$  and let  $|\psi\rangle, |\phi\rangle \in \mathcal{H}$  be eigenstates of the pseudo-Hermitian operator  $\hat{O}$ , where  $\hat{O}, \hat{O} \in \mathcal{B}(\mathcal{H})$  are linear operators. It thus follows that

$$\langle \tilde{\psi} | \hat{O} \tilde{\phi} \rangle = \langle \tilde{\psi} | \eta \eta^{-1} \hat{O} \eta \eta^{-1} \tilde{\phi} \rangle = \langle \tilde{\psi} | (\eta^\dagger)^{-1} \eta^\dagger \eta \hat{O} \eta^{-1} \tilde{\phi} \rangle = \langle \psi | \rho \hat{O} \phi \rangle,$$

where we have used that  $\hat{O} = \eta^{-1} \hat{O} \eta$ . It thus follows that the eigenvectors of the Hermitian and pseudo-Hermitian operators are related as  $\langle \tilde{\psi} | = \langle \psi | \eta^\dagger$  and  $|\tilde{\phi}\rangle = \eta |\phi\rangle$ . Note that these relations are in fact the same relations that were given by non-Hermitian postulate 4, in the sense that  $\eta = \sqrt{\rho}$  when  $\rho$  is a positive operator.

It should now be clear why sections 4.3 and 4.4 have been so focused with pseudo-Hermitian operators and their properties. Furthermore, to conclude the discussion of the non-Hermitian postulates in relation to  $\mathcal{PT}$ -symmetry, Mostafazadeh made the following remark on the nature of the postulates when the operators are pseudo-Hermitian:

Pseudo-Hermitian quantum mechanics shares all the postulates of conventional quantum mechanics except that the inner product of the physical Hilbert space  $\mathcal{H}_{\text{phys}}$  is not a priori fixed but determined by the eigenvalue problem for a linear (Hamiltonian) operator that acts on a reference Hilbert space  $\mathcal{H}$ . [88]

A pseudo-Hermitian formulation of  $\mathcal{PT}$ -symmetric quantum mechanics is thus closely related to the standard formulation of quantum mechanics, as seen in section 3.2. Furthermore, as an unbroken  $\mathcal{PT}$ -symmetry ensures that operators with discrete spectra have purely real eigenvalues, it is by theorem 4.9 equivalent to the operators being pseudo-Hermitian. Thus the condition of para-Hermiticity, the condition for non-Hermitian postulates 3 to 5, or equivalently pseudo-Hermiticity with real spectra can be seen as a result of requiring unbroken  $\mathcal{PT}$ -symmetry.

Furthermore, equipped with corollary 4.24 the relations between observables of Hermitian and non-Hermitian may be evaluated. Importantly, as noted by Fring, assigning physical meaning to non-Hermitian operators must be done with care. For example, the operators  $\hat{p}$  and  $\hat{x}$  associated with the Bender-Boettcher Hamiltonian, eq. (2.3), cannot be directly interpreted as the operators associated with observable momenta and positions. These are auxiliary operators which are associated to the momentum and position operators in the non-Hermitian system through the map  $\eta$  as  $\hat{P} \equiv \eta^{-1} \hat{p} \eta$  and  $\hat{X} \equiv \eta^{-1} \hat{x} \eta$ , respectively. A misidentification of which operators are associated physical

observables can thus lead to false conclusion. As noted by [80] an apparent violation of the Heisenberg uncertainty principle may appear as in general

$$[\hat{p}, \hat{x}] \not\geq \frac{\hbar}{2} \text{ while } [\hat{P}, \hat{X}] \geq \frac{\hbar}{2}. \quad (4.6)$$

The uncertainty principle holds for the physical operators  $\hat{X}$  and  $\hat{P}$  and not for the unphysical  $\hat{x}$  and  $\hat{p}$ .

## 4.7 Unitary Time Evolution

As noted above, the non-Hermitian operators does not necessarily correspond to observables in the same manner as Hermitian operators. Thus somewhat more care must be taken in generalising the time-evolution of states in order to ensure that the time-evolution remains unitary. A non-unitary time-evolution would be highly non-desirable as it would destroy the correspondence between the states and probabilities.

In Hermitian Quantum Mechanics, the time-evolution is governed by the Hamiltonian which also corresponds to the operator corresponding to the observable energy of the system. However, the non-Hermitian Hamiltonian cannot *a priori* be taken to possess this dual purpose. Following [80], the in general time-dependent Hamiltonian operator  $\hat{H}(t)$  is the operator associated with the time-dependent Schrödinger equation, eq. (3.1). Whilst energy measurements of the system is associated with an energy operator  $\hat{\mathcal{E}}(t)$ , whose time-dependence is generated by  $\hat{H}(t)$ . In this sense, the Hamiltonian is taken to *generate time evolution*.

### 4.7.1 Conservation of Norms – Implications

By the notion of *unitary time evolution* we refer to the conservation of norms. For Hermitian Hamiltonians the usual time evolution operator  $U(t', t)$  is unitary such that the Dirac norm is time-independent, i.e.

$$\langle \psi(t) | \phi(t) \rangle = \langle \psi(0) | U^\dagger(t) U(t) | \phi(0) \rangle = \langle \psi(0) | \phi(0) \rangle \quad \text{for any } |\psi\rangle, |\phi\rangle \in \mathcal{H}.$$

If the Hamiltonian is non-Hermitian on the other hand this is generally not the case, the usual time-evolution operator is thus not unitary in the sense that  $U^\dagger U = \mathbb{1}$ .

Following [90], let us for simplicity consider a time-independent Hamiltonian  $\hat{H} \in \mathcal{B}(\mathcal{H})$ , which generally can be non-Hermitian. Then similarly to both Hermitian postulate 5 and non-Hermitian postulate 6, let us assume that the time-evolution is given by the usual Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad \text{where } |\psi\rangle \in \mathcal{H}. \quad (4.7)$$

Moreover, the Hermitian conjugate of eq. (4.7) we have the associated Schrödinger equation for the covectors  $\langle \psi | \in \mathcal{H}$ :

$$i\hbar \frac{d}{dt} \langle \psi(t) | = \langle \psi(t) | \hat{H}^\dagger \quad \text{where } |\psi\rangle \in \mathcal{H}. \quad (4.8)$$

As per usual for non-Hermitian operators the eigenvectors of  $\hat{H}$  and  $\hat{H}^\dagger$  are generally not the same, such that the norms  $\langle \psi | \psi \rangle$  are not strictly positive. Then let us assume a

metric inner product by introduce the time-independent metric  $V$ , which generally can be any type of metric operator ensuring that

$$\langle \psi | V | \psi \rangle \geq 0 \quad \text{where} \quad \langle \psi | V | \psi \rangle = 0 \quad \text{only if} \quad |\psi\rangle = 0.$$

By requiring that the  $V$ -norm is time-independent, it follows that

$$\frac{d}{dt} \langle \psi(t) | V | \psi(t) \rangle = \frac{d \langle \psi(t) |}{dt} V | \psi(t) \rangle + \langle \psi(t) | V \frac{d | \psi(t) \rangle}{dt} = 0$$

It thus follows from the Schrödinger equation, eqs. (4.7) and (4.8), that

$$i\hbar \frac{d}{dt} \langle \psi(t) | V | \psi(t) \rangle = \langle \psi(t) | \left( V \hat{H} - \hat{H}^\dagger V \right) | \psi(t) \rangle = 0.$$

The requirement of conservation of norms thus implies that

$$V \hat{H} - \hat{H}^\dagger V = 0, \tag{4.9}$$

which is merely the pseudo-Hermiticity condition, definition 4.6, given that the metric,  $V$ , is invertible. This brief calculation thus illustrates a striking fact:

*Remark 4.25.* For time-independent Hamiltonian and metric operators, conservation of norms is equivalent to requiring pseudo-Hermitian Hamiltonians.

Moreover, we note that the usual time-evolution operator and its Hermitian conjugate are solutions to eqs. (4.7) and (4.8) respectively. Furthermore, the pseudo-Hermiticity relation ensures that

$$U^\dagger(t) = \exp \left\{ \frac{i}{\hbar} \hat{H}^\dagger t \right\} = V \exp \left\{ \frac{i}{\hbar} \hat{H} t \right\} V^{-1} = V U^{-1}(t) V^{-1},$$

giving a  $U$  a new relation between its Hermitian conjugate and inverse

$$U^\dagger(t) = V U^{-1}(t) V^{-1}. \tag{4.10}$$

From this relation it follows that

$$U^\dagger(t) V U(t) = V U^{-1}(t) V^{-1} V U(t) = V,$$

such that

$$\langle \psi(t) | V | \phi(t) \rangle = \langle \psi(0) | V | \phi(0) \rangle. \tag{4.11}$$

The construction of the metric norm thus ensures that norms behave in a similar manner as the Dirac norm but also the pseudo-Hermiticity of the Hamiltonian. The above results can reformulated into the following theorem:

**Theorem 4.26.** For a system with time-independent Hamiltonian operator  $\hat{H} \in \mathcal{B}(\mathcal{H})$ , the time-evolution operator,

$$U(t) = \exp \left\{ -\frac{i}{\hbar} \hat{H} t \right\},$$

is unitary with respect to the metric inner product

$$\langle \psi | \phi \rangle_V \equiv \langle \psi | V | \phi \rangle \quad \forall |\psi\rangle, |\phi\rangle \in \mathcal{H}$$

iff  $\hat{H}$  is pseudo-Hermitian.

Furthermore, it is clear that by multiplying eq. (4.8) by the metric,  $V$ , from the right,

$$i\hbar \frac{d}{dt} \langle \psi(t) | V = \langle \psi(t) | \hat{H}^\dagger V = \langle \psi(t) | V \hat{H},$$

it forms the Schrödinger equation for the left eigenvectors of  $\hat{H}$ :

$$-i\hbar \frac{d}{dt} \langle \phi(t) | = \langle \phi(t) | \hat{H} \quad \text{where } \langle \phi(t) | = \langle \psi(t) | V \quad (4.12)$$

Before generalising these results to time-dependent systems: Note that although the above construction implies both conservation of norms and pseudo-Hermiticity, it does not imply para-Hermiticity and real spectra. Thus as long as the operator in the Schrödinger equation, the *generator of time-translations*, does not correspond to a physical observable there is *a priori* nothing preventing the time-evolution to be generated from an operator with a complex spectrum. By theorem 4.9, the complex part of spectrum of the generator of time-translations is only constrained to appear in pairs of complex conjugates.

### 4.7.2 Unitary Evolution Operator

Similarly to Hermitian quantum mechanics, the time-evolution of a state is given by a time-evolution operator which is the solution to the Schrödinger equation. Similarly to [80], the general construction of a time-evolution operator is given by the following theorem.

**Theorem 4.27.** *Let  $U(t, t') \in \mathcal{B}(\mathcal{H})$  be the time-evolution operator such that for a generally time-dependent Hamiltonian operator  $\hat{H}(t) \in \mathcal{B}(\mathcal{H})$  acting on states  $|\psi(t)\rangle \in \mathcal{H}$ . Then the states evolve as*

$$|\psi(t)\rangle = U(t, t') |\psi(t')\rangle, \quad (4.13a)$$

*under the time-evolution operator*

$$U(t, t') = \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t'}^t d\tau \hat{H}(\tau) \right\}. \quad (4.13b)$$

*Where  $\hat{T}$  denotes the time-ordering operator.*

Note that the time-evolution operator, eq. (4.13b), is the same as the time-evolution operator in Hermitian quantum mechanics. More specifically, eq. (4.13b) takes the exact same form as the unitary time-evolution operator of Quantum Field Theory [10]. However as we saw in section 4.7.1, the operator is not unitary in the ordinary sense that  $U^\dagger(t, t')U(t, t') = \mathbb{1}$ .

Moreover, from theorem 4.27 some essential properties of the unitary time-evolution operator follows rather straightforwardly.

**Corollary 4.28.** *Let  $\hat{H}(t) \in \mathcal{B}(\mathcal{H})$  be a time-dependent Hamiltonian operator with a time-evolution operator  $U(t, t') \in \mathcal{B}(\mathcal{H})$ . Then  $U(t, t')$  satisfies the Schrödinger equation,*

$$i\hbar \frac{\partial}{\partial t} U(t, t') = \hat{H}(t)U(t, t'), \quad (4.14a)$$

and has the following properties

$$U(t, t')U(t', t'') = U(t, t'') \quad (4.14b)$$

$$U(t, t) = \mathbb{1} \quad (4.14c)$$

For consistency, a short proof of these properties can be found in appendix A.4

As noted, the time-evolution operator is not unitary in the ordinary sense. However, that does not mean that it does not conserve norms as seen in section 4.7.1. Thus let us generalise theorem 4.26 to time-dependent systems:

**Theorem 4.29.** *The time-evolution operator  $U(t, t')$  is unitary with respect to some generally time-dependent metric inner product,*

$$\langle \psi(t) | \phi(t) \rangle_{\rho(t)} \equiv \langle \psi(t) | \rho(t) | \phi(t) \rangle \quad \forall |\psi(t)\rangle, |\phi(t)\rangle \in \mathcal{H},$$

if the Hamiltonian operator  $\hat{H}(t)$  satisfies the condition,

$$i\hbar \frac{d\rho(t)}{dt} = \hat{H}^\dagger(t)\rho(t) - \rho(t)\hat{H}(t), \quad (4.15)$$

at all times,  $t$ , and  $\rho(t) = \rho^\dagger(t)$ .

*Proof.* Similarly to section 4.7.1, by requiring the conservation of norms and imposing a generally time-dependent metric  $\rho(t)$  on the inner product, we find that

$$\frac{d}{dt} \langle \psi(t) | \rho(t) | \psi(t) \rangle = \frac{d}{dt} \langle \psi(t) | \rho(t) | \psi(t) \rangle + \langle \psi(t) | \frac{d\rho(t)}{dt} | \psi(t) \rangle + \langle \psi(t) | \rho(t) \frac{d|\psi(t)\rangle}{dt} = 0.$$

Then from the Schrödinger equations, eqs. (4.7) and (4.8), now with time-dependent Hamiltonians we find that

$$i\hbar \frac{d}{dt} \langle \psi(t) | \rho(t) | \psi(t) \rangle = \left\langle \psi(t) \left| \left( \rho(t)\hat{H}(t) - \hat{H}^\dagger(t)\rho(t) - \frac{i}{\hbar} \frac{d\rho(t)}{dt} \right) \right| \psi(t) \right\rangle = 0.$$

Thus implying that

$$i\hbar \frac{d\rho(t)}{dt} = \hat{H}^\dagger(t)\rho(t) - \rho(t)\hat{H}(t),$$

in order for norms to be conserved. Furthermore as the most general solution of eq. (4.15) is [86, 87]:

$$\rho(t) = U^{-1\dagger}(t, 0)\rho(0)U^{-1}(t, 0),$$

which can be rewritten as

$$U^\dagger(t, 0) = \rho(0)U^{-1}(t, 0)\rho^{-1}(t),$$

if  $\rho(t)$  is Hermitian. It thus follows that

$$U^\dagger(t, 0)\rho(t)U(t, 0) = \rho(0)U^{-1}(t, 0)\rho^{-1}(t)\rho(t)U(t, 0) = \rho(0),$$



thus implying that

$$\langle \psi(t) | \rho(t) | \psi(t) \rangle = \langle \psi(0) | \rho(0) | \psi(0) \rangle.$$

Showing that the time-evolution operator is unitary with respect to the  $\rho$ -inner product.  $\square$

Furthermore, from eq. (4.15) it follows that the inner product structure of non-Hermitian systems is not only given by the static parameters of a Hamiltonian. In general, the inner product is dynamically dependent on the Hamiltonian. Moreover, we see that theorem 4.29 reduces to theorem 4.26 except for the detail on the Hermiticity of the metric. This detail will not be of practical use as the Hermiticity of metric follows from theorem 4.12 if the Hamiltonian has a real spectrum. Note however that if the pseudo-Hermiticity condition, definition 4.6, to be fully invertible the metric in theorem 4.26 should also be Hermitian<sup>5</sup>.

From the proof of corollary 4.28 we can also make the following remark:

*Remark 4.30.* The existence of the generalisation of pseudo-Hermiticity relation in time,

$$i\hbar \frac{d\rho(t)}{dt} = \hat{H}^\dagger(t)\rho(t) - \rho(t)\hat{H}(t),$$

is a necessary and sufficient condition for unitary evolution with respect to the  $\rho$ -metric inner product.

Note that the metric map,  $\rho$ , clearly ensures unitary evolution by theorem 4.12. However, as noted by [90], the existence of the pseudo-Hermitian map  $\eta$  is not necessary. That is, the connection to a Hermitian operator is not a necessary requirement and unitary evolution is supported even when the eigenvalues of the Hamiltonian form complex conjugate pairs.

Having established these general properties of the unitary time evolution induced by the Hamiltonian, let us now briefly make some comments on the case where  $\hat{H}(t)$  is of a para-Hermitian type.

### 4.7.3 Time-dependent Pseudo-Hermiticity

Continuing with a time-dependent non-Hermitian Hamiltonian operator  $\hat{H}(t)$  acting on states  $|\psi(t)\rangle \in \mathcal{H}$ . Let us now assume that there exists a time-dependent Hermitian Hamiltonian operator  $\hat{h}(t)$  acting on states  $|\phi(t)\rangle \in \mathcal{H}'$  associated with  $\hat{H}$ . Both Hamiltonians are generators of the time-evolution of the states in their respective Hilbert spaces through the Schrödinger equation. Generalising theorem 4.7 the Hamiltonians are related through the *time-dependent Dyson equation* [80]:

---

<sup>5</sup>The general argument is as follows: Because  $\hat{H}^\dagger = V\hat{H}V^{-1}$  and  $V$  is invertible, then  $\hat{H} = V^{-1}\hat{H}^\dagger V$ . However, by taking the Hermitian adjoint of the latter, it follows that

$$V^\dagger \hat{H} V^{-1\dagger} = V \hat{H} V^{-1},$$

which is fulfilled if  $V = V^\dagger$ .

**Theorem 4.31.** *Let  $\hat{H}(t) \in \mathcal{B}(\mathcal{H})$  be a non-Hermitian operator and  $\hat{h}(t) \in \mathcal{B}(\mathcal{H}')$  a time-dependent Hermitian operator. Suppose there exists a map  $\eta(t) : \mathcal{H} \rightarrow \mathcal{H}'$  such that the Hamiltonians are related through a pseudo-Hermitian similarity transformation at some time  $t_0$ . At any given time, the Hamiltonians are related by the time-dependent Dyson equation:*

$$\hat{h}(t) = \eta(t)\hat{H}(t)\eta^{-1}(t) + i\hbar\frac{\partial\eta(t)}{\partial t}\eta^{-1}(t). \quad (4.16)$$

The proof of this is rather simple, but for reference it can be found in appendix A.4.

From theorem 4.31 it is clear that although a pseudo-Hermitian map can be constructed at every time  $t$  as long as the pseudo-Hermiticity relation, definition 4.6 or more specifically theorem 4.7, exists at some time  $t_0$ . The power of theorem 4.31 is that the evolution of the map in time can be highly non-trivial, it allows us to relate the eigenstates of the Hermitian and non-Hermitian operators at all times. However, the map can be highly non-trivial such that in practice it might not be an easy task to construct the map. Theorem 4.31 can similarly to remark 4.30 be seen as the equation generating the time-evolution of the pseudo-Hermitian map  $\eta$ . Moreover, construction of a metric operator  $\rho(t)$  similarly to theorem 4.12 ensures that the metric operator satisfies remark 4.30.

Furthermore, as noted by Fring, [80], eq. (4.16) takes the same form as gauge-transformation<sup>6</sup>. That is, if there exists a class of similarity transformations  $\eta$  satisfying eq. (4.16), then choosing one of these similarity transformations should not change observables. As the transformation maps are in general not unique, such a choice should exist. Furthermore, as noted by Mostafazadeh, [82], multiple such maps are associated with symmetries of the Hamiltonian. Thus in comparison to gauge-transformations, if the symmetry is unphysical then the choice of maps should not impact observables.

Moreover, from theorem 4.14 it is clear that  $\mathcal{PT}$ -symmetry implies unitary evolution with respect to a metric inner product, as seen from the proof of theorem 4.29. However, the result is even stronger. In fact,  $\mathcal{PT}$ -symmetry is both a necessary and sufficient condition for unitary evolution [90]. The unitary evolution in Hermitian quantum mechanics follows directly from theorem 4.29 when the operator is Hermitian, implying a time-independent metric – the identity operator.

Having formulated the necessary foundations of  $\mathcal{PT}$ -symmetric quantum mechanics, let us now consider a simple example to illustrate some of the features previously listed in this chapter and other subtitles.

## 4.8 $\mathcal{PT}$ -Symmetric Two-Level System

Similarly to Fring<sup>7</sup> [80], let us choose the simplest example of a quantum system, a two-level system. In particular let us choose the special case of a two-level system, given by the Hamiltonian

$$H = -\frac{1}{2}(\omega\mathbb{I} + i\kappa\sigma_x + \lambda\sigma_z) = -\frac{1}{2}\begin{pmatrix} \omega + \lambda & i\kappa \\ i\kappa & \omega - \lambda \end{pmatrix}, \quad (4.17)$$

where  $\omega, \kappa, \lambda \in \mathbb{R}$  and  $\sigma_x, \sigma_z$  are the usual Pauli matrices. From the matrix expression, eq. (4.17), it is immediately clear that the Hamiltonian is non-Hermitian due to the  $\sigma_x$

<sup>6</sup>For some details on gauge-transformations and gauge-symmetries, there exists plenty of available sources. For example see any introductory book on quantum field theory, e.g. [10–12]

<sup>7</sup>It should be noted that the following example follows an example by [80] very closely.

components being imaginary.

Furthermore, it is easily verified that condition (i) of definition 4.1, eq. (4.1a), satisfied if

$$\mathcal{PT} \equiv \sigma_z \tau, \quad (4.18)$$

where  $\tau$  represents the operation of complex conjugation to the right. Note, that eq. (4.1a) is satisfied for all allowed values of  $\omega$ ,  $\kappa$  and  $\lambda$ . Thus, for this particular choice of Hamiltonian the  $\mathcal{PT}$ -symmetry is parameter-independent. This would of course not be the case for generic Hamiltonians. Generally, the  $\mathcal{PT}$ -operator could be dependent on the parameters of the Hamiltonian,  $\mathcal{PT}(\omega, \kappa, \lambda)$ , and in principle parameters could be allowed to be time-dependent as well.

Moreover, the energy eigenvalues of the Hamiltonian, eq. (4.17), are

$$E_{\pm} = -\frac{\omega}{2} \pm \frac{\sqrt{\lambda^2 - \kappa^2}}{2}. \quad (4.19)$$

From which we see that there are three possible categorisations of the eigenvalues:

- If  $|\lambda| > |\kappa|$  then both of the energy eigenvalues are real,  $E_{\pm} \in \mathbb{R}$ .
- If  $|\lambda| < |\kappa|$  then the energy eigenvalues form a complex conjugate pair,  $E_+ = E_-^* \in \mathbb{C}$ .
- If  $|\lambda| = |\kappa|$  then the energy eigenvalues becomes degenerate  $E_+ = E_- = -\frac{\omega}{2}$ .

It is thus clear that energy eigenvalues form two distinct regions in parameter space, one of purely real eigenvalues and one of complex eigenvalues. By varying the parameters, the eigenvalues can be continuously shifted between the two regions. A plot of the eigenvalues as a function of the parameter  $\lambda$  are shown in fig. 4.1a where we have chosen  $\omega$  to be a function of  $\lambda$ , more specifically  $\omega(\lambda) = -\lambda/4$ . This particular choice is not of any significance the overall argument, but is merely to illustrate that the real part of the energy can increase across the  $\mathcal{PT}$ -broken region. Figure 4.1a shows that the eigenvalues are real in two symmetric regions and that the imaginary parts of the two eigenvalues are always of equal magnitude.

Furthermore, the normalised right eigenvectors of the Hamiltonian are

$$|\psi_{\pm}\rangle = \frac{1}{N_{\pm}} \begin{pmatrix} -\lambda \pm \sqrt{\lambda^2 - \kappa^2} \\ -i\kappa \end{pmatrix} \quad (4.20)$$

where  $N_{\pm}$  is a normalisation constant. From theorem 4.18 we know that the the right eigenvectors are related to the left by the parity operator  $\mathcal{P}$ , as  $\mathcal{P}|\psi_{\pm}\rangle = s_{\pm}|\phi_{\pm}\rangle$ , where  $s_{\pm}$  is the signature. By identifying the parity operator as  $\mathcal{P} = \sigma_z$  it follows that

$$|\phi_{\pm}\rangle = \frac{s_{\pm}}{N_{\pm}} \begin{pmatrix} i(-\lambda \pm \sqrt{\lambda^2 - \kappa^2}) \\ -\kappa \end{pmatrix}.$$

As the signature is always  $\pm 1$ , it can be obtained by evaluating the inner product between left and right eigenvectors. By calculation, we find that

$$\langle \phi_{\pm} | \psi_{\mp} \rangle = 0 \quad \text{and} \quad \langle \phi_{\pm} | \psi_{\pm} \rangle = \mp s_{\pm},$$

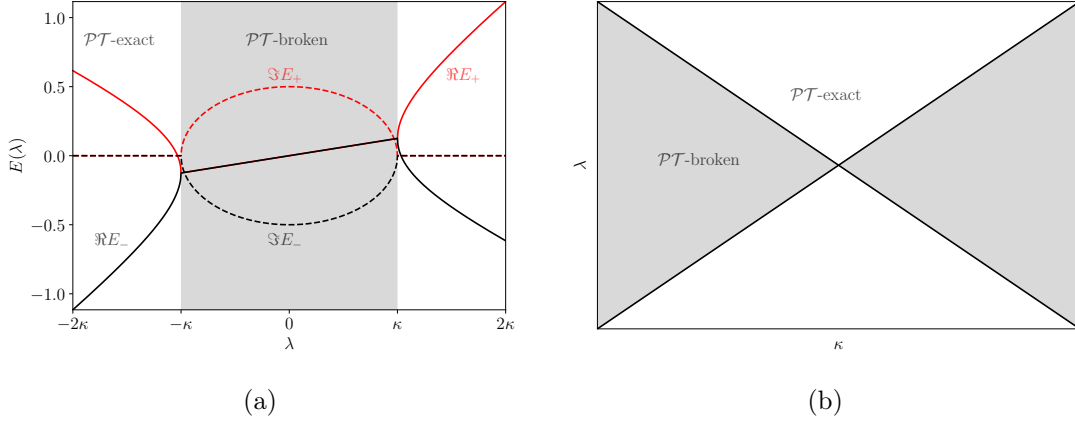


Figure 4.1: The figures shows the energy and parameter space associated with eq. (4.17), as a function of the parameter  $\lambda$ . The shaded regions represent the  $\mathcal{PT}$ -broken region and the unshaded region(s) the  $\mathcal{PT}$ -exact. (a) shows the energy eigenvalues, eq. (4.19), as a function of  $\lambda$ . The solid lines represent the real parts of the energy and the dashed lines the imaginary parts. The lower energy  $E_-$  is shown in black and the higher energy  $E_+$  in red. (b) shows the 2D parameter space of eq. (4.17). The solid lines represent  $\lambda^2 - \kappa^2 = 0$ , i.e. the singularity boundary of the phase diagram.

when the normalisation constant takes the form

$$N_{\pm} = \sqrt{2} \sqrt{\lambda^2 - \kappa^2 \pm \lambda \sqrt{\lambda^2 - \kappa^2}}.$$

It is thus clear that left and right eigenvectors form a biorthonormal basis,

$$\langle \phi_i | \psi_j \rangle = \langle \psi_j | \phi_i \rangle = \delta_{i,j},$$

when the signature takes the form  $s_{\pm} = \mp 1$ . Furthermore, note that the left and right eigenvectors form a biorthonormal basis for all choices of parameters, except  $|\lambda| = |\kappa|$ . We recognise that the point  $\lambda^2 - \kappa^2 = 0$  is troublesome, as the normalisation constant becomes zero but also because the eigenvalues coalesce. This type of singularity point is known as an *exceptional point*, which will be discussed further in section 5.2.

By using the signature,  $s_{\pm} = \mp 1$ , the left eigenvectors can thus be written as

$$|\phi_{\pm}\rangle = \frac{1}{N_{\pm}} \begin{pmatrix} i(\pm\lambda - \sqrt{\lambda^2 - \kappa^2}) \\ \pm\kappa \end{pmatrix}, \quad (4.21)$$

which also satisfies the left eigenvalue equation  $H^{\dagger} |\phi_{\pm}\rangle = E_{\pm} |\phi_{\pm}\rangle$ .

Disregarding the special point,  $\lambda^2 - \kappa^2 = 0$ , for the moment, it is clear that condition (ii) of definition 4.1 breaks down when  $|\lambda| < |\kappa|$ . That is, the eigenvectors of the Hamiltonian, eqs. (4.20) and (4.21), are no longer eigenvectors of the  $\mathcal{PT}$ -operator. This is easily seen because the root in the first component of both the left and right eigenvectors becomes imaginary and is thus affected differently by the complex conjugation part of the  $\mathcal{PT}$ -operator compared to when  $|\lambda| > |\kappa|$ . The region where the eigenvalues are in complex conjugate pairs, is thus a  $\mathcal{PT}$ -broken phase of the parameter space. Shown as a shaded region in fig. 4.1a. Furthermore, fig. 4.1b shows the *phase diagram* of the

Hamiltonian, where the shaded regions are the  $\mathcal{PT}$ -broke phases and the unshaded are the  $\mathcal{PT}$ -exact. Although, the phase diagram does not show any particularly interesting features for this simple system, phase diagrams can be of help guiding intuition when considering more exotic systems. For completeness, the solid lines indicates the position(s) of the exceptional points of the Hamiltonian, which discussed further in section 5.2. We also note that the biorthogonal basis even holds in the  $\mathcal{PT}$ -broken phase.

Furthermore, the Dyson map  $\eta$  associated with the system can be constructed directly from the right eigenvectors. The transpose of  $\eta$  takes a matrix from with the right eigenvectors as column vectors, i.e.  $\eta = (|\psi_+\rangle \quad |\psi_-\rangle)^\top$ . This map allows us to construct a metric of the desired type, i.e. satisfying theorem 4.12. The metric thus takes the form

$$\rho = \eta^\dagger \eta = \frac{1}{\sqrt{\lambda^2 - \kappa^2}} \begin{pmatrix} \lambda & i\kappa \\ -i\kappa & \lambda \end{pmatrix}, \quad (4.22)$$

which is easily seen to be Hermitian in the  $\mathcal{PT}$ -exact phase. Using the metric, the relation between the Hamiltonian and its Hermitian conjugate  $\rho H \rho^\dagger = H^\dagger$  can be verified. Looking at the metric, it is easily seen that  $\det \rho = 1$  and that the eigenvalues of the metric can be found to be

$$R_1 = \frac{\sqrt{\lambda^2 - \kappa^2}}{\lambda + \kappa} \quad \text{and} \quad R_2 = \frac{\lambda + \kappa}{\sqrt{\lambda^2 - \kappa^2}}$$

Note that both the map and metric breaks down at  $|\lambda| = |\kappa|$ , thus illustrating that this procedure cannot be used to circumvent the problem of the singularity of the Hamiltonian at that point.

Furthermore, it can be verified that the map satisfies the definition of pseudo-Hermiticity, theorem 4.7,

$$h = \eta H \eta^{-1} = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}. \quad (4.23)$$

The Dyson map  $\eta$ , thus allows us to find the Hermitian counterpart of theorem 4.7 and as a bonus, the Hermitian matrix is in this case diagonal. Note that in the  $\mathcal{PT}$ -broken phase the eigenvalues becomes complex conjugate pairs, breaking the Hermiticity of the matrix  $h$ . This is not unexpected as the Dyson map was constructed in one regime of theorem 4.9, that is purely real eigenvalues. In the  $\mathcal{PT}$ -broken regime another Dyson map could be constructed according to theorem 4.9. However as  $\eta$  is constructed from the eigenvectors, which are biorthogonal and span the eigenspace of  $H$ , except at  $|\lambda| = |\kappa|$ , the map  $\eta$  still exists in the  $\mathcal{PT}$  broken phase as a similarity transform. Note however, that the transformed matrix will not be Hermitian, nor will it be the Hermitian adjoint of the Hamiltonian. The square of  $\eta$ , the metric operator on the other hand retains its property as a pseudo-Hermitian map in accordance with definition 4.6 in both the  $\mathcal{PT}$ -broken and exact phases.

As demonstrated above the metric  $\rho$  satisfies the pseudo-Hermiticity relation,  $\rho H \rho^{-1} = H^\dagger$ . However, the parity operator  $\mathcal{P}$  also satisfies satisfies this relation, but as noted in section 4.4.2 it cannot be a metric operator as it is not guaranteed to give a positive semi-definite inner product. The key difference between the two operators is that  $\rho$  has only positive eigenvalues and is thus suitable for generating a positive semi-definite inner product. Whilst the parity operator have both positive and negative eigenvalues, in this case both  $\pm 1$ . Still, remembering section 4.4.2, the parity operator can be used to form an equivalent inner product, which is positive semi-definite.

Having established the Dyson map and corresponding metric, let us obtain the equivalent  $\mathcal{CPT}$ -operator. From theorem 4.19, the left and right eigenvectors forms the new operator

$$\mathcal{C} = \frac{1}{\sqrt{\lambda^2 - \kappa^2}} \begin{pmatrix} \lambda & i\kappa \\ i\kappa & -\lambda \end{pmatrix}. \quad (4.24)$$

Combined with the parity operator, we see that

$$\mathcal{PC} = \frac{1}{\sqrt{\lambda^2 - \kappa^2}} \begin{pmatrix} \lambda & i\kappa \\ -i\kappa & \lambda \end{pmatrix} = \rho.$$

That is, the  $\mathcal{T}$  operator acts only as complex conjugation in this example, such that  $\mathcal{T}|\Psi\rangle = |\Psi\rangle^*$  for some  $|\Psi\rangle \in \mathcal{H}$ . The  $\mathcal{CPT}$ -inner product thus becomes

$$\langle \Psi | \Phi \rangle_{\mathcal{CPT}} = \langle \Psi | \mathcal{PC} | \Phi \rangle = \langle \Psi | \rho | \Phi \rangle.$$

It is thus immediately clear that the  $\mathcal{CPT}$ - and metric-inner products are equivalent for this system. Note, that both the  $\mathcal{P}$  and  $\mathcal{C}$  operators are not fundamentally invertible maps, but rather an independent operation and constructed directly from the eigenvectors of the Hamiltonian. It thus becomes clearer why the  $\mathcal{CPT}$ -inner product, and equivalently the metric-inner product, remains positive semi-definite also in the  $\mathcal{PT}$ -broken phase. The border between the two phases and the resulting physics should be considered with care as the span of the eigenvectors of the Hamiltonian no longer span the Hilbert space. This border and its characteristic properties will be the topic of section 5.2.

## Chapter 5

# Effects of Non-Hermitian Quantum Mechanics

Having established the fundamentals of non-Hermitian Quantum Mechanics, chapter 3, and  $\mathcal{PT}$ -symmetric Quantum Mechanics, chapter 4, let us now consider some emergent effects unique to non-Hermitian dynamics. There are several effects of systems being non-Hermitian, many of which has been extensively studied. A typical examples are *exceptional points* (EPs) and *non-Hermitian skin effects*, of which only the former will be addressed. For a review of non-Hermitian skin effects, see [39, 94]. Before considering EPs, let us look at a constraint on physically realisable systems with  $\mathcal{PT}$ -symmetry.

As noted in section 2.2.3, the field of optics was one of the first areas of physics where  $\mathcal{PT}$ -symmetry was implemented, both theoretically and experimentally.  $\mathcal{PT}$ -symmetry in optics was first realised in 2005 by Ruschhaupt *et al.* [95] using balanced gain and loss of energy. This and subsequent realisations, discussed in section 2.2.3, were realisations of  $\mathcal{PT}$ -symmetry in quantum systems interacting with classical potentials. As previously noted, realisations of  $\mathcal{PT}$ -symmetry in systems quantum mechanical interactions, proved difficult. The explanation of this apparent problem of  $\mathcal{PT}$ -symmetric quantum mechanics can be attributed to result by Scheel & Szameit [2] from 2018. Thus let us firstly introduce a *no-gain theorem* by Scheel & Szameit, [2], resolving ambiguities regarding loss and gain in quantum systems. The theorem provides a bound on the properties and dynamics of realisable systems described by non-Hermitian quantum mechanics. The theorem explains why initial attempts at observations  $\mathcal{PT}$ -symmetric quantum mechanics failed, whereas the classical and semi-classical systems was observed. Note that not long after the paper by Scheel & Szameit, Klauck *et al.* [53] experimentally demonstrated two-particle quantum interference in a  $\mathcal{PT}$ -symmetric system. Equipped with the result by Scheel & Szameit, Klauck *et al.* studied the dynamics of two-photon interference in an  $\mathcal{PT}$ -symmetric optical structure by utilising asymmetric loss [53].

Furthermore, as seen in chapter 4, non-Hermitian quantum mechanics need a non-trivial metric structure in order to have positive-semidefinite and conserved norms. The dynamics of these systems may thus exhibit a fundamentally different behaviour than that of Hermitian quantum mechanics. More specifically, the notion of EPs in parameter space is a recurring phenomena in studying  $\mathcal{PT}$ -symmetric quantum mechanics but also in several other areas of physics [39, 96–98]. Anticipating the analysis of solutions of a system with a non-Hermitian time-evolution equation in chapter 6, a brief presentation of EPs in quantum mechanics and their characteristic properties will be given. Although

it will not be given much attention below, the notion of EPs appear more than only quantum mechanical systems. For instance, EPs can appear in classical mechanics as well, see [97] for a very short summary.

## 5.1 A No-Gain Theorem

The difficulty in realising the generalisation of classical and semi-classical  $\mathcal{PT}$ -symmetric systems in physical quantum mechanical systems can be attributed to a phenomenon described by Scheel & Szameit. This result, however, was not found until 2018 [2], twenty years after the first paper by Bender & Boettcher discussing  $\mathcal{PT}$ -symmetric systems [1].

Although shown by considering the harmonic oscillator modes of photons, the result actually takes a stronger form applicable to a much wider range of systems [2]. The result can be stated as the following theorem:

**Theorem 5.1.** *If a quantum system,  $S$ , has a complex potential,  $V$ , where  $V$  is derived from a coupling to a reservoir and admits a description by a Langevin equation. Then the quantum eigenstates of a Hamiltonian describing  $S$  cannot be eigenstates of the  $\mathcal{PT}$ -operator.*

See [2] for the details and an explicit example of theorem 5.1.

In other words, the theorem proves that no  $\mathcal{PT}$ -symmetric quantum system that admits a complex potential can exist. Furthermore, by extending to all reservoir that can be described by Langevin's equation, the theorem effectively covers all reasonable realisations of systems coupled to physical environments. That is because any quantum mechanical system that admits a description by a Liouvillian super operator, can be shown to satisfy the generalised Langevin equation<sup>1</sup> [60]. This can be seen in relation to the Langevin equation incorporating both deterministic sources, such as external fields and classical sources, as well as fluctuating sources, such as thermal contributions [100].

Theorem 5.1 thus effectively prevents descriptions with a net gain in the system. A net gain on the system will ensure that coherent states will become thermally mixed in time [2], a similar example will be presented below. This prevents realisations of  $\mathcal{PT}$ -symmetric quantum systems in the most naive way of having a system coupled to two reservoirs, with only gain from one and loss from the other. A way around this would be through the construction of noiseless amplifiers, but such a deterministic gain process would violate the no-cloning theorem of quantum mechanics [2]. This indicates that in order to realise  $\mathcal{PT}$ -symmetric quantum systems, one must abandon the most naive constructs. Furthermore, theorem 5.1 may some sense be seen as an extension of the no-cloning theorem.

Although the result is a bit surprising, the fact that the processes of loss and gain to an external reservoir are not opposites is not unique to  $\mathcal{PT}$ -symmetric quantum mechanics. This manifestly different natures of loss and gain may also be seen through the following simple example from the realm of the quantum mechanics of open systems.

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<sup>1</sup>The traditional Langevin equation, first introduced by Paul Langevin in 1908 [99], applies to classical Brownian motion. Study of Brownian motion is concerned with random motion, however this is not a purely classical phenomenon. Steps to generalise random processes to quantum systems has been proposed, amongst which the referenced work by Kawasaki, [60].



### 5.1.1 Example – Quantum Harmonic Oscillator

As an example, let us consider a simple system described by the Hermitian Hamiltonian  $H = \hbar\omega\hat{a}^\dagger\hat{a}$  where  $\hat{a}$  and  $\hat{a}^\dagger$  are the usual harmonic oscillator ladder operators. Let the system be in contact with an environment modelled as an infinite thermal reservoir. Let the system be connected to the environment in such a way that the dynamics of system can be described by the Lindblad equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{\gamma}{2} \left( \left\{ \hat{a}\hat{a}^\dagger, \rho \right\} - 2\hat{a}^\dagger\rho\hat{a} \right), \quad (5.1)$$

where  $\rho(t)$  is the density operator of the system.

For this system the Lindblad operator  $L = \hat{a}^\dagger$  is the harmonic oscillator creation operator. Thus eq. (5.1) describes the evolution of a system with constant gain. Moreover, because the gain is constant and independent of the energy in the system, it is analogous to a system connected to a reservoir at infinite temperature ( $T = \infty$ ). Had the Lindblad operator been the annihilation operator  $\hat{a}$ , then the Lindblad equation would give the dynamics of a system of constant loss instead. Then as the loss is constant and independent of the energy of the system, it is analogous to a system connected to a reservoir at zero temperature ( $T = 0$ ). Then the interchange of  $\hat{a}^\dagger$  and  $\hat{a}$  effectively acts as interchanging gain with loss. Thus if we consider the average excitation of the oscillator,  $n = \langle \hat{a}\hat{a}^\dagger \rangle$ , eq. (5.1) ensures that  $n(t) \propto e^{+\gamma t}$  if the oscillator is exposed to gain and  $n(t) \propto e^{-\gamma t}$  for loss as shown in appendix B.1 Thus, not surprisingly, the average excitations evolves oppositely in time when comparing the net gain and net loss cases. Gain induces an increase in the excitation number and loss a decrease. Similarly, when calculating the density matrix of the system in the energy basis, starting from a single energy state, the system with gain is shown to have an increasing probability of being in energy states above the initial state. For a system with loss, the calculation shows an increasing probability of the system being in the ground state with a decaying probability of being in other states.

From looking at average excitations and probabilities of being in energy states, gain and loss appears to be reversible process. However, gain and loss are not opposite processes on a quantum system. The significant difference between gain and loss dominated processes appears when we calculate the density matrix when the initial state is a coherent state. As shown in appendix B.1, the time-evolution of the density matrix can be calculated using the transformation

$$C(\lambda, \lambda^*, t) \equiv \text{Tr} \left[ \rho e^{\lambda\hat{a}^\dagger} e^{-\lambda^*\hat{a}} \right]. \quad (5.2)$$

Then using this transformation, the Lindblad equation, eq. (5.1), can be transformed into eq. (B.9). This transformed equation can be solved using the method of characteristics [101] as shown in appendix B.1.

The time-evolution of  $\rho(t)$  can be found by finding a function  $f(\zeta, \zeta^*, t)$  such that

$$\rho(t) = \int d\zeta d\zeta^* f(\zeta, \zeta^*, t) |\zeta\rangle\langle\zeta|, \quad (5.3)$$

where  $f(\zeta, \zeta^*, t)$  can be seen as an inverse function of eq. (5.2). As shown in appendix B.1, the function  $f(\zeta, \zeta^*, t)$  can be found by insertion into the solution of the transformed Lindblad equation, eq. (B.9), when assuming the function to be Gaussian. Then if the system is in a coherent state  $|z_0\rangle$  at some initial time  $t_0$ , the amplitude,  $\langle z|\rho|z\rangle$ , for the

system in contact with a reservoir at infinite temperature to be in a coherent state  $|z\rangle$  at a time  $t$  can be found using eq. (5.3). The complete expression for this amplitude can be seen from eq. (B.14), where  $F(z(t), \zeta)$  is the integrand found from the expectation value of eq. (5.3) with respect to  $|z\rangle$ . From eq. (B.14), we identify the amplitude distribution of the system expressed in terms of a coherent basis  $|\zeta\rangle$  as

$$F_{T=\infty}(z(t), \zeta) = \frac{1}{\pi(e^{\gamma t} - 1)} e^{-\frac{|\zeta - z(t)|^2}{1 - e^{-\gamma t}}} \quad \text{where } z(t) = z_0 e^{(\frac{\gamma}{2} - i\omega)t}. \quad (5.4)$$

Stated in this manner, the distribution is only a function of time through the rotating state  $z(t)$ . Furthermore, note that the amplitude distribution takes the form of a Gaussian, where the initial distribution has zero width. That corresponds to the initial amplitude distribution of the system being a delta function. Moreover, note that the width of the distribution eq. (5.4),

$$2\sigma^2 = 1 - e^{-\gamma t}, \quad (5.5)$$

does not give the normalisation of the distribution as it would for a proper Gaussian. That is the coefficient in front of the exponential in eq. (5.4) is not  $1/2\pi\sigma^2$ , which is the proper normalisation constant for a complex Gaussian [102]. That is because the coefficient is the normalisation for the inverse transformation of eq. (5.2), not  $\langle z|\rho(t)|z\rangle$ . Hence the integral of eq. (5.4) over all values of  $\zeta$  does not give one. This implies that the probability of the system being in a coherent state is not conserved.

For comparison, a similar calculation can be performed for the QHO at zero temperature as well. As shown in appendix B.2.2 the amplitude distribution, eq. (B.17), remains a delta function at all times. Thus showing that a system prepared in a coherent state will remain in coherent state indefinitely. Furthermore, the evolution of the coherent state was found to be

$$z(t) = z_0 e^{-(\frac{\gamma}{2} + i\omega)t}. \quad (5.6)$$

It is thus clear that the harmonic oscillator behaves quite differently in the two cases. Figure 5.1 shows the magnitude,  $z(t)$ , state of the coherent state  $|z(t)\rangle$  for a short period of time. For simplicity we have set the ratio  $\gamma/\omega = 0.1$ . From fig. 5.1, as well as the explicit expressions of  $z(t)$ , we see that the two solutions rotates in different directions in the complex plane. Moreover, the solution for  $T = 0$  is seen to decay away, which is not surprising as the environment will constantly pull energy from the system. The solution for  $T = \infty$  however, is shown to grow in time. Due to the signs of the  $\omega$  terms in the exponents being the same it is clear that reversing the time-evolution of in one of the expressions for  $z(t)$  does not yield the other.

Furthermore, from eq. (5.4) it is clear that although the initial amplitude distribution of the QHO at  $T = \infty$  delta function, it will not remain a delta function. The amplitude will broaden in time as shown by fig. 5.2 where the amplitude distribution is plotted over the complex plane, at six select times. From the figure, we see that if the system starts out in a sharply defined state, it becomes smeared as time passes. Similarly to the QHO at  $T = 0$ , the peak of the distribution rotates. The direction and exact evolution of the rotation is not easily seen from fig. 5.2, but from fig. 5.1 we see that it will spiral outwards in a clock-wise direction. Moreover, note that the peak values of the distributions, as seen from the colour bars in fig. 5.2 takes very different values. However, fig. 5.2 does not depict the evolution of the amplitude in time very well.

The time evolution of the amplitude distribution for  $T = 0$  is easily enough visualised as it is constant in time, the time evolution of the amplitude distribution  $T = \infty$ , however,

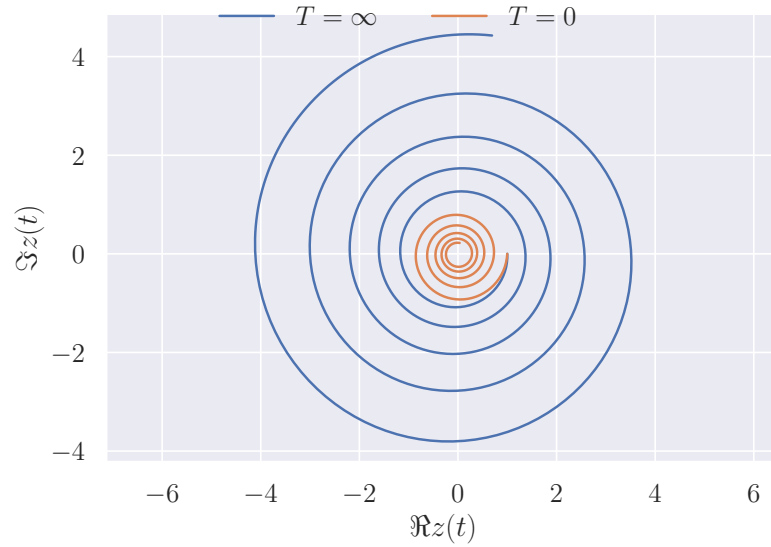


Figure 5.1: The plot shows the solution  $z(t)$  over a short time  $t$  for  $\gamma/\omega = 0.1$ . The solution for  $T = \infty$  is in blue and the solution for  $T = 0$  is in orange.

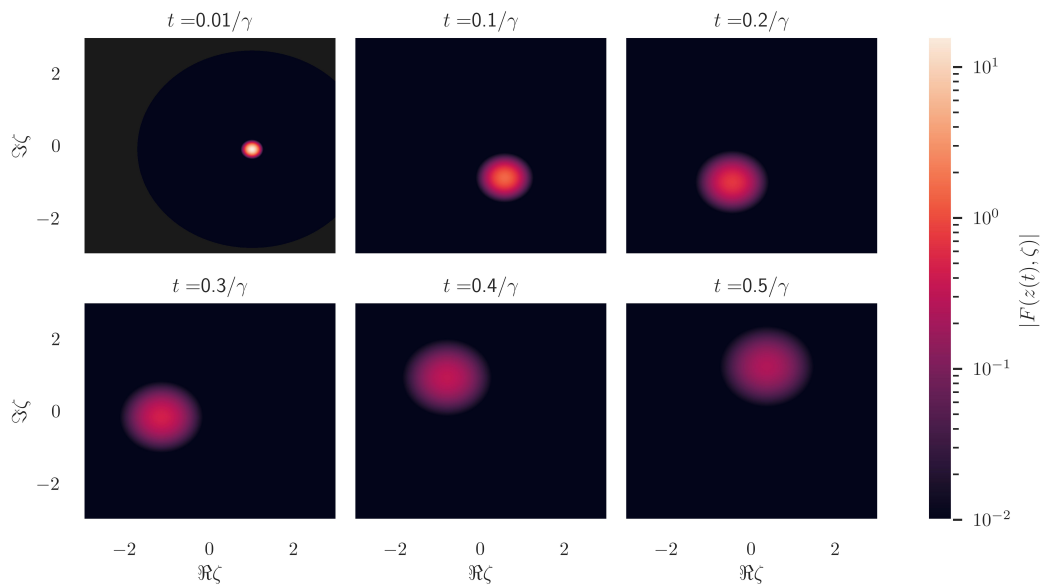


Figure 5.2: The figure shows the amplitude distribution  $F_{T=\infty}(z(t), \zeta)$  of the quantum harmonic oscillator at  $T = \infty$  at six select times, for  $\gamma/\omega = 0.1$ . In order to compare, the contour lines have a logarithmic spacing as seen from the colour bar.

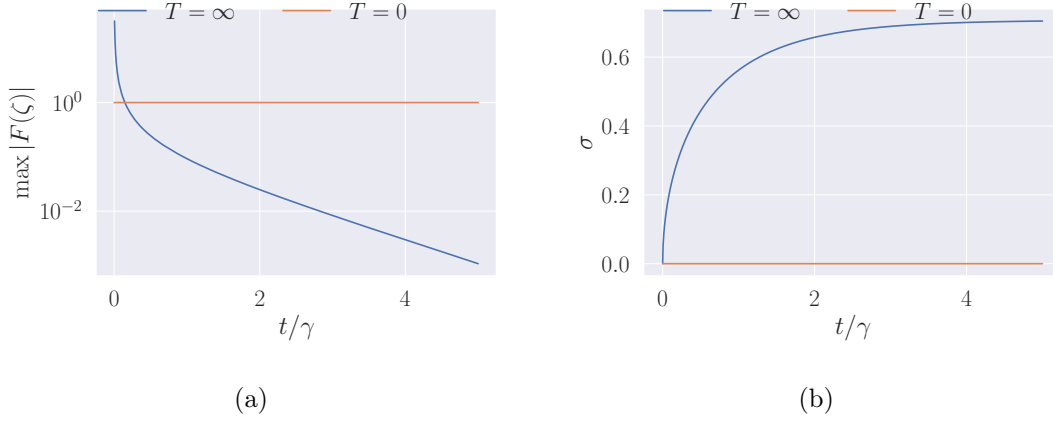


Figure 5.3: (a) The figure shows amplitude of the distributions  $F(z(t), \zeta)$  as a function of time, for both  $T = \infty$  and  $T = 0$ . (b) The figure shows width of the distributions  $F(z(t), \zeta)$  as a function of time, for both  $T = \infty$  and  $T = 0$ . In both figures  $\gamma/\omega = 0.1$ .

is not as obvious. From  $F_{T=0}(z(t), \zeta) = \delta(z(t) - \zeta)$  it is clear that the amplitude is constantly one. From fig. 5.3a we see that the peak of the amplitude  $F_{T=\infty}$ , eq. (5.4), decays rapidly in time. Note that the y-axis in fig. 5.3a is logarithmic, indicating that at early times the amplitude decays with a faster than linearly in the exponent. At later times however, the amplitude decays linearly in the exponent, which is as expected from the coefficient in eq. (5.4). That is, for  $e^{\gamma t} \gg 1$  eq. (5.4) behaves as  $F_{T=\infty}(z(t), \zeta) \sim e^{-\gamma t}$ .

Moreover, the width of the distribution, characterised by the standard deviation,  $\sigma$ , can be visualised in a similar manner. The standard deviation in amplitude distribution for  $T = 0$  is clearly zero at all times, whereas the standard deviation for the amplitude distribution at  $T = \infty$  is given by eq. (5.5). From fig. 5.3b, we see that the standard deviation for  $T = \infty$  starts out as zero, corresponding to the initial delta function. However, as time passes it increases, and very rapidly at early times. As time passes further, fig. 5.3b clearly shows that standard deviation approaches the limit of eq. (5.5),  $\sigma_{T=\infty} \rightarrow \sqrt{2}/2$  as  $t \rightarrow \infty$ . Then in comparing figs. 5.3a and 5.3b it is clear that both the broadening of  $F_{T=\infty}(z(t), \zeta)$  and its decay are greater at small times than larger. The system at  $T = \infty$  is thus driven rapidly away from a coherent state. Lastly, we could worry that for  $T = \infty$  fig. 5.3a, shows the peak growing to infinity as  $t \rightarrow 0$ . This is not a problem as the associated standard deviation goes as rapidly to zero, ensuring that the integral of  $F_{T=\infty}(z(t), \zeta)$  remains bounded to the range from zero to one.

It is thus clear that although the average excitations of the system in the two cases can be related by reversing time, it has become clear from the above discussion that a system dominated by gain cannot be related to a system dominated by loss through reversing time. From a classical standpoint this is a bit surprising, especially that we can coherently drain energy from the system whilst pumping energy cannot be done while preserving a coherent state of the system. This type of behaviour is only possible because the evolution of the system is only probabilistically deterministic, not completely deterministic as a classical system would be. The destruction of the coherent state when subjected to gain can thus be interpreted as an inevitable entanglement of the system with the reservoir, whereas we have demonstrated the similar evolution with loss does not induce an entanglement.

The above example of the Quantum Harmonic Oscillator does thus provide a simple example of the aforementioned No-Gain theorem, theorem 5.1: It clearly shows that in quantum mechanics gain and loss are not opposite dynamics. Theorem 5.1 is thus important in attempting to construct non-Hermitian systems, including systems with a  $\mathcal{PT}$ -symmetric quantum mechanical description.

## 5.2 Exceptional Points

As seen in the simple example of a  $\mathcal{PT}$ -symmetric system in section 4.8, for non-Hermitian systems there can be points in the space of parameters where the system exhibits a sudden change in some characteristic. From section 4.8, remember that the eigenvalues of the matrix

$$H \sim \begin{pmatrix} \omega + \lambda & i\kappa \\ i\kappa & \omega - \lambda \end{pmatrix} \quad (5.7)$$

suddenly changed from being real to complex conjugate pairs at  $\kappa = \lambda$ . Additionally, the two eigenvectors of  $H$  *coalesced* into one eigenvector at this point. This characteristic change in  $H$  can be attributed to the Jordan normal<sup>2</sup> form of  $H$  exhibiting a singularity at  $\kappa = \lambda$ . That is, the Jordan normal form of  $H$  is diagonal for all  $\omega, \kappa, \lambda \in \mathbb{R}$ , except  $\kappa = \lambda^3$ . This type of singularity is known as an *exceptional point* (EP) [39].

Following [96], let us define an exceptional point as

**Definition 5.2.** An *exceptional point* is a point in parameter space where the matrix,  $H$ , describing the system is defective, i.e. the geometric multiplicity is smaller than the algebraic multiplicity.

Equivalently, the EP is a point in parameter space where two or more eigenvalues of the matrix,  $H$ , are degenerate and their associated eigenvectors coalesce. The notion of the matrix being *defective* thus becomes clear as the eigenvectors can no longer span the entire vector space of which the eigenvectors are elements. It is thus clear that  $H$  is no longer diagonalisable. Furthermore, before discussing the multiplicity of matrices, let us make a few comments.

Some authors, such as Ashida *et al.*, make additional distinctions by dividing the EPs into two classes. According to the characterisation by [39], the EP in eq. (5.7) is of *first type* and can be characterised by occurring only at spectral degeneracies. Whereas EPs of the *second type* are characterised by the change in rank of the nilpotent part of the matrix [39]. EPs of the second type can thus appear without a spectral degeneracy. Lastly note, that definition 5.2 is equivalent to the definition of EPs by [22].

In literature, a distinction is sometimes made when the matrix exhibiting the EP is not the Hamiltonian matrix of the system. E.g., when EPs occur in the Liouvillian super operators, they are sometimes referred to as *Liouvillian exceptional points* (LEPs) [103] rather than EPs or Hamiltonian EPs. Furthermore, some authors also make the distinction of using EPs referring to discrete spectra and *spectral singularity* when referring to continuous spectra [89, 104]. In the following, these distinctions will usually be omitted and the generalisation of definition 5.2 to operators with continuous spectra see [89].

Before continuing on with EPs, let us take a brief look at characteristics of the algebraic and geometric multiplicity of matrices.

<sup>2</sup>Also known as Jordan canonical form, see [22] for details.

<sup>3</sup>Technically we must also require that  $\omega, \kappa, \lambda \neq 0$ .

### 5.2.1 Multiplicity of Matrices

The *algebraic multiplicity* of an eigenvalue is its multiplicity as root in the characteristic polynomial. That is, the largest integer  $k$  such that  $(\lambda - \lambda_i)^k$  divides evenly in the characteristic polynomial. The integer  $k$  is thus the dimension of the eigenspace generated by the associated eigenprojection [22].

The *geometric multiplicity* of an eigenvalue  $\lambda_i$  is the number of linearly independent eigenvectors associated with  $\lambda_i$ . That is the dimensionality of the set  $N_{\lambda_i}$  of all  $\mathbf{x} \in M$ , where  $M$  is some matrix, satisfying the eigenvalue equation

$$M\mathbf{x} = \lambda_i\mathbf{x}$$

for some eigenvalue  $\lambda_i \in \mathbb{C}$  [22]. The geometric multiplicity is thus  $\ell = \dim N_{\lambda_i}$ , or

$$\ell = \dim \ker (M\mathbf{x} - \lambda_i\mathbf{x})$$

where  $\ker$  denotes the kernel or nullspace. Moreover, it is clear that the geometric multiplicity cannot be greater than the algebraic multiplicity [22]. Due to the origins of the multiplicities as solutions to eigenvalue problems, the multiplicities are generally constrained to

$$1 \leq \ell \leq k \leq n.$$

Where  $n$  is the dimensionality of the vector space.

From the above it becomes clear that an Hermitian matrix cannot be defective. In fact neither can real symmetric matrices nor unitary matrices. Generally, a normal matrix<sup>4</sup> cannot be defective as it would imply that  $k \neq \ell$ . It is thus clear that EPs can only appear in non-Hermitian system and any system exhibiting EPs cannot be governed by Hermitian mechanics. EPs are thus a purely non-Hermitian effect.

Let us now consider a couple of examples of EPs in simple quantum systems.

### 5.2.2 Two-Level Non-Hermitian Models

Let us start with the simplest quantum system, two-level systems. Following Bergholtz *et al.*, let us consider a NH model Hamiltonian in reciprocal space [96]. For some lattice momentum  $k$ , the Hamiltonian takes the generic form

$$H(k) = d_0(k) \mathbf{1} + \mathbf{d}(k) \cdot \boldsymbol{\sigma}. \quad (5.8)$$

Let the vector  $\mathbf{d}(k)$  be written as  $\mathbf{d}(k) = \mathbf{a}(k) + i\mathbf{b}(k)$ , where  $\mathbf{a}(k), \mathbf{b}(k) \in \mathbb{R}^3$  and  $d_0 \in \mathbb{C}$ . Furthermore, let  $\boldsymbol{\sigma}$  be the usual vector of Pauli matrices such that eq. (5.8) is ensured to span all possible Hilbert spaces of two-level systems. This model was introduced by Bergholtz *et al.* as a general model for quantum systems dominated by two energy levels in order to theoretically explore the topological properties of non-Hermitian band structures in a simple manner. The calculation does however hold for arbitrary systems described by two-level systems as eq. (5.8) is the most generic Hamiltonian for quantum systems with Hilbert spaces of dimension two<sup>5</sup>. This model is thus applicable to a large variety of physical systems across physics, including the usual qubit and spin-1/2 problems [69].

<sup>4</sup>A matrix  $A$  is normal iff it commutes with its conjugate transpose  $A^\dagger$  [22]. That is,  $AA^\dagger = A^\dagger A$ , which is simply an explicit representation of the normal operators introduced in section 2.1.1

<sup>5</sup>This follows from theorem 1.3 and the fact that the Lie algebra coefficients are generally complex numbers.

We will return to the applications and experimental verifications of such non-Hermitian two-level systems in section 7.1. Note that this model is also the same model as given in [98].

As eq. (5.8) is non-Hermitian for non-zero  $\mathbf{B}$ , the eigenvalues  $E_{\pm}(k)$  are complex. The eigenvalues of  $H$  are

$$E_{\pm} = d_0 \pm \sqrt{|\mathbf{a}|^2 - |\mathbf{b}|^2 + 2i\mathbf{a} \cdot \mathbf{b}}. \quad (5.9)$$

As usual, the dependence on  $k$  has been left implicit for the sake of readability. The corresponding right eigenvectors of the system are

$$|\psi_{\pm}\rangle = \begin{pmatrix} -\frac{(a_3+ib_3) \pm \sqrt{|\mathbf{a}|^2 - |\mathbf{b}|^2 + 2i\mathbf{a} \cdot \mathbf{b}}}{a_1 + ia_2 + ib_1 - b_2} \\ 1 \end{pmatrix}, \quad (5.10)$$

and the left eigenvectors take a similar form.

From eqs. (5.9) and (5.10) it is clear that the Hamiltonian has an EP when the root becomes zero, that is when

$$|\mathbf{a}|^2 - |\mathbf{b}|^2 = 0 \quad \text{and} \quad \mathbf{a} \cdot \mathbf{b} = 0. \quad (5.11)$$

Note however that the EP does not occur at a single point in parameter space. From eq. (5.11) we see that values of  $\mathbf{a}$  form a circle of EPs in the plane perpendicular to  $\mathbf{b}$  of radius  $|\mathbf{b}|$  [98]. In general the EPs can form multi-dimensional surfaces in parameter space, but also other types of geometrical structures [96]. Although slightly misleading, the term EP is conventional and can be seen in older textbooks such as [22].

Furthermore, from eqs. (5.9) and (5.10) it is also clear that in continuously deforming the system such that parameters pass through the EP, the roles of the plus and minus solutions will be reversed. More generally, due to the EP the eigenvalues do not have two separate Riemann sheets, instead the Riemann sheets are connected such that by encircling the EP the eigenvectors interchange [98]. EPs can thus be said to induce a non-trivial topology, see [39, 96] for some general remarks on the topological properties of EPs.

The EP of this type of system is known as a *second order EP* and is characterised by having two eigenvectors coalesce, or equivalently the eigenvalue having a square root dependence in the degenerate part [96]. More generally we have that

**Theorem 5.3.** *A  $n$ -th order exceptional point has  $n$  eigenvectors coalescing and has a characteristic  $n$ -th order root dependence of the degenerate part of the associated eigenvalue.*

Theorem 5.3 is equivalent with the matrix having a  $n$ -dimensional non-diagonalisable Jordan block [105]. It should also be clear that the order of the exceptional point can at most be the dimension of the Hilbert space, as the multiplicities are bounded by the dimension.

### 5.2.3 Three-Level Model

In the above example, the EP was of the same order as the dimension of the Hilbert space. In order to see that the order of the exceptional point does not necessarily increase with the dimension of the problem, let us construct an example of a three-level system. For the general two-level system, only the three generators of  $SU(2)$  along with the identity

are needed to describe the system. It is thus fairly simple to consider completely generic systems as above. However, in order to describe generic three-level systems, the eight generators of  $SU(3)$  plus the identity are needed. It is thus significantly more difficult to consider generic systems in the same manner. The number of real parameters needed to describe the Hamiltonian in the same manner as eq. (5.8) would thus be 18, compared to the eight for the above. As the dimensionality of the associated Hilbert spaces increases, this number just grows.

Let us thus consider the following artificial Hamiltonian

$$H = \begin{pmatrix} \mu & \alpha & 0 \\ 1 & \mu & \beta \\ 0 & 1 & \mu \end{pmatrix}, \quad (5.12)$$

where  $\alpha, \beta, \mu \in \mathbb{C}$ . This Hamiltonian can be seen as a generalisation of the very simple example Hamiltonian

$$H = \begin{pmatrix} 0 & \alpha \\ 1 & 0 \end{pmatrix},$$

used by [96], which technically is a special case of the two-level Hamiltonians described by [91, 98, 105].

The energy eigenvalues of eq. (5.12) are

$$E_0 = \mu \text{ and } E_{\pm} = \mu \pm \sqrt{\alpha + \beta}, \quad (5.13)$$

and associated right eigenvectors are

$$|\psi_{R,0}\rangle = \begin{pmatrix} -\beta \\ 0 \\ 1 \end{pmatrix} \text{ and } |\psi_{R,\pm}\rangle = \begin{pmatrix} \alpha \\ \pm\sqrt{\alpha + \beta} \\ 1 \end{pmatrix}, \quad (5.14a)$$

whilst the corresponding left eigenvectors are

$$\langle\psi_{L,0}| = (-\beta \ 0 \ 1) \text{ and } \langle\psi_{L,\pm}| = \left(-\frac{1}{\alpha} \ \pm\frac{\sqrt{\alpha+\beta}}{\beta} \ 1\right). \quad (5.14b)$$

It thus becomes immediately clear that the Hamiltonian, eq. (5.12), exhibits an EP at  $\alpha = -\beta$ . At the EP, all three eigenvalues become degenerate  $E_0 = E_{\pm} = \epsilon$  but more importantly, all three eigenvectors coalesce. It should however be noted that the EP is not a third-order EP, only a second-order EP by theorem 5.3. That is, although at the EP the Hamiltonian has only one left and one right eigenvector, the EP can be reached by continuously tuning the system without changing  $|\psi_{R,0}\rangle$  and  $\langle\psi_{L,0}|$ . The coalescing can thus be seen as only happening for  $|\psi_{R,\pm}\rangle$  and  $\langle\psi_{L,\pm}|$ , respectively. This could be seen most easily from eq. (5.13), which exhibits a square root dependence in  $\alpha$  and  $\beta$ . Furthermore, from eq. (5.13) it is clear that for  $\alpha > -\beta$  the eigenvalues are all real, whereas for  $\alpha < -\beta$  the  $E_{\pm}$  are imaginary and  $E_0$  is real. The EP thus coincides with eigenvalues of the Hamiltonian, eq. (5.12), transitioning from being real to having a complex conjugate pair of eigenvalues.

A third order exceptional point can be obtained by changing the lower left entry of eq. (5.12) from zero to one, i.e.

$$H = \begin{pmatrix} 0 & \alpha & 0 \\ 1 & 0 & \beta \\ 1 & 1 & 0 \end{pmatrix}. \quad (5.15)$$



For simplicity, the diagonal elements,  $\mu$ , has also been removed, however this does not affect the analysis.

The eigenvalues of eq. (5.15) are

$$\lambda_0 = \frac{\sqrt[3]{2}(\alpha + \beta)}{\sqrt[3]{\sqrt{(27\alpha\beta)^2 - 4(3\alpha + 3\beta)^3 + 27\alpha\beta}}} + \frac{\sqrt[3]{\sqrt{(27\alpha\beta)^2 - 4(3\alpha + 3\beta)^3 + 27\alpha\beta}}}{3\sqrt[3]{2}} \quad (5.16a)$$

and

$$\lambda_{\pm} = \frac{-(1 \pm i\sqrt{3})(\alpha + \beta)}{2^{2/3}\sqrt[3]{\sqrt{(27\alpha\beta)^2 - 4(3\alpha + 3\beta)^3 + 27\alpha\beta}}} - \frac{(1 \mp i\sqrt{3})\sqrt[3]{\sqrt{(27\alpha\beta)^2 - 4(3\alpha + 3\beta)^3 + 27\alpha\beta}}}{6\sqrt[3]{2}} \quad (5.16b)$$

From the eigenvalues it is clear that  $\alpha = -\beta$  is no longer a degeneracy as it was for eq. (5.13). However, from the characteristic polynomial of eq. (5.15),

$$\lambda^3 - \lambda(\alpha + \beta) - \alpha\beta = 0,$$

it is clear that the eigenvalues all becomes degenerate at  $\alpha = \beta = 0$  but also all eigenvectors coalesce<sup>6</sup>, making it a third order EP. And from eqs. (5.16a) and (5.16b) it is clear that for  $\alpha, \beta \ll 1$  near the EP, the third roots will dominate the eigenvalues and it is easily verifiable that  $\lim_{\alpha, \beta \rightarrow 0} \lambda_0 = \lim_{\alpha, \beta \rightarrow 0} \lambda_{\pm} = 0$ .

### 5.2.4 Dependence on External Perturbations

One of the significant features of EPs are their characteristic dependence on external perturbations. Adding a small perturbation,  $\epsilon$ , to one component in eq. (5.12) corresponds to a small perturbation in the energy associated with a specific state transition. That is if we let the basis of  $H$  be

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

then  $\alpha$  is the energy associated with the transition  $|0\rangle \rightarrow |1\rangle$  because  $\langle 0|H|1\rangle = \alpha$ . Then if we add a small perturbation  $\epsilon$  to one transition, say  $|0\rangle \rightarrow |1\rangle$ , the perturbed Hamiltonian is thus

$$H' = H + \epsilon|0\rangle\langle 1| = \begin{pmatrix} \mu & \alpha + \epsilon & 0 \\ 1 & \mu & \beta \\ 0 & 1 & \mu \end{pmatrix}. \quad (5.17)$$

The eigenvalues the perturbed Hamiltonian are

$$E_0 = \mu \text{ and } E_{\pm} = \mu \pm \sqrt{\alpha + \epsilon + \beta}, \quad (5.18)$$

---

<sup>6</sup>The explicit expressions of the left and right eigenvectors take a complicated form and have thus been omitted. However, all three eigenvectors exhibit a simultaneous coalescing.

such that  $\alpha = -\beta$  will be close to the second order EP, now formally at  $\alpha = -\beta - \epsilon$ . Close to an EP, two of the energy eigenvalues are  $\lambda_{\pm} \propto \sqrt{\epsilon}$  for  $\epsilon \ll \alpha, \beta$ . We may thus conclude that close to an second order EP, the system can be have a square root dependence in external perturbations.

More generally, the dependence on external perturbations to non-Hermitian matrices is limited by the following theorem.

**Theorem 5.4.** *Non-Hermitian matrices with a  $n$ -th order exceptional point can at most exhibit a  $n$ -th root dependence in external perturbations near the exceptional point.*

The origin of theorem 5.4 can be seen from considering a small perturbation  $\epsilon$  on a Hamiltonian near its EP. Because the EP occurs at degeneracies in the eigenvalues then near an EP, then the degenerate part of the characteristic polynomial is  $\tilde{p}(\lambda) \approx \lambda^n$  with being  $n$  is the order of the exceptional point. Then adding  $\epsilon \ll 1$  in a manner similar to eq. (5.17) will at most shift the characteristic polynomial as  $p(\lambda) \rightarrow p(\lambda) - \epsilon = p'(\lambda)$ . Near the EP, the relevant part of the characteristic polynomial will thus be  $\tilde{p}' \approx \lambda^n - \epsilon$ . The dependence on the external perturbation in the eigenvalues can thus at most be  $\lambda \propto \sqrt[n]{\epsilon}$ . This simple explanation can be generalised and made rigorous by the following proof.

*Proof of theorem 5.4.* Let  $\mathcal{H}$  be a complex separable Hilbert space of dimension  $n$  and let  $A, B \in \mathcal{B}(\mathcal{H})$  be two non-normal<sup>7</sup> operators. Then [106, Lemma VIII.2.1] states that

$$d(\sigma(A), \sigma(B)) \leq 4 \frac{\|A - B\|^{1/n}}{(\|A\| + \|B\|)^{1/n-1}}.$$

Where  $\|\cdot\|$  denotes the unitarily invariant norm<sup>8</sup> and

$$d(\sigma(A), \sigma(B)) = \min_{\tau} \max_{1 \leq j \leq n} |\sigma_j(A) - \sigma_{\tau_j}(B)|,$$

where  $\tau$  denotes the minimum take over all possible permutations and  $\sigma_j(A)$  denotes an element in the spectrum of  $A$ . Moreover,

$$d(\sigma(A), \sigma(B)) \geq \max_{1 \leq j \leq n} |\lambda_j(A) - \lambda_j(B)|,$$

where  $\{\lambda_j(A)\}$  is the set of ordered eigenvalues of  $A$ .

Then if  $B$  is a perturbation on  $A$ , that is  $\|A - B\| = \epsilon \ll 1$ , it follows that

$$\max_{1 \leq j \leq n} |\lambda_j(A) - \lambda_j(B)| \leq \frac{4 \sqrt[n]{\epsilon}}{(\|A\| + \|B\|)^{1/n-1}}. \quad (5.19)$$

Moreover, if the perturbed operator  $B$  can be written as a series in  $\epsilon$ ,

$$B(\epsilon) = A + \sum_{k=1}^{\infty} \epsilon^k B_k$$

<sup>7</sup>It is here important that the operators are not normal operators, as [106, Lemma VIII.2.1] do not hold for normal operators. More specifically, if the operators are normal a much stricter condition exists, see comments in proof of theorem 5.5, and Hermitian operators are constrained by Weyl's perturbation theorem [106, Theorem VI.2.1].

<sup>8</sup>The specifics of this particular norm is are not very important for our current purposes. For interested readers, please consult [106] for details.

where  $B_k \in \mathcal{B}(\mathcal{H})$  are equipped with the order-by-order convergence criteria  $\|B_k\| \ll \epsilon^{-k}, \forall k \in \mathbb{N}_+$ . Then by requiring that the expansion is convergent [22],

$$\|B(\epsilon)\| = \left\| A + \sum_{k=1}^{\infty} \epsilon^k B_k \right\| \leq \|A\| + \sum_{k=1}^{\infty} \epsilon^k \|B_k\|,$$

then eq. (5.19) reduces to

$$\max_{1 \leq j \leq n} |\lambda_j(A) - \lambda_j(B)| \lesssim \frac{4 \sqrt[n]{\epsilon}}{(2\|A\|)^{1/n-1}},$$

assuming that the perturbation is small compared to  $A$ , i.e.  $\epsilon^k \|B_k\| \ll \|A\|, \forall k \in \mathbb{N}_+$ . It is thus clear that

$$\sup_{B(\epsilon) \in \mathcal{B}(\mathcal{H})} \max_{1 \leq j \leq n} |\lambda_j(A) - \lambda_j(B)| \propto \sqrt[n]{\epsilon}. \quad (5.20)$$

□

Hermitian matrices, however, cannot exhibit EPs this root dependence in external perturbations. However, an equivalent theorem can be given for Hermitian matrices.

**Theorem 5.5.** *Hermitian matrices can at most exhibit a linear dependence in external perturbations.*

This can quite easily be seen from adding perturbations in a similar manner to eq. (5.17). However, if the perturbed Hamiltonian is to be Hermitian, a perturbation cannot be added to only one transition rate. In order for the Hermiticity to be kept in the presence of perturbations it must also be added to the reverse. That is a perturbations to a Hermitian Hamiltonian  $h$  must be on the form

$$h' = h + \epsilon |i\rangle\langle j| + \epsilon^* |j\rangle\langle i|$$

in order for  $h'$  to be Hermitian. The characteristic polynomial  $p(\lambda)$  will thus be dependent on  $|\epsilon|^2$  due to the Hermitian symmetry of  $h'$ , i.e.  $p(\lambda) \propto \lambda^2 |\epsilon|^2$ . The eigenvalues can thus be at most dependent on  $|\epsilon|$ . More generally, theorem 5.5 follows from the following proof.

*Proof of theorem 5.5.* Theorem 5.5 follows straightforwardly from [106, Theorem VI.5.4] by the same general argument as the proof of theorem 5.4, if the matrices  $A$  and  $B$  are required to be normal matrices and that the matrix  $A - B$  is normal as well. This bound can also be extended in cases where  $A - B$  is no longer normal, e.g. [106, Theorem VI.5.1], such that theorem 5.5 holds as long as  $\|A - B\|$  is small compared to the distance between two distinct eigenvalues of  $A$ . Alternatively, theorem 5.5 also follows directly from *Weyl's Perturbation Theorem* [106, Theorem VI.2.1]. □

From theorems 5.4 and 5.5 it is clear that non-Hermitian systems can exhibit a much stronger dependence on small external perturbations than Hermitian system. Figure 5.4 explicitly shows the difference between the linear and root bounds, and it is clear that for small values of  $\epsilon$  the difference is significant. For large values, i.e.  $\epsilon > 1$  the polynomial dependencies will be dominant and a separate analysis would be needed. Moreover, from theorem 5.4 and fig. 5.4 it is clear that higher order EPs are significantly more

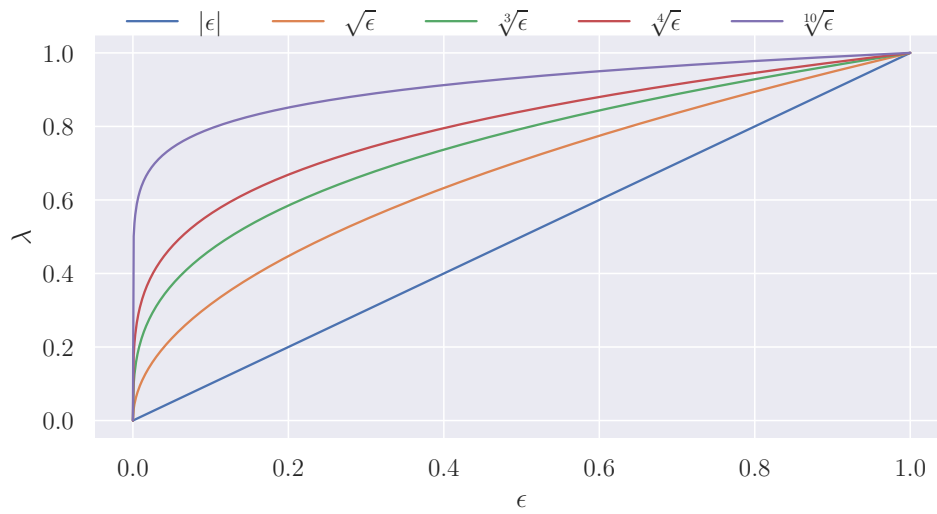


Figure 5.4: The figure shows the dependence on small external perturbations  $\epsilon$  for matrices.  $|\epsilon|$  corresponds to the bound for Hermitian matrices and the others non-Hermitian matrices near EPs.

sensitive to small perturbations, especially very small perturbations, than even second order EPs. That is a small shift in the energy near an EP will thus induce a relatively large change energy. Higher order EPs thus provide an exciting avenue for systems with beyond Hermitian sensitivity to external perturbations, this will be discussed further in section 7.1.

## Chapter 6

# Quantum System in Stochastic Environment

As noted in chapter 2, the presence of non-Hermitian dynamics in many physical systems is often attributed to the system being in contact with some environment. Quantum systems in contact with an environment are commonly known as *open quantum systems*, and have a wide range of applications to physical systems. For example, in section 5.1.1 we saw an example of a quantum system in contact with a thermal bath. Moreover, as noted section 5.2, exceptional points (EPs) is a phenomenon found only in non-Hermitian systems. Open quantum systems is arguably an excellent starting point in searching for EPs in systems beyond the simple models presented in section 5.2. Thus let us construct the following example of a *quantum system in a stochastic environment* and analyse the effect of EPs in the time-evolution.

There exists several schemes used to describe open quantum systems and dynamics are typically was either categorised as either *Markovian* or *non-Markovian*, but other categorisations exists such as Gaussian, Poisson and Bernoulli processes [107]. The dynamics of the system are said to be Markovian if the probabilities satisfies the *Markov property* [107, 108]. That is, predicting the future probabilities of the system is dependent only on the present state of the system and not previous states. Such systems are often said to be memoryless and is thus applicable to both classical and quantum systems with time-independent dynamics. Open systems are often taken to be Markovian if the interactions between the system and the environment is small compared to the internal dynamics of the system or if the interactions are of a type that prevents energy exchanged with the environment from reentering the system, e.g. exchange without reflection back into the system. That is, systems with strong interactions or so-called back-scattering are typically dependent on the history of the system, hence violating the Markov property.

There exists several derivations of the equations of motion for Markovian systems, these equations of motion are often known as *master equations* [3]. Notable examples of such master equations can be found in the Caldeira-Leggett model, the Redfield and Lindblad equations. Of these the Lindblad equation is the most commonly found in literature and the dynamics of such systems has been extensively studied [42]. E.g., the system of Harmonic oscillators discussed in section 5.1.1 was described using the Lindblad equation.

In this chapter we will derive the master equation for a class of quantum systems where the interaction with the environment can be quantified in a manner such that

the system can be treated as a closed quantum system with noise. We will consider an interaction with the environment described as a so-called *telegraph process*. In section 6.1 we will briefly introduce the notion of noise from telegraph processes before deriving the master equations for quantum systems of arbitrary, finite dimension in section 6.2. Equipped with the master equation we will in sections 6.3.1 and 6.3.3 demonstrate some characteristics of the dynamics using two-level systems as an example, in particular the existence of an exceptional point in the parameter space.

## 6.1 Telegraph Noise

In physical systems it is not uncommon that there exists two or more configurations of a system that are statistically favourable, especially for large systems. Examples of this are spin-chain configurations, magnetisation directions, charge configurations, etc. Such systems will be extremely sensitive to small perturbations, and can in many cases exhibit spontaneous transitions between the configurations. These transitions thus commonly appears to be random processes giving sudden configurational changes of the system. However, as long as the configurations are overall energetically similar, the changes will only induce changes in the equations of motion of the states of the interacting with it and not its energy expectation values.

Let us consider a quantum system governed by the free Hamiltonian  $H_{\text{free}}(t)$ . Then similarly to the *spin-fluctuator* model<sup>1</sup>, let the interactions of the quantum system with the environment be described by the Hamiltonian  $H_{\text{int}}(t)$ . Where both  $H_{\text{free}}$  and  $H_{\text{int}}$  are operators on states in the same Hilbert space. Then if we assume the at the configurational changes in the environment happen at times much longer than the relaxation times of the system, then the changes in the environment can be treated as classical [109]. Then the effect of the random changes in the environment can be encoded in a fluctuator  $\eta(t)$ , such that the dynamics of the quantum system would be fully governed by the Hamiltonian

$$H(t) = H_{\text{free}}(t) + \underbrace{H_0(t) + \eta(t)H_1(t)}_{H_{\text{int}}(t)}. \quad (6.1)$$

Where  $H_0$  and  $H_1$  are two Hamiltonians decomposing the interaction Hamiltonian into a part independent fluctuator  $\eta(t)$  and a part affected by  $\eta(t)$ . In particular,  $H_0$  is the part of the interaction Hamiltonian that is unchanged under the action of the fluctuator  $\eta(t)$  and  $H_1$  denotes the part affected by the fluctuator, but with the action of the fluctuator it self removed. In general, both  $H_0$  and  $H_1$  can be time-dependent but in practice, at least  $H_0$  will be time-independent. In complete generality, the fluctuator  $\eta(t)$  can itself be be an operator and not necessarily an unitary operator thus inducing changes in the operator norm  $\|H_{\text{int}}\|$  in time.

If we assume that the switchings between fluctuation states are random, independent events and the rates of random switching are between the fluctuation states are equal, the fluctuation model is a stochastic process [111]. The fluctuations is then often referred to as a *random telegraph process*, see [108] for a review. Furthermore, the probability  $P_k$

<sup>1</sup>The spin-fluctuator model is describes the interaction of a quantum system with a set of two-level entities, where the entities fluctuates randomly due to thermal interactions with a bath [109]. Spin-fluctuator models have been applied to describe dissipation effects in solid states, see [108], and decoherence in charge qubits, see [109] and the references therein. Spin fluctuation theory as also been applied to superconductors, see [110] for a review.

for the fluctuator to switch states  $k$  times within a time interval  $t$  is then given by the *Poisson distribution* [107],

$$P_k = \frac{(\gamma t)^k}{k!} e^{-\gamma t}. \quad (6.2)$$

Where  $\gamma$  denotes the rate of random switching between the levels of the fluctuator.

From the physical description above, it should not be surprising that telegraph noise appears in a variety of physical systems, such as metals, semi-metals, tunnel junctions and superconductors[108]. Telegraph noise is thus a viable candidate for modelling noise in quantum systems that are realisable in solid state physics, including qubit systems. In particular for systems that inherently cannot be completely separated from the environment. For further details and examples of such noise in solids, as well as the connection to the noise with  $1/f$  power spectral densities, see [108].

In the following section we will limit ourselves to the case of only two fluctuator states, but the procedure may readily be extended to several fluctuator states. An example of the extension to several fluctuator states can be found in [109], although only for two-level systems in a special case.

## 6.2 The Master Equations

Similarly Vestgård *et al.*[111] and Bergli *et al.*[109], let us derive the master equations from a probability argument. Let the states of the quantum system be described  $\rho(t)$ , then the dynamics of the system is given by the usual von-Neumann equation

$$i\hbar \frac{d\rho}{dt} = [H(t), \rho], \quad (6.3)$$

Furthermore as noted in theorem 1.3, for any quantum system represented by states in a finite dimensional Hilbert space, the density operator can be represented as<sup>2</sup>

$$\rho(t) = \frac{1}{N} \left( \mathbb{1} + \sum_i^N r_i(t) \tau_i \right). \quad (6.4)$$

Where  $N$  denotes the dimension of the Hilbert space  $\mathcal{H}$ ,  $\mathbb{1}$  is the  $N$ -dimensional identity operator and  $r_i(t) \in \mathbb{C}$  is the coefficients of the generators,  $\tau_i$  of the Lie algebra,  $\mathfrak{su}(N)$ , of  $SU(N)$ . The dynamics of the system is thus fully represented by the coefficients  $r_i(t)$ .

Conventionally, the coefficients  $r_i$  are represented by an ordered Euclidian vector  $\mathbf{r}$ , such that eq. (6.4) takes the form

$$\rho(t) = \frac{1}{N} (\mathbb{1} + \mathbf{r}(t) \cdot \vec{\tau}),$$

where  $\vec{\tau} = (\tau_1, \tau_2, \dots, \tau_N)$ .

Due to the presence of noise in the Hamiltonian, i.e. the random fluctuator, let us average over the noise. That is by averaging over eq. (6.3), any state of the system will only be known to a certain probability. The average value of  $\mathbf{r}$  is as usual

$$\langle \mathbf{r} \rangle = \int d^N r p(t, \mathbf{r}) \mathbf{r}, \quad (6.5)$$

---

<sup>2</sup>A more intuitive origin of representation of the density operators than theorem 1.3 follows doing an operator expansion of the density operator around the identity. Moreover, as the generator  $\tau_i$  are traceless the coefficient  $N^{-1}$  follows from the requirement of  $\text{Tr}\{\rho\} = 1$ .

where  $p(t, \mathbf{r})$  is the probability of the system being in a state represented by  $\mathbf{r}$ .

Assuming that there are only two fluctuator states, denoted  $\pm$ , the associated Hamiltonians can for simplicity be denoted  $H_{\pm}$ . Then let  $p_+(t, \mathbf{r})$  ( $p_-(t, \mathbf{r})$ ) denote the probability of being in a state evolving under a von-Neumann equation with the Hamiltonian  $H_+$  ( $H_-$ ). The total probability is given as the sum of the two probabilities  $p_{\pm}(t, \mathbf{r})$ , i.e.  $p(t, \mathbf{r}) = p_+(t, \mathbf{r}) + p_-(t, \mathbf{r})$ , and integrates to one at all times

$$\int d^N r p(t, \mathbf{r}) = 1.$$

Equivalently, the probability of the system being in a state represented by the density operator  $\rho$  at a time  $t$  is

$$p(t, \rho) = p_+(t, \rho) + p_-(t, \rho).$$

Then the probability that the system will evolve under  $H_+$  at a time  $t + \epsilon$ , where  $\epsilon \ll 1$ , is given by

$$p_+(t + \epsilon, \rho) = \alpha p_+(t, \rho - U_+(\epsilon) \rho U_+^\dagger(\epsilon)) + \beta p_-(t, \rho - U_-(\epsilon) \rho U_-^\dagger(\epsilon)). \quad (6.6)$$

Where coefficients  $\alpha$  and  $\beta$  are given by the Poisson distribution, eq. (6.2), and are to leading order epsilon  $\alpha \approx P_0 = 1 - \gamma \epsilon + \mathcal{O}(\epsilon^2)$  and  $\beta \approx P_1 = \gamma \epsilon + \mathcal{O}(\epsilon^2)$ .  $\alpha$  is thus the probability of the fluctuator not changing during the time interval and  $\beta$  the probability of it changing. Furthermore,

$$U_{\pm}(\epsilon) = \exp\left\{-\frac{i}{\hbar} \int_t^{t+\epsilon} dt' H_{\pm}(t')\right\} \quad (6.7)$$

is the usual unitary time-evolution operator from  $t$  to  $t + \epsilon$  according to  $H_{\pm}(t)$ . Furthermore, by the same argument, the probability of the system evolving under  $H_-$  at a time  $t + \epsilon$  is

$$p_-(t + \epsilon, \rho) = \alpha p_-(t, \rho - U_-(\epsilon) \rho U_-^\dagger(\epsilon)) + \beta p_+(t, \rho - U_+(\epsilon) \rho U_+^\dagger(\epsilon)). \quad (6.8)$$

Then by expanding eq. (6.7) as well as eqs. (6.6) and (6.8) to first order in  $\epsilon$  we find that

$$\dot{p}_+(t, \rho) = -\gamma(p_+(t, \rho) - p_-(t, \rho)) + \frac{i}{\hbar} [H_+, \rho] \nabla p_+, \quad (6.9a)$$

$$\dot{p}_-(t, \rho) = +\gamma(p_+(t, \rho) - p_-(t, \rho)) + \frac{i}{\hbar} [H_-, \rho] \nabla p_- \quad (6.9b)$$

where  $\nabla p_{\pm}$  denotes the gradient<sup>3</sup> of  $p_{\pm}$  with respect to  $\rho$ .

<sup>3</sup>On a technical; The commutator in eq. (6.9) is an operator of the same dimension as its entries, then in a similar fashion as eq. (6.11) it can be represented as

$$[H_{\pm}, \rho] \nabla p_{\pm} = A = a_0 \mathbb{1} + \mathbf{a} \cdot \vec{\tau}.$$

The product with  $\nabla p_{\pm}$  is thus formally

$$[H_{\pm}, \rho] \nabla p_{\pm} = A_{\pm} \nabla p_{\pm} = \sum_i^N a_i \frac{\partial p_{\pm}}{\partial r_i},$$

which is a scalar quantity. The dimensionality of eq. (6.9) is thus correct, although the notation perhaps a bit confusing if read carefully.



These are thus the master equations for the evolution of the probabilities of the system. The necessary steps to arrive at the above equations are explained in somewhat more detail in appendix C.1.1, but note that it is necessary to assume that the rate of change of  $H_{\pm}(t)$  in time is much smaller than  $\epsilon$ . That is, if the Hamiltonians changes abruptly in time, then the expansion of eq. (6.7) in terms of  $\epsilon$  will no longer hold.

The master equations, eq. (6.9), are the immediate generalisation to the master equations found for  $p_+$  and  $p_-$  in [109, 111]. These master equations were explicitly found for two-level systems, whilst eq. (6.9) holds for systems of arbitrary countable dimension.

Furthermore, let us define the expectation values

$$\mathbf{m}_{\pm}(t) = \int d^N r p_{\pm}(t, \mathbf{r}) \mathbf{r}, \quad (6.10)$$

in accordance with eq. (6.5).  $\mathbf{m}_{\pm}(t)$  thus purely auxiliary quantities introduced for calculations convenience with the property that

$$\mathbf{m}_+(t) + \mathbf{m}_-(t) = \langle \mathbf{r}(t) \rangle.$$

Similarly to eq. (6.4), let Hamiltonians  $H_{\pm}$  be expressed in terms of the generators of  $\mathfrak{su}(N)$  Lie algebra, such that

$$H_{\pm} = d_0^{\pm} \mathbf{1} + \mathbf{d}_{\pm} \cdot \vec{\tau}. \quad (6.11)$$

Where  $d_0 \in \mathbb{C}$  and  $\mathbf{d}_{\pm} \in \mathbb{C}^N$ .

The master equations, eq. (6.9), may thus be rewritten as

$$\dot{m}_i^{\pm} = \mp \gamma (m_i^+ - m_i^-) + \frac{1}{\hbar} d_j^{\pm} m_k^{\pm} f_{i,j,k} \quad (6.12)$$

as shown in appendix C.1.2, where  $m_i^{\pm}$  denotes  $i$ th component of eq. (6.10) and  $f_{i,j,k}$  are the structure constants of the  $\mathfrak{su}(N)$  algebra. Through eq. (6.4), it could equivalently have been written representation independent manner

$$\dot{\rho}_{\pm} = \mp \gamma (\rho_+ - \rho_-) - \frac{i}{\hbar} [H_{\pm}, \rho_{\pm}], \quad (6.13)$$

where  $\rho_{\pm}$  are averaged and purely auxiliary quantities. The definitions of  $\rho_{\pm}$  is given by eq. (C.4).

The averaged dynamics of the system under the influence of the stochastic telegraph noise can thus be found by solving eq. (6.13). However it is not clear how to do so for a system of arbitrary size  $N$ , let us thus consider the simplest case of a two-level system to explore the dynamics. First, note that in the limit that  $\gamma \rightarrow 0$ , eq. (C.4) decouples and readily reduces expected von-Neumann equation,

$$\lim_{\gamma \rightarrow 0} \dot{\rho}_{\pm} = -\frac{i}{\hbar} [H_{\pm}, \rho_{\pm}].$$

### 6.3 Two-Level Systems

As usual when demonstrating the workings of a procedure, let us consider the case of a two-level system. Let us consider a generic two-level system under the influence of a

fluctuator with two states, as described in the previous sections. The Hamiltonian be given by eq. (6.11) where the generators  $\tau_i$  of the  $\mathfrak{su}(2)$  are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Furthermore, the Pauli matrices obey the commutation relation

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{i,j,k}\sigma_k,$$

where the Einstein summation convention is implied and  $\varepsilon_{i,j,k}$  is the anti-symmetric Levi-Civita symbol. The master equations can thus be written as the vector equation

$$\dot{\mathbf{m}}_{\pm} = \pm\gamma(\mathbf{m}_+ - \mathbf{m}_-) + \frac{2}{\hbar}\mathbf{d}_{\pm} \times \mathbf{m}_{\pm}, \quad (6.14)$$

using the fact that  $(\mathbf{d}_{\pm} \times \mathbf{m}_{\pm})_k = \varepsilon_{i,j,k}d_i^{\pm}m_j^{\pm}$ . From eq. (6.14) it is clear that it is coupled in two different ways. Firstly, the two first terms couples  $\mathbf{m}_+$  and  $\mathbf{m}_-$ , whilst the last term couples the different elements of  $\mathbf{m}_+$  and  $\mathbf{m}_-$ , respectively. In order to solve this, note that the cross product can be rewritten as

$$\frac{2}{\hbar}\mathbf{d}_{\pm} \times \mathbf{m}_{\pm} = \frac{2}{\hbar} \begin{pmatrix} 0 & -d_3^{\pm} & d_2^{\pm} \\ d_3^{\pm} & 0 & -d_1^{\pm} \\ -d_2^{\pm} & d_1^{\pm} & 0 \end{pmatrix} \begin{pmatrix} m_1^{\pm} \\ m_2^{\pm} \\ m_3^{\pm} \end{pmatrix} = D_{\pm}\mathbf{m}_{\pm}. \quad (6.15)$$

It is thus clear that eq. (6.14) can be rewritten as the matrix equation

$$\begin{pmatrix} \dot{\mathbf{m}}_+ \\ \dot{\mathbf{m}}_- \end{pmatrix} = \gamma \begin{pmatrix} \frac{D_+}{\gamma} - \mathbf{1}_3 & \mathbf{1}_3 \\ \mathbf{1}_3 & \frac{D_-}{\gamma} - \mathbf{1}_3 \end{pmatrix} \begin{pmatrix} \mathbf{m}_+ \\ \mathbf{m}_- \end{pmatrix},$$

where  $\mathbf{1}_3$  denotes the  $3 \times 3$  identity matrix. Then if we define the ordered vector  $\mathbf{m} = [\mathbf{m}_+, \mathbf{m}_-]$  of vectors, eq. (6.14) can be expressed as the simplified matrix equation

$$\dot{\mathbf{m}} = \gamma \begin{pmatrix} \alpha & \mathbf{1}_3 \\ \mathbf{1}_3 & \beta \end{pmatrix} \mathbf{m} = \gamma A\mathbf{m}, \quad (6.16)$$

where  $\alpha = \frac{D_+}{\gamma} - \mathbf{1}_3$  and  $\beta = \frac{D_-}{\gamma} - \mathbf{1}_3$ . The problem of solving eq. (6.14) has thus been reduced to diagonalising  $A$ , which in general is not easy. Furthermore, from eq. (6.15) it is clear that the matrices  $D_{\pm}$  cannot be Hermitian for non-zero<sup>4</sup>  $d_i^{\pm}$ , thus implying that in general neither is the matrix  $A$ .

### 6.3.1 A Simplified Two-Level System

Let us first consider a system with the Hamiltonians  $H_{\pm}$  taken to be on the form

$$H_{\pm} = \frac{1}{2} \begin{pmatrix} \Delta \pm v & 0 \\ 0 & \Delta \pm v \end{pmatrix} \Rightarrow \mathbf{d}_{\pm} = \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ \Delta \pm v \end{pmatrix}, \quad (6.17)$$

<sup>4</sup>If all components of the Hamiltonian are zero the entire problem reduces to a trivial stationary problem,  $\dot{\mathbf{m}} = 0$ . Thus in practice  $A$  cannot be Hermitian.

where  $\Delta, v \in \mathbb{R}$  are constants. In decomposing the Hamiltonians  $H_{\pm}$  in terms of the Pauli matrices, the vectors  $\mathbf{d}_{\pm}$  can be represented as vectors on a Bloch sphere. Where for this simple system, the Hamiltonians are simply two vectors of different length along the  $\sigma_3$  direction.

Moreover, as the Hamiltonians are time-independent then transforming eq. (6.16) will not induce additional terms. Thus  $A$  can be diagonalised by the matrix  $S$  such that  $J = S^{-1}AS$  is a diagonal matrix such that eq. (6.16) reduces to the diagonal differential matrix equation

$$\dot{\mathbf{n}} = \gamma J \mathbf{n}, \quad (6.18)$$

where we defined  $\mathbf{n} = S^{-1}\mathbf{n}$ . Through this transformation, solving eq. (6.18) has reduced to solve a set of 6 linearly independent first order differential equations – one for each component of  $\mathbf{n}$ .

For simple Hamiltonians given by eq. (6.17), the eigenvalues of  $A$  are

$$\lambda_1 = -2 \quad \lambda_{3,4} = -\left(1 \pm \frac{i}{\gamma\hbar} \left(\Delta + \sqrt{v^2 - \gamma^2\hbar^2}\right)\right) \quad (6.19a)$$

$$\lambda_2 = 0 \quad \lambda_{5,6} = -\left(1 \pm \frac{i}{\gamma\hbar} \left(\Delta - \sqrt{v^2 - \gamma^2\hbar^2}\right)\right). \quad (6.19b)$$

In the notation above if there are multiple indices, the first refers to the plus and the second to the minus sign. Moreover, these eigenvalues are the diagonal elements of  $J$ . It is thus immediately clear that the solution of eq. (6.18) is

$$n_i(t) = e^{\gamma\lambda_i t} n_i(0), \quad (6.20)$$

due to the diagonal nature of  $J$ . Furthermore, from eq. (6.19) we see that the eigenvalues are generally complex and comes in complex conjugate pairs, thus explicitly demonstrating that the matrix  $A$  is non-Hermitian.

Let us define the decoherence rates  $T_i$  and oscillation frequencies  $\omega_i$  such that any eigenvalue  $\gamma\lambda_i = -T_i^{-1} + i\omega_i$ . That is, in general the solutions  $\mathbf{n}(t)$  can be written in component form as

$$n_i(t) = n_i(0) e^{-t/T_i} e^{i\omega_i t}. \quad (6.21)$$

It is thus clear that the decoherence rates are the negative real parts of  $\gamma\lambda_i$  and the frequencies the imaginary parts. It thus follows from eq. (6.19) that the non-zero decoherence rates are

$$T_0^{-1} = 2\gamma, \quad T_{\pm}^{-1} = \gamma \pm \gamma \operatorname{Re} \left\{ \sqrt{1 - \frac{v^2}{\gamma^2\hbar^2}} \right\}. \quad (6.22)$$

We recognise that the slowest decoherence rate,  $T_-$ , is the exact same result as found by [109] in the same case, albeit using a slightly different method of calculation.

Furthermore, it is clear that the point  $v^2 = \gamma^2\hbar^2$  is a point of particular interest, as the square root in eq. (6.22) suddenly becomes imaginary. This is easily seen from fig. 6.1 where the decoherence rates  $T_{\pm}$  abruptly becomes constant at  $v = \gamma\hbar$ . Moreover, the decoherence rates exhibit the characteristic square root behaviour of second order EP and as we will see in section 6.3.2, it is in fact an EP. Furthermore, fig. 6.1 also includes the Gaussian expectation<sup>5</sup> for reference, the figure is thus very much similar to [109,

<sup>5</sup>As demonstrated in [109] the slower decoherence rate can be approximated using a Gaussian approximation. The particulars are not of interest for the current discussion, but the result is included for reference. See [109] for details.

Figure 2]. We note from fig. 6.1 that the decoherence rates form a pair mirrored around  $T^{-1} = \gamma$  but also that for  $v \ll \gamma$ , the slower decoherence rate  $T_-^{-1}$  follows the Gaussian expectation,  $T^{-1} = v^2/2\gamma$  [109], closely. For  $v \lesssim \gamma\hbar$ , the deviation from the Gaussian expectation increases and for  $v \approx \gamma\hbar$  it is significant.

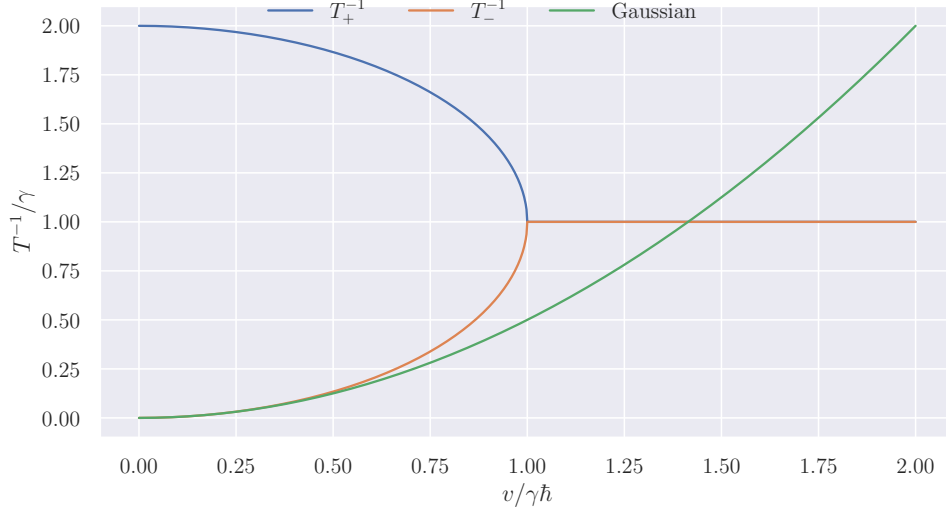


Figure 6.1: The figure show the dimensionless decoherence rates  $T_{\pm}/\gamma$  as a function of the dimensionless parameter  $v/\gamma\hbar$ . The decoherence rates are mirror images and additionally, the figure shows the expected decoherence rate from the Gaussian approximation.

Similarly to the decoherence rates, the non-zero oscillation frequencies are

$$\omega_{\pm} = \frac{\Delta}{\hbar} \pm \gamma \operatorname{Im} \left\{ \sqrt{1 - \frac{v^2}{\gamma^2 \hbar^2}} \right\}. \quad (6.23)$$

Similarly to the decoherence rates, the frequencies also exhibits a sudden change at  $v^2 = \gamma^2 \hbar^2$ . At this point the absolute value of the frequencies suddenly start to grow as seen from fig. 6.2. Furthermore, as seen from fig. 6.2 and eq. (6.23) there is only one oscillation frequency below  $v = \gamma\hbar$  and it is fully given by  $\Delta$ . Note however, that the oscillation frequency can appear in eq. (6.21) as both positive and negative. Above  $v = \gamma\hbar$ , the frequencies  $\omega_{\pm}$  split into a pair, mirrored about  $\Delta/\hbar$ .

In fear of confusion in the naming of the decoherence rates and associated frequencies, table 6.1 shows the correspondence between the solutions  $q_i$ , eigenvalues, decoherence rates and frequencies. Note especially the oscillation frequencies as some of them are accompanied with an additional negative sign.

Then to investigate if the point  $v = \gamma\hbar$  is in fact an EP, let us find the eigenvectors of  $A$  and check if they coalesce. That is the column vectors of the diagonalisation matrix  $S$ .

### 6.3.2 Exceptional Point

Let us for simplicity introduce the dimensionless variables  $\tilde{v} = v/\gamma\hbar$  and  $\mu = \sqrt{1 - \tilde{v}^2}$ , then represented as column vectors of a diagonalisation matrix  $S$  the eigenvectors of  $A$

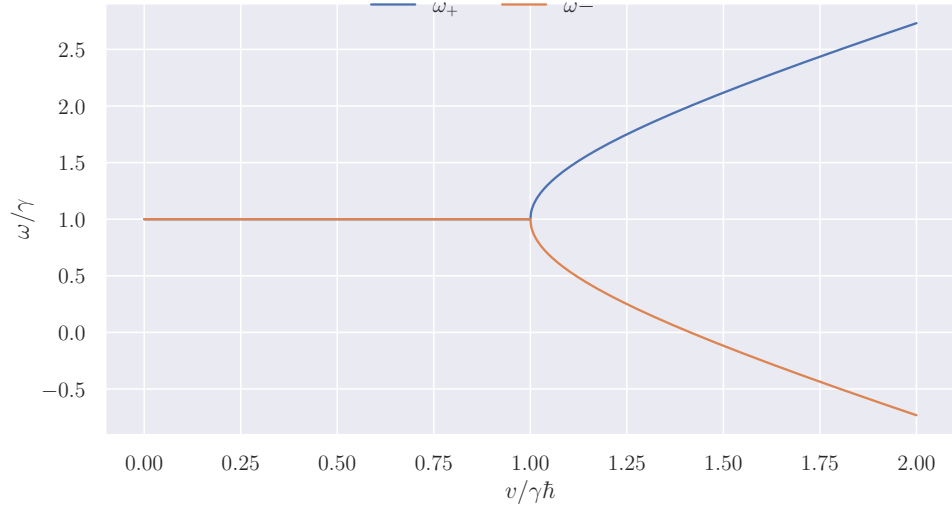


Figure 6.2: The figure show the rotational frequencies  $\omega_{\pm}$  as a function of the parameter  $v/\gamma\hbar$  for for  $\Delta/\hbar = \gamma$ . The figure shows that  $\omega_+ = \omega_-$  up to exceptional point at  $v = \gamma\hbar$ .

Table 6.1: The figure shows the correspondence between labels on solutions  $n_i$ , eigenvalues, decoherence rates and frequencies.

Index, $i$	Decoherence rate, $T^{-1}$	Frequency, $\omega$
$n_1, \lambda_1$	$T_0^{-1}$	-
$n_2, \lambda_2$	-	-
$n_3, \lambda_3$	$T_-^{-1}$	$-\omega_-$
$n_4, \lambda_4$	$T_+^{-1}$	$\omega_-$
$n_5, \lambda_5$	$T_+^{-1}$	$-\omega_+$
$n_6, \lambda_6$	$T_-^{-1}$	$\omega_+$

are

$$S = \begin{pmatrix} 0 & 0 & -\tilde{v} - i\mu & -\tilde{v} - i\mu & -\tilde{v} + i\mu & -\tilde{v} + i\mu \\ 0 & 0 & -i\tilde{v} + \mu & i\tilde{v} - \mu & -i\tilde{v} - \mu & i\tilde{v} + \mu \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & i & -i & i \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (6.24)$$

where we for simplicity has assumed both  $\Delta$  and  $v$  to be positive. We thus see that  $A$  has 6 linearly independent eigenvectors as long as  $v \neq \gamma\hbar$ . However at  $v = \gamma\hbar$ , we see that the third and fifth eigenvector coalesce but also that the fourth and sixth eigenvector coalesce. This is exactly what we would expect from the eigenvalues, eq. (6.19), where we see that at this point  $\lambda_3 = \lambda_5$  and  $\lambda_4 = \lambda_6$ . The coalescing of the eigenvectors confirms that  $A$  becomes defective at this point, and that it is in fact an exceptional point.

Furthermore, we note that for  $v \approx \gamma\hbar$ , the square roots of both the eigenvalues, eq. (6.19), and the eigenvectors, eq. (6.24), becomes strongly dependent on the ratio  $v/\gamma\hbar$ . In particular, if one of the Hamiltonians are subject to a small perturbation  $\epsilon$  then the dimensionless quantity  $\mu$  will near the EP exhibit the characteristic  $\mu \propto \sqrt{\epsilon}$  dependence.

This dependence is manifested in figs. 6.1 and 6.2, where we see large changes in  $T_{\pm}^{-1}$  and  $\omega_{\pm}$  near the exceptional point. Moreover we note, that although the number of linearly independent vectors are reduced by two at the EP, the EP is only a second order EP. This is because are two pairs of eigenvectors that coalesce, however the two pairs do not coalesce. That is row three and five becomes identical at the same point as row four and six, however row three and four (five and six) are always linearly independent.

Moreover, note from fig. 6.1 that the decoherence rate  $T_{-}^{-1}$  ( $T_{+}^{-1}$ ) has a response that increases (decreases) it well beyond linear response near the exceptional point, albeit only for  $v < \gamma\hbar$ . At the exceptional point, the behaviour is suddenly changed and for  $v > \gamma\hbar$  the decoherence rates exhibits no dependence in  $v$ . We thus see from eq. (6.22) the system has only two decoherence rates, where  $T_{0}^{-1}$  is double that of  $T_{\pm}^{-1}$ . The decoherence of the system is thus given solely by the rate  $\gamma$ . A similar argument of course holds for the frequencies as well, only with the inequalities reversed.

Note however, that the eigenvectors of matrix  $A$  does not represent the energy eigenvalues and the  $\lambda_i$  of eq. (6.19) are not energy eigenvalues. Nor can  $A$  be said to be what we usually refer to as a Liouvillian. Regardless, the exceptional point appears in the matrix responsible for the time-evolution of the system. In order to confirm that it is in fact a feature appearing in the physical dynamics of the system, let us calculate the evolution of the components of the averaged Bloch vector  $\mathbf{r}$ . Then using that  $\mathbf{m}(t) = S\mathbf{n}(t)$  and that the averaged Bloch components are  $r_i(t) = m_i(t) + m_{i+3}(t)$  by construction, eq. (6.16), it follows from eq. (6.24) that

$$r_1(t) = -(i+a)n_3(t) + (i-a)n_4(t) - (i+b)n_5(t) + (i+b)n_6(t), \quad (6.25a)$$

$$r_2(t) = (1-ia)n_3(t) + (1+ia)n_4(t) + (1-ib)n_5(t) + (1+ib)n_6(t), \quad (6.25b)$$

$$r_3(t) = r_3(0) \quad (6.25c)$$

The particular form of the components of  $\mathbf{m}(t)$  and the parametric functions  $a = \tilde{v} + i\mu$  and  $b = \tilde{v}i\mu$  appear for readability. See appendix C.2.3 for the expressions for  $\mathbf{m}_{\pm}$ . We immediately note that the third component,  $r_3$  is fully decoupled from the two others and is constant in time. This is expected as the cross product in eq. (6.14) ensures that the third components of  $\mathbf{m}_{\pm}$  remains unchanged in this special case.

Moreover, let us assume that the initial state is an average over  $\mathbf{m}_{+}$  and  $\mathbf{m}_{-}$ , i.e.  $\mathbf{m}_{+} = \mathbf{m}_{-}$ , and that the system begins in the state  $r_1(0) = 1$ . Let us for simplicity define

$$\lambda_{\pm} \equiv i\frac{\Delta}{\hbar} \pm \sqrt{1 - \frac{v^2}{\gamma^2\hbar^2}} = i\frac{\Delta}{\hbar} \pm \mu.$$

The averaged Bloch vector components thus take the form

$$r_1(t) = \frac{e^{-\gamma t}}{2} \left[ \frac{\mu+1}{\mu} e^{\gamma\mu t} + \frac{\mu-1}{\mu} e^{-\gamma\mu t} \right] \cos(\Delta t) \quad (6.26a)$$

$$r_2(t) = -\frac{e^{-\gamma t}}{2} \left[ \frac{\mu+1}{\mu} e^{\gamma\mu t} + \frac{\mu-1}{\mu} e^{-\gamma\mu t} \right] \sin(\Delta t) \quad (6.26b)$$

where the third averaged Bloch vector has been omitted as it zero by eq. (6.25c). Figure 6.3 shows the  $r_1(t)$  component for a set of values of both  $v/\gamma\hbar$  and  $\Delta/\hbar$ . It is thus clear that for  $\Delta = 0$ , the solution decays at an increasing rate as the value of  $v$  is increased towards  $\gamma\hbar$ . However, once passed the EP, increasing the value of  $v$  further does not increase

the decoherence rate further, as eq. (6.22) has a constant maximum value above the EP. Instead increasing  $v$  further induces rapid oscillations anticipated from eq. (6.23).

Furthermore, from eq. (6.26) it follows that the norm of the Bloch vector is

$$|\mathbf{r}(t)| = \frac{e^{-\gamma t}}{2} \left[ \frac{\mu + 1}{\mu} e^{\gamma \mu t} + \frac{\mu - 1}{\mu} e^{-\gamma \mu t} \right]. \quad (6.27)$$

From which we note that the Bloch vector components in the plane can be written as

$$r_1(t) = |\mathbf{r}(t)| \cos(\Delta t) \quad \text{and} \quad r_2(t) = -|\mathbf{r}(t)| \sin(\Delta t).$$

The the time-evolution of the system can thus be seen to rotate counter-clockwise in the plane with a decaying amplitude for  $v < \gamma \hbar$ . Above the EP  $\mu$  becomes imaginary, it is thus clear from eq. (6.27) that it will induce additional oscillations, exactly as seen from eq. (6.27).

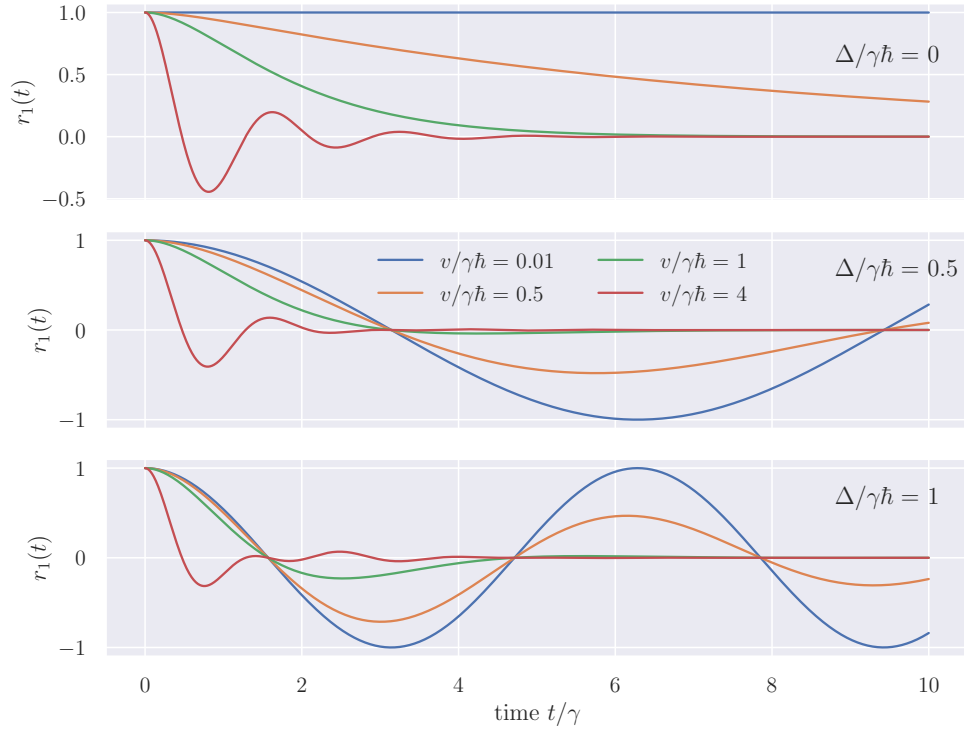


Figure 6.3: The figure shows the time-evolution of the first averaged Bloch component vector  $r_1$  as a function of time for select values of  $v$ . The three plots shows select values of  $\Delta/\gamma \hbar$  where the colour of the line represents the same value of  $v/\gamma \hbar$  in all plots.

Moreover, from fig. 6.3 we see that for non-zero values of  $\Delta$ , the solutions gain oscillations. From eq. (6.23) it is clear that these oscillators has a period of  $2\pi\Delta/\hbar$  and will thus be responsible for slow oscillations as long as  $v$  is small or comparable to  $\Delta$ . From eq. (6.23) and fig. 6.3 we identify thus  $\Delta$  as responsible for inducing rotations in the solutions. This is also seen by considering the  $r_2$  components, as shown by fig. 6.4. From fig. 6.4 it is clear that for small values of  $v$  that the averaged state vector of the system rotates in a counter clockwise direction, whereas for large values of  $v$  the rapid

oscillations dominate. This effect becomes especially clear by looking at the largest value of  $v$  in fig. 6.4.

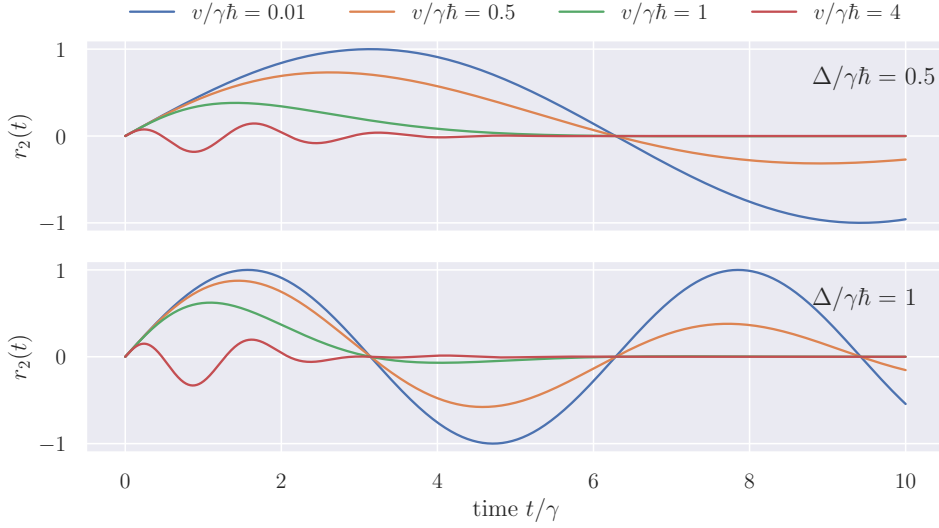


Figure 6.4: The figure shows the time-evolution of the second averaged Bloch component vector  $r_2$  as a function of time for select values of  $v$  at  $g = 0$ . The two plots shows select values of  $\Delta/\gamma\hbar$  where the colour of the line represents the same value of  $v/\gamma\hbar$  in all plots.

By setting  $\Delta = 0$  we effectively choose a rotating frame of reference. Then if we use that  $\mu = \sqrt{1 - \frac{v^2}{\gamma^2\hbar^2}}$ , eq. (6.26) reduces to

$$r_1(t) = \frac{e^{-\gamma t}}{2\mu} ((\mu + 1)e^{\gamma\mu t} + (\mu - 1)e^{-\gamma\mu t}) \quad (6.28a)$$

$$r_2(t) = 0. \quad (6.28b)$$

Note that eq. (6.28a) is the result found by [109] for the average Bloch components in the plane of the Bloch sphere. More generally, the average Bloch vectors are

$$r_1(t) = r_1(0) \frac{e^{-\gamma t}}{2\mu} ((\mu + 1)e^{\gamma\mu t} + (\mu - 1)e^{-\gamma\mu t}) \quad (6.29a)$$

$$r_2(t) = r_2(0) \frac{e^{-\gamma t}}{2\mu} ((\mu + 1)e^{\gamma\mu t} + (\mu - 1)e^{-\gamma\mu t}), \quad (6.29b)$$

where  $r_1(0)$  and  $r_2(0)$  are left as free parameters. It is thus clear that the solutions are decaying as long as  $\mu$  is real and will acquire oscillations once  $\mu$  becomes imaginary, which happens at the EP. The EP thus appear in the full dynamics of the system. For values of  $v$  above the EP, the solution can thus be rewritten in terms of trigonometric functions as

$$\frac{r_{1,2}(t)}{r_{1,2}(0)} = e^{-\gamma t} \left( \frac{\sin(\gamma\sqrt{\varepsilon}t)}{\sqrt{\varepsilon}} + \cos(\gamma\sqrt{\varepsilon}t) \right), \quad \varepsilon \equiv \frac{v^2}{\gamma^2\hbar^2} - 1.$$

It is thus clear that for  $v \gtrsim \gamma\hbar$  the solutions will both decay and oscillate, and for  $\varepsilon \ll 1$  the oscillations will be dominated in size by the sinus oscillations. For  $\varepsilon \gg 1$  on the other hand, the oscillations will be dominated by the cosine.



### 6.3.3 Generalised Qubit

Let us now consider the more general case, that is we allow the system to have a minimal energy gap  $g \in \mathbb{R}$  such that the Hamiltonians take the form

$$H_{\pm} = \frac{1}{2} \begin{pmatrix} \Delta \pm v & g \\ g & \Delta \pm v \end{pmatrix} \Rightarrow \mathbf{d}_{\pm} = \frac{1}{2} \begin{pmatrix} g \\ 0 \\ \Delta \pm v \end{pmatrix}. \quad (6.30)$$

In decomposing the Hamiltonians  $H_{\pm}$  in terms of the Pauli matrices, the vectors  $\mathbf{d}_{\pm}$  can be represented as vectors on a Bloch sphere. Figure 6.5 shows the vectors  $\mathbf{d}_{\pm}$ , where the axes has been chosen such that the 1- and 3-axes are almost in the plane of the paper. This seems a convenient choice as  $\mathbf{d}_{\pm}$  does not have any component along the 2-axis.

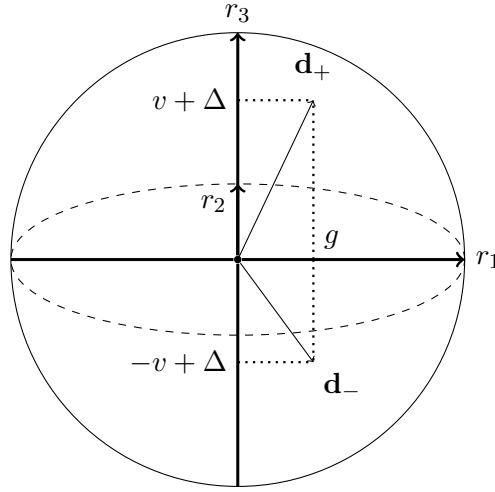


Figure 6.5: The Hamiltonians  $H_{\pm}$  of a two-level system represented in terms of the vectors  $\mathbf{d}_{\pm} = (g, 0, \Delta \pm v)$  on the Bloch sphere. The 2-axis, i.e. the  $y$ -axis, of the Bloch-coordinates is taken to point into the page (barely visible behind the 3-axis).

Although, the specific form of eq. (6.30) has been chosen for the analysis in this section, it should be noted that this is in fact a quite general form. As shown in appendix C.2.2, any pair of Hamiltonians exhibiting fluctuations along one direction can be brought to the form of eq. (6.30) through coordinate transformations. The analysis below is thus more general than it would seem at first glance, in fact the analysis will hold for all two-level systems where the fluctuator states are anti-parallel of each other. The Hamiltonians shown in eq. (6.17) can thus be seen to be the quite general for qubit systems with time-independent Hamiltonians.

For this particular system, the time-evolution is given by the matrix

$$A = \begin{pmatrix} -1 & -(\Delta + v) & 0 & 1 & 0 & 0 \\ \Delta + v & -1 & -g & 0 & 1 & 0 \\ 0 & g & -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 & -(\Delta - v) & 0 \\ 0 & 1 & 0 & \Delta - v & -1 & -g \\ 0 & 0 & 1 & 0 & g & -1 \end{pmatrix}. \quad (6.31)$$

Moreover  $\det A = 4g^2v^2$ , thus by the invertible matrix theorem it follows that  $A$  is invertible for all  $g \neq 0$  and  $v \neq 0$ . It thus follows that  $A$  has no EP for nonzero values of  $g$ , as it cannot be both invertible and defective as defective matrices are not diagonalisable.

Anyhow, in diagonalising  $A$ , we find that the eigenvalues are in general quite complicated expressions. Thus let us for simplicity state the eigenvalues for the special case of  $\Delta = 0$ :

$$\lambda_{1,2} = -\frac{\sqrt[3]{2}\xi}{3\sqrt[3]{\sqrt{4\xi^3 + 4\chi^2} \pm 2\chi}} + \frac{3}{\sqrt[3]{2}}\sqrt[3]{\sqrt{4\xi^3 + 4\chi^2} \pm 2\chi} - \frac{2}{3} \quad (6.32a)$$

$$\lambda_{3,4} = \frac{(1 + i\sqrt{3})\xi}{3 \cdot 2^{2/3}\sqrt[3]{\sqrt{4\xi^3 + 4\chi^2} \pm 2\chi}} - \frac{1 - i\sqrt{3}}{\sqrt[3]{2}}\sqrt[3]{\sqrt{4\xi^3 + 4\chi^2} \pm 2\chi} - \frac{2}{3} \quad (6.32b)$$

$$\lambda_{5,6} = \frac{(1 - i\sqrt{3})\xi}{3 \cdot 2^{2/3}\sqrt[3]{\sqrt{4\xi^3 + 4\chi^2} \pm 2\chi}} - \frac{1 + i\sqrt{3}}{\sqrt[3]{2}}\sqrt[3]{\sqrt{4\xi^3 + 4\chi^2} \pm 2\chi} - \frac{2}{3} \quad (6.32c)$$

where  $\chi$  and  $\eta$  are the parametric expressions

$$\chi = 18g^2 - 9v^2 + 8 \quad \text{and} \quad \xi = 3g^2 + 3v^2 - 4.$$

From eq. (6.32) we see that the eigenvalues form three pairs, of which eqs. (6.32b) and (6.32c) also forms two complex conjugate pairs. Unfortunately the expressions for the eigenvalues are very complicated, such that analysing them becomes much more difficult than in section 6.3.1. In order to avoid unnecessary complications, let us find the eigenvectors of  $A$  numerically in order to show the time-evolution of states, then also for non-zero values of  $\Delta$ .

Furthermore, let us consider the evolution of the averaged states  $\mathbf{r}$  for non-zero values of  $g$ . For simplicity let us choose the initial state  $\mathbf{r}(0) = (1, 0, 0)$  as in the previous subsection. Firstly, let us consider the case of  $\Delta = 0$ . The components of the average Bloch vector can be seen in fig. 6.6. By comparison to fig. 6.3 we see that the behaviour of the first component is seemingly unchanged and from the two other components in fig. 6.6, we see only small deviations from zero. Note however, that the small oscillations seemingly disappear at  $v = \gamma\hbar/2$ . We see that for  $v/\gamma\hbar = 0.01$  the oscillations are both of the largest period and amplitude, and that similarly to the case of  $g = 0$  the frequency of the oscillations increase with  $v$ . From the lower plot in fig. 6.6 we see that the oscillations of the  $r_3$  component do not appear to oscillate about zero, rather both the smaller and larger value of  $v$  clearly oscillates about a negative value.

Although some the non-zero value of  $g$  showed some effect in fig. 6.6, it did not appear that there was a significant transfer into the  $r_3$  state. Let us now instead consider the case where we set  $\Delta = g = \gamma\hbar$ . All components of the average Bloch vector can be seen from fig. 6.7. By comparison to figs. 6.3 and 6.4 we see that the non-zero  $g$  has induced a significant transfer into the previously unavailable  $r_3$  component. From fig. 6.7 it is clear that the transfer is especially significant for small values of  $v$  and that the decoherence now acts in all components of the Bloch vector. However, for the largest value of  $v$  there does not appear to be much transfer into the  $r_3$  component.

Furthermore, fig. 6.7 shows that the  $r_1$  and  $r_3$  components remains strictly positive for values of  $v$  below the EP. In comparison to fig. 6.3, we thus see that the non-zero  $g$  seemingly decouples three fourths of the Bloch sphere from the evolution. This is however not the case for large values of  $v$ . Our assumption in the previous section that  $\Delta$  induces

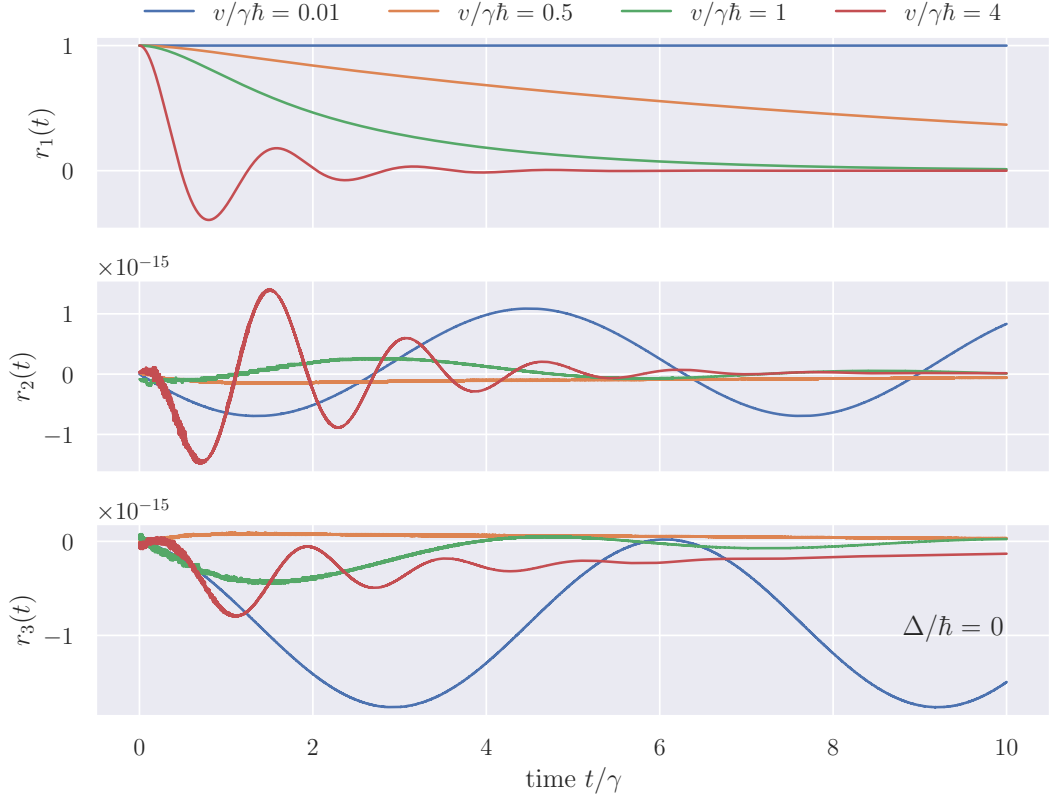


Figure 6.6: The figure shows the time-evolution of all components of the averaged Bloch vector  $\mathbf{r}(t)$  for select values of  $v$  at  $\Delta = 0$  and  $g = \gamma\hbar$ .

a rotating frame of reference no longer holds in fig. 6.7, it thus seems that a rotating frame approximation will fail in this more general case.

In order to better understand the transfer to and from the  $r_3$  component, let us instead look at the a system with the initial state  $\mathbf{r}(0) = (0, 0, 1)$ . Figure 6.8 shows the  $r_3$  component as a function of both time,  $t/\gamma$  and  $v/\hbar$  at  $\Delta = g = \hbar$ . We thus see that  $v \leq 1$  the solution oscillates onto the  $r_1$  and  $r_2$  components with an oscillation period less than  $2\pi\Delta$  as we saw from  $g = 0$ . Moreover, for  $\hbar < v \lesssim 2\hbar$  the  $r_3$  component rapidly decays without any oscillations. It in fact decays much faster than for both larger and smaller values of  $v$ . Lastly, for values of  $v \gtrsim \hbar$  the system shows a significantly slowed decoherence rate.

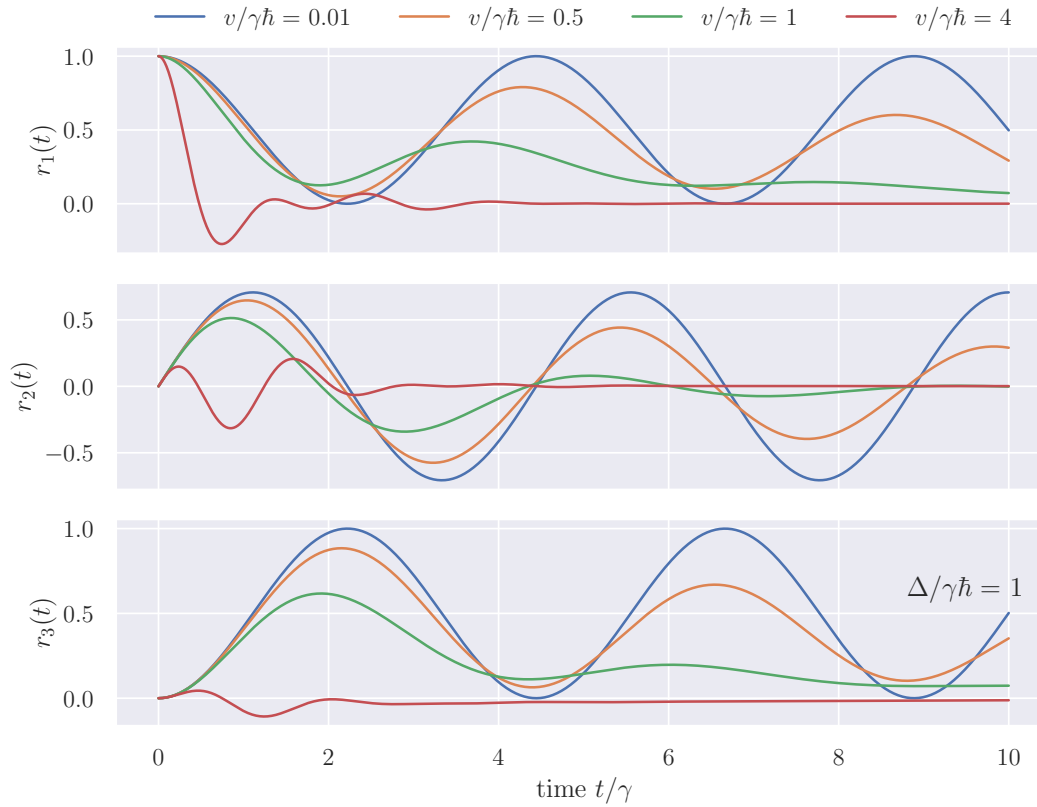


Figure 6.7: The figure shows the time-evolution of all components of the averaged Bloch vector  $\mathbf{r}(t)$  for select values of  $v$  at  $\Delta = \gamma\hbar$  and  $g = \gamma\hbar$ .

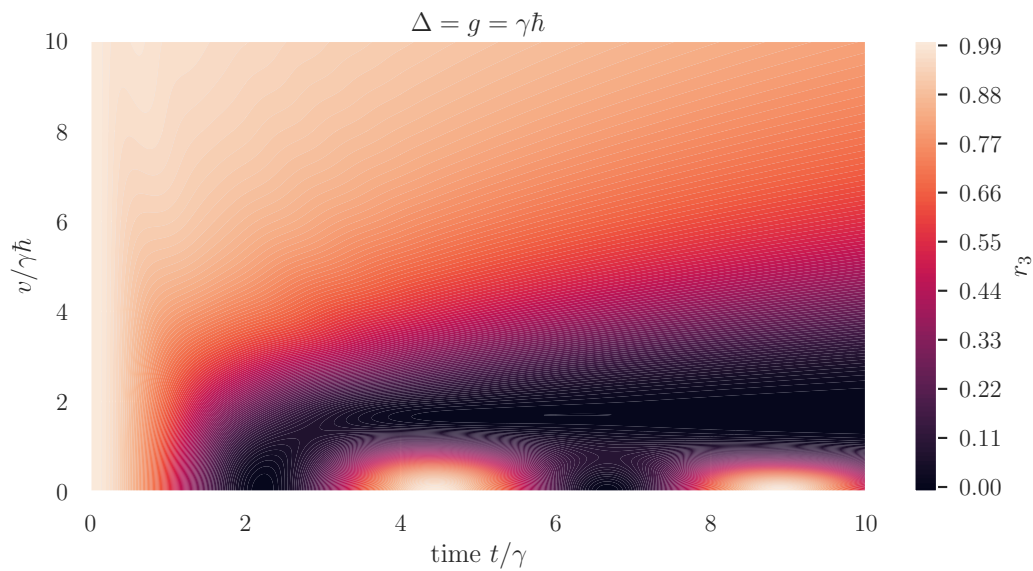


Figure 6.8: The figure shows dependency of the third averaged Bloch vector  $r_3(t)$  in both  $t$  and  $v$  at  $\Delta = g = \gamma\hbar$ .

## Chapter 7

# Recent Developments & Applications

Although only 25 years has past since the seminal paper by [1], a significant amount of work has been done on the subject of  $\mathcal{PT}$ -symmetric quantum mechanics both theoretically and experimentally. In 2016 Bender [112] reported that more than two thousand articles and more than two dozen conferences had been held since 1998. A quick search for  $\mathcal{PT}$ -symmetry and quantum using Google Scholar [113] reveals more than ten thousand results including preprints, books and conference proceedings, of which more than seven thousand has been published since 2016. In a related search using Web Of Science [114], which is slightly more restricted in terms available sources, shows an increasing amount of publications per year as shown by fig. 7.1. It should of course be noted that these searches are not particularly refined and that other related search terms do appear in them. Regardless there has been a significant increase in the number of published papers, especially in the last decade, as depicted by fig. 7.1. The increased publishing could be attributed to several factors, including being a relatively new area of study. It should also be noted that general advances in our abilities to engineer experiments and increasingly sensitive equipment is likely to be important factors.

The subjects of the articles published on  $\mathcal{PT}$ -symmetry since 1998 span almost all areas of physics and explore a wide range of phenomena. In relation to the discussion in the preceding chapters, let us look at a few topics which recently has gained some interest within  $\mathcal{PT}$ -symmetry and the greater realm of non-Hermitian physics. Moreover, let us also make a few comments on the applications of non-Hermitian phenomena to sensors, quantum computing and technology.

### 7.1 $\mathcal{PT}$ -Symmetry & EPs

In section 4.8 we saw that the breakdown of  $\mathcal{PT}$ -symmetry happened at a point where the eigenvalues became degenerate, and the associated eigenvectors coalesced. In section 5.2, this behaviour of the eigenvectors was identified with an EP in the parameters space of the Hamiltonian. As it turns out, this connection between EPs and the breakdown of  $\mathcal{PT}$ -symmetry is not coincidental. As we saw in section 4.3,  $\mathcal{PT}$ -symmetric operators are pseudo-Hermitian where the properties of pseudo-Hermitian operators were constrained by theorem 4.9. Moreover as the eigenvectors coalesce at EPs and thus no longer form a biorthogonal basis, as required for theorem 4.9. The presence of an EP thus implies

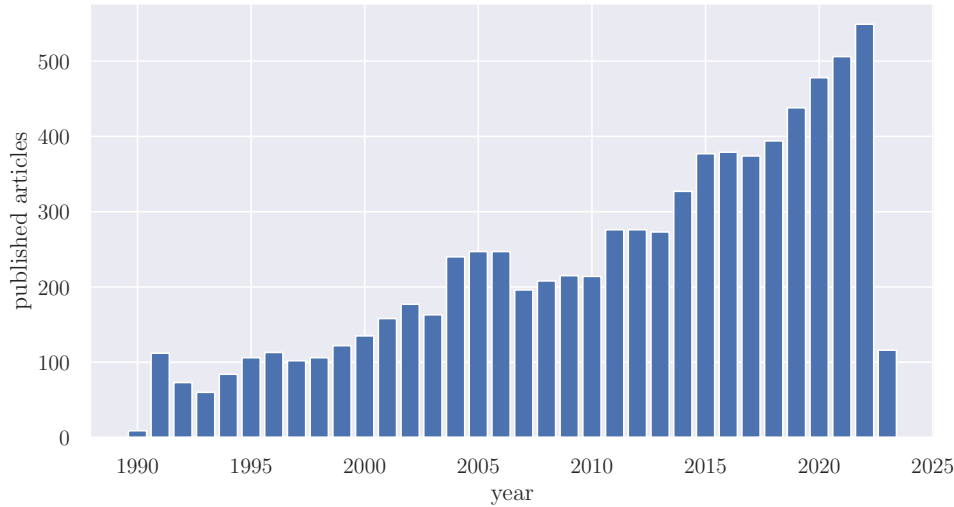


Figure 7.1: Articles published on  $\mathcal{PT}$ -symmetry per year, as of April 2023. Data from Web Of Science [114].

the breakdown pseudo-Hermiticity and the  $\mathcal{PT}$ -symmetry as well. Although introduced in the context of quantum mechanics, these properties of operators are not inherently quantum properties but can also be found in classical dynamics as noted in section 2.3.1.

As previously noted, the existence of  $\mathcal{PT}$ -symmetry and non-Hermitian effects in quantum systems are not only theoretical but have also been experimentally observed, e.g. in [53]. Moreover, as noted in section 2.2.3 observations of  $\mathcal{PT}$ -symmetry was originally confined to optical systems, but has later been extended to other areas of physics. Then not surprisingly, optics is one of the areas where non-Hermitian effects such as EPs were first observed and exploited. In particular as noted in [115], the first realisation of a fully  $\mathcal{PT}$ -symmetric system of coupled waveguides explicitly demonstrated a spontaneous breaking of  $\mathcal{PT}$ -symmetry by parametrically tuning the system [48]. More specifically, Rüter *et al.*, [48], experimentally demonstrated that for a gain below some critical threshold, the two propagation modes exhibit asymmetric power oscillations and non-reciprocal response. At some critical gain, the propagation modes coalesced and spontaneously broke the  $\mathcal{PT}$ -symmetry of the system. Above the critical gain the system showed a broken  $\mathcal{PT}$ -symmetry with an asymmetric distribution between the waveguides [48]. The sudden change in the propagation properties of the system at some critical ratio of the gain to the coupling between the waveguides can be attributed to an EP [115]. The optical experiment by Rüter *et al.* is not to dissimilar to the experimental system used by Klauck *et al.* in order to demonstrate  $\mathcal{PT}$ -symmetry breaking in two-photon quantum interference [53].

Later,  $\mathcal{PT}$ -symmetry and EPs has been applied to the study and engineering of lasers but also to construct exotic phenomena such as coherently perfect absorption, see [58, 115] for a review. Perfect absorption has also been observed for more general non-Hermitian systems in optics exhibiting EP-surfaces [116, 117].

Although it might seem like it from the above discussion, EPs and  $\mathcal{PT}$ -symmetry as not only been observed in optical systems. By studying the energy levels of a single

trapped ion as a qubit system with the  $\mathcal{PT}$ -symmetric Hamiltonian

$$H = J\sigma_x + i\Gamma\sigma_z, \quad (7.1)$$

Ding *et al.*, [118], experimentally determined the position of the EP. Here  $\Gamma$  denotes the dissipation rate and  $J$  is the coupling strength. Note that the Hamiltonian is phenomenologically<sup>1</sup> identical to our example Hamiltonian, eq. (4.17), of a  $\mathcal{PT}$ -symmetric system in section 4.8. Similarly to section 4.8 it is easy to verify that the  $\mathcal{PT}$ -operator of eq. (7.1) is  $\mathcal{PT} = \sigma_z\tau$ , where  $\tau$  denotes complex conjugation, and that it has an EP at  $|J| = |\Gamma|$ . The Hamiltonian, eq. (7.1), is through a mapping onto another Hamiltonian, still symmetric under the same  $\mathcal{PT}$  operator, experimentally realised in a dissipative single qubit-system. Theoretically, the dissipative qubit system can be calculated using the usual Lindblad master equation [119].

By an experimental protocol similar to quantum state tomography, Ding *et al.* are able to determine both the eigenvalues and the position of the EP without a fitting parameter. Furthermore, Ding *et al.* also demonstrates how the procedure also applies to more general Hamiltonians on the form of eq. (7.1) with time-dependent coefficients. E.g. the time-dependent  $\mathcal{PT}$ -symmetric Hamiltonian

$$H(t) = J[1 + \cos(\omega t)]\sigma_x + i\Gamma\frac{1 - \text{sign}\{\cos(\omega t)\}}{2}\sigma_z, \quad (7.2)$$

where  $\omega$  is a modulation frequency [118]. This periodically driven Hamiltonian represents a Floquet system, and is thus applicable to a much wider range of systems. By use of numerical calculations, [118] calculated a theoretical prediction for the phase diagram of this Floquet system. Figure 7.2 shows the numerical prediction on the right along with the results obtained from experiment on the left at a time  $t = 2\pi\hbar/\omega$ . The amplitude in fig. 7.2, as shown by the colour bar, displays the difference

$$P_J(t) - P_\Gamma(t) = |\langle\uparrow|\mathcal{U}(t)|\downarrow\rangle|^2 - |\langle\leftarrow|\mathcal{U}(t)|\rightarrow\rangle|^2$$

where  $\mathcal{U}(t)$  is the generalised unitary time evolution operator, see theorem 4.27. The vectors

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \quad \text{and} \quad |\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$$

where  $|\uparrow\rangle, |\downarrow\rangle \in \mathcal{H}(2)$  is the spin-representation of the basis states [69]. For positive values of the difference  $P_J(t) - P_\Gamma(t)$ , the system is in a  $\mathcal{PT}$ -exact phase [118]. Conversely, the system is in a  $\mathcal{PT}$ -broken phase if the difference is negative, with EPs when  $P_J(t) - P_\Gamma(t) = 0$ .

From fig. 7.2 we see that the experimental results are in good agreement with the theoretical predictions. Moreover, fig. 7.2 shows the  $\mathcal{PT}$ -broken regions becoming increasingly narrower with decreasing decoherence rates  $\Gamma$ , merging into points as  $\Gamma \rightarrow 0$ . These points of broken  $\mathcal{PT}$ -symmetry can be attributed to multi-photon resonances which are predicted and observed in different forms of periodically modulated non-Hermitian systems as well [118].

The type of experimental protocol presented in [118] provides exciting new possibilities. Similarly to quantum state tomography it provides new possibilities in experimentally

<sup>1</sup>The only notable difference is that the imaginary unit is placed in front of  $\sigma_x$  rather than  $\sigma_z$  in eq. (4.17). This difference is however not of importance as eq. (4.17) can easily be retrieved by setting  $J = i\kappa$  and  $\Gamma = -i\lambda$ .

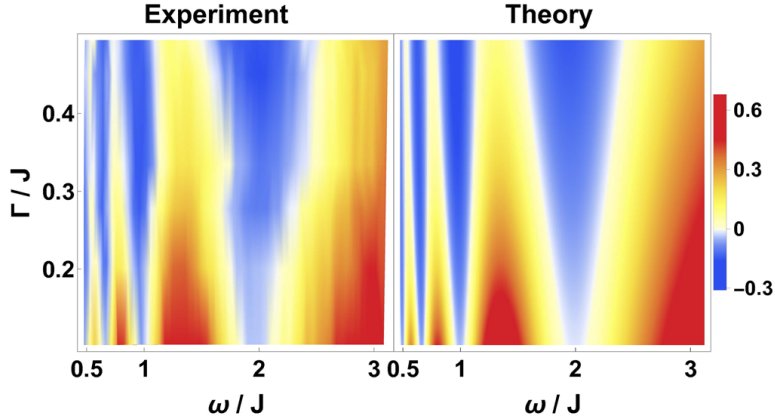


Figure 7.2: Phase diagram for the  $\mathcal{PT}$ -symmetric time-dependent Hamiltonian, eq. (7.2), at the time  $t = 2\pi\hbar/\omega$  with experimental measurement on the left and theoretical prediction on the right. The colour bar shows  $P_J(t) - P_\Gamma(t)$ , where positive values corresponds to the  $\mathcal{PT}$ -exact phase and negative values the  $\mathcal{PT}$ -broken. Reprinted from [118] with permission from the American Physical Society.

determining the quantum state of systems, especially in non-Hermitian systems [118]. Being able to determine the  $\mathcal{PT}$ -symmetric regions and eigenvalues allows for novel access to quantum systems near EPs, where the density matrix of the systems are accessible thorough regular quantum state tomography. Moreover, protocols applicable to static and periodically driven systems allows experimental access to a wide variety physical systems. Lastly, Ding *et al.* suggests that ability to precisely determine EPs can be utilised to measure weak unknown time-dependent signals by the enhanced sensitivity to perturbations [118, 119] which will be further discussed in section 7.3.

## 7.2 Decoherence in Qubits

$\mathcal{PT}$ -symmetry can also be utilised as a measure to protect the quantum states of a system from decoherence. As physical systems are almost always in contact with some uncontrollable environment, decoherence is almost always present and Liouvillian super-operators has been suggested as a means to capture both energy loss and decoherence [103]. The dynamics of dissipative systems are usually described using the Lindblad master equation, as noted in section 2.2.2. Moreover, similarly to Hamiltonian dynamics, Liouvillian dynamics can also exhibit EPs.

A recent study by Chen *et al.*, [103], demonstrates the presence of EPs in the dynamics of a superconducting qubit, induced from both energy loss and decoherence. The study is concerned with dynamics of a qubit system, where the Hamiltonian of the Lindblad master equation is Hermitian. Moreover, the Lindblad equation does not appear to be  $\mathcal{PT}$ -symmetric, in particular due an one-component jump operator. Nevertheless, as the Liouvillian operator of the system is non-Hermitian it can be shown to exhibit EPs [103]. By dynamically tuning the parameters of the system, Chen *et al.* obtains similar relations between the decay rates and oscillation frequencies as the stochastic qubit, section 6.3.1. Figure 7.3a displays the decoherence rate (red) and oscillation frequency (blue) for the



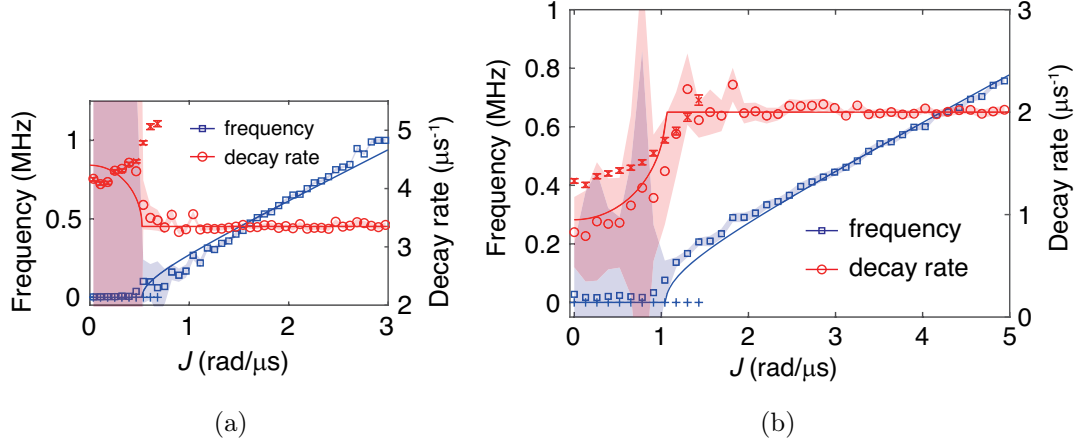


Figure 7.3: (a) Decoherence rate and oscillation frequency of driven dissipative qubit, with Liouvillian EP at the breaking point. (b) Decoherence rate and oscillation frequency of driven dissipative three level system, with Liouvillian EP at the breaking point ( $J = 1$ ). The solid lines represents the theoretical predictions and circles/squares represents observations, the shaded areas represents the standard error. Reprinted from [103] with permission from the American Physical Society.

driven dissipative qubit, the circles/squares<sup>2</sup> shows the experimental result and the solid lines the theoretical prediction [103]. In comparing the decoherence rate and oscillation frequencies to that of the stochastic qubit discussed in section 6.3.1, in particular figs. 6.1 and 6.2, the two systems displays similar dependencies in the parameters  $J/v$ . The result shown in fig. 7.3a would correspond to a state with the slower decoherence rate  $T_-^{-1}$ , eq. (6.22), and the quicker oscillation frequency  $\omega_+$ , eq. (6.23). Note that the system are different and the comparison should be taken as superficial<sup>3</sup> but both systems exhibit a similar response to the Liouvillian EP, shown as a breaking point in fig. 7.3a.

Although the standard deviations form an exponential fit to the data (shaded area) in fig. 7.3a are quite significant below the EP, especially for the decay rate, the experimental results appears to agree well with the theoretical prediction. Moreover, Chen *et al.* generalises the study to three-level systems by introducing a third and higher energy level with a spontaneous decay rate. Without introducing the particulars of the three level system, we can see from fig. 7.3b that the decoherence rate and oscillation frequency displays a similar behaviour to the qubit. Moreover, the experimental results appear to agree slightly better with predictions. These results motivates a new look at open quantum systems for the purpose of utilising non-Hermitian effects such as EPs on a large variety of systems [103]. The immediate benefit of obtaining precise knowledge of the decoherence qubit systems is for the engineering of more efficient or stable qubit systems, e.g. for the purpose of quantum computing.

Moreover, the  $\mathcal{PT}$ -symmetry of open systems has been proposed as method to protect states from decoherence. Through a theoretical investigation, Gardas *et al.*, [120], demonstrates how the  $\mathcal{PT}$ -symmetry of a quantum system can slow down

<sup>2</sup>The crosses/plusses indicates values from an exponential fit and the shaded regions represents the standard deviation to the fit.

<sup>3</sup>Although I have not been able to verify it, it is possible that the result by [103] could follow as a special case of the stochastic qubit discussed in chapter 6.

decoherence when in contact with a bath. The example system showing a critical slowing of decoherence was a simple  $\mathcal{PT}$ -symmetric two-level Hamiltonian, modelled by a Hermitian Hamiltonian in contact with a bath, where the bath components was traced out [120]. This simple example thus demonstrates a possible avenue for utilising  $\mathcal{PT}$ -symmetry to engineer qubits which are inherently protected against decoherence, or at least much more stable.

### 7.3 Enhanced Sensing

One application of  $\mathcal{PT}$ -symmetry and especially EPs that has been highlighted by many authors is enhanced sensing [39, 58, 103, 115, 121]. Highly sensitive sensors such as micro-cavity sensors for detection of single or a few particles relies on energy degeneracies for detection, as a small perturbation can lift the degeneracy and give a detectable energy splitting [121]. Then as noted in section 5.2.4, a Hermitian system subject to an external perturbation of the size  $\epsilon$ , it has a maximal response of  $\epsilon$  to small perturbations, see theorem 5.5. This maximally one-to-one dependence in external perturbations is thus the benchmark for traditional quantum and classical sensors. However, as noted in section 5.2.4, non-Hermitian systems can exhibit a root-dependence to external perturbations. From theorem 5.4 we remember that near EPs of order  $n$ , non-Hermitian systems can show a  $\sqrt[n]{\epsilon}$ -dependence to perturbations for  $\epsilon \ll 1$ . The basic idea is thus to utilise this dependence near EPs to achieve a energy splitting beyond  $\epsilon$  in sensors, thus achieving an enhanced sensitivity compared to the Hermitian benchmark.

Micro-cavity sensors for detection of single particles was one of the first sensors where the utilisation of EPs was suggested. In a paper from 2014, Wiersig showed through theoretical calculations and numerical simulations how a two-fold degeneracy could be lifted well beyond the Hermitian benchmark to achieve enhanced sensitivity in the splitting of resonant frequencies or energy levels [121]. Later, similar utilisations of higher order EPs to further enhance sensitivity has also been proposed, e.g. [122].

Hodaei *et al.*, [122], experimentally demonstrated enhanced sensitivity using  $\mathcal{PT}$  micro-ring lasers. The first physical system realised by Hodaei *et al.* was a set up two coupled micro-rings, one with gain and one with loss, exhibiting a second order EP. Near the EP, the splitting in eigenfrequencies of the system Hamiltonian exhibit the characteristic square root dependency to external perturbations, as shown by fig. 7.4a (top figure). The theoretical prediction is shown as a solid line and the experimental results as the green dots with accompanying error bars, and the inset shows the logarithm of the data showing a good agreement with the predicted square root. Moreover, fig. 7.4a (bottom figure) shows the sensitivity enhancement compared to the Hermitian benchmark. By adding another neutral micro-ring between the gain and loss rings, Hodaei *et al.* were also able to realise a third order EP in a similar experimental setup. Figure 7.4b (top figure) shows the predicted and observed splitting of the eigenfrequencies to be well within the error margins and as seen from the inset, the frequency splitting shows a clear cubic root dependence. Moreover, Figure 7.4b (bottom figure) shows the sensitivity enhancement compared to the Hermitian benchmark which compared to the second order EP, fig. 7.4a (bottom figure), shows a significantly increased sensitivity. In particular the maximally observed enhancement for the third order EP was 23 times the benchmark, whereas the second order EP had an enhancement of 13 times the benchmark [122].

Although important progress has been made in constructing enhanced sensing devices,

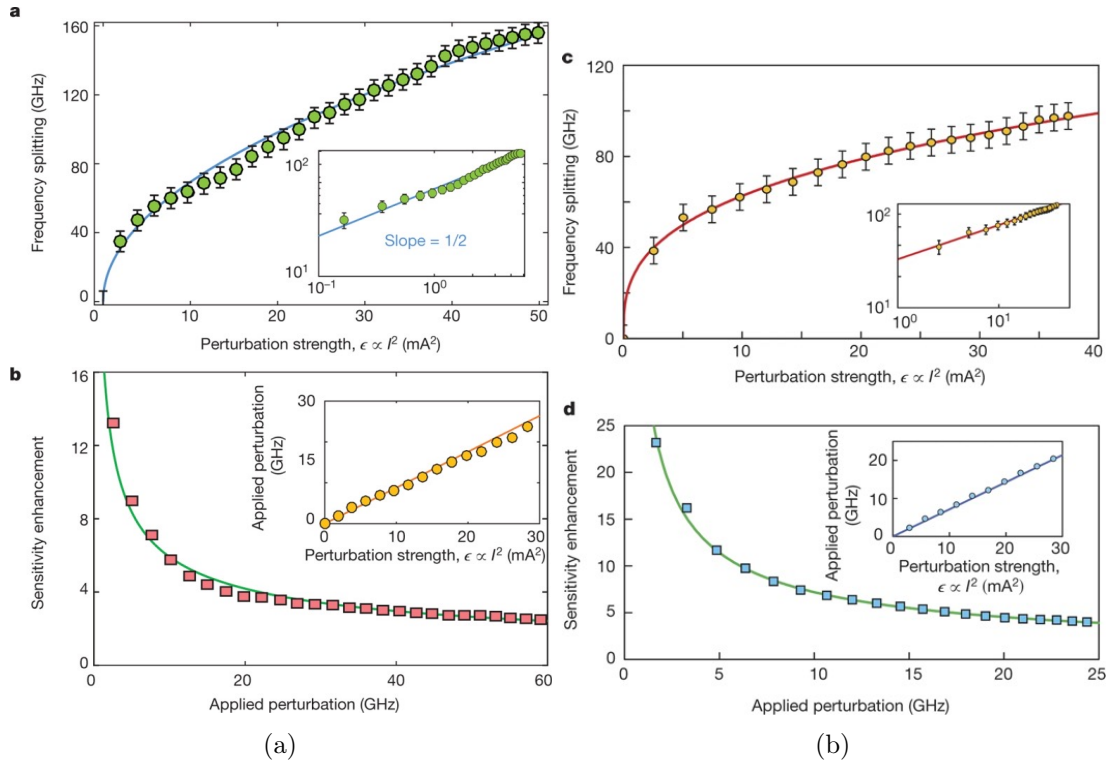


Figure 7.4: (a top) Observed frequency splitting in  $\mathcal{PT}$ -symmetric system of two coupled micro-rings displaying existence of second order EP. Solid line represents expectation, dots observations and error bars uncertainty in frequency measurements due to spectrometer. The inset shows the data on a logarithmic scale. (a bottom) Sensitivity enhancement compared to Hermitian benchmark near second order EP. (b top) Observed frequency splitting in  $\mathcal{PT}$ -symmetric system of three coupled micro-rings displaying existence of third order EP. (b bottom) Sensitivity enhancement compared to Hermitian benchmark near third order EP. Reprinted from [122] with permission from Springer Nature.

such as the above examples<sup>4</sup>. Enhanced quantum sensors have been far more elusive, however recent studies have shown promising result on  $\mathcal{PT}$ -symmetric quantum systems [103, 118, 123]. For example Yu *et al.*, [123], observed an enhancement almost 9 times above the Hermitian benchmark in a quantum optics experiment.

The aforementioned enhanced sensing experiments, both proposed and experimentally verified, all rely on exploiting EPs. However, other methods for enhanced sensing has also been proposed [124–126]. In particular McDonald & Clerk, [124], illustrates how the non-Hermitian effects beyond EPs can be advantageous to quantum sensing problems. Through an example using the Hatano-Nelson model<sup>5</sup> exhibiting  $\mathcal{PT}$ -symmetry<sup>6</sup>, McDonald & Clerk develops a novel measurement protocol utilising the non-Hermitian dynamics in lattice models to enhance sensitivity and show that the quantum Fisher information<sup>7</sup> per photon increases exponentially with system size as well as verify the persistence of the advantage in the non-perturbative regime [124]. A similar exponential response has also been found in other systems [125, 126].

These enhanced sensing protocols provide an exiting avenue for exploring new physics as they can push sensor technology to previously unavailable accuracy. Moreover, systems displaying enhanced sensitivity could be used to infer knowledge about very weakly interacting processes in Nature. Although the field of non-Hermitian physics is relatively new and studies of EPs and other non-Hermitian effects are newer still, the aforementioned developments and others not included show promising results for applications to optical systems, quantum systems, quantum technologies and sensors in general. Personally, I find the possibilities of utilising symmetry-protection and EPs to improve stability in qubit systems and the enhanced sensing possibilities especially intriguing.

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<sup>4</sup>Note the above examples [121, 122] are concerned with optical type sensors large enough that the dynamics are given by Maxwells equations rather than the Schrödinger equation. In this sense they are classical sensors.

<sup>5</sup>The Hatano-Nelson model is a one dimensional tight-binding model with asymmetric hopping with nearest neighbours. The particulars of this model is not of importance to the current discussion, for details on the model see [124] and the references therein.

<sup>6</sup>Technically McDonald & Clerk refers to the symmetry as a  $\mathbb{Z}_2$ -symmetry of the combined action of time-reversal,  $\mathcal{T}$ , and a discrete rotation,  $\mathcal{R}$ . However, as this constitutes a  $\mathcal{PT}$ -symmetry by definition 4.1, we will not make a distinction.

<sup>7</sup>The *quantum Fisher information* is a measure of the carried by some variable and is bounded the classical Fisher information [127]

# Final Remarks

In this thesis we have reviewed several aspects of non-Hermitian physics, especially focusing on  $\mathcal{PT}$ -symmetry and its roles. Over the course of the previous chapters many different concepts and formulations have been introduced and discussed, thus some final remarks are in order. Let us thus briefly summarise and highlight the most important results. Moreover, let us also give a few concluding remarks from the preceding chapters as well as indicate possible future applications of  $\mathcal{PT}$ -symmetry.

## Summary

In chapter 1, we briefly reviewed the general role of symmetries in physics and saw how parity and time-reversal symmetries are important symmetries of Nature. In particular, due to their relation to conservation laws symmetries is often used as a guiding premise for generalising existing theories or building new ones. As a result of the previous success in utilising symmetries, it seemed a natural starting point for extending ordinary quantum mechanics beyond Hermitian operators.

Aiming to extend quantum mechanics, we reviewed the role of hermiticity in chapter 2. In particular, from the analysis of the canonical Bender-Boettcher Hamiltonian, eq. (2.2), we saw that the condition of Hamiltonians being Hermitian is not a necessary condition for having real eigenvalues. The properties of the eigenspectrum of the Bender-Boettcher Hamiltonian was linked to its  $\mathcal{PT}$ -symmetry – indicating that  $\mathcal{PT}$ -symmetry is an important symmetry for non-Hermitian systems. Moreover, we saw through a few examples that non-Hermitian systems are in fact not something new in classical nor quantum physics. In particular, non-Hermitian systems often appear as open systems or as effective descriptions, in both which degrees of freedom have been omitted.

Moreover, motivated from examples of non-Hermitian systems in both classical and quantum physics we have reviewed the traditional formulation of quantum mechanics, through the Dirac-von Neumann postulates [33, 34], can be extended to include non-Hermitian systems. In chapter 3, we saw that the postulates of Hermitian and non-Hermitian quantum mechanics can be given in a very similar manner. In particular the only two significant amendments to the Dirac-von Neumann postulates are needed to generalise Hermitian quantum mechanics:

1. Observables are represented by *para-Hermitian* operators rather than Hermitian operators.
2. The inner product structure of the Hilbert space is dynamically determined by observables, in particular the Hamiltonian operator.

The first amendment to the postulates ensures that the observables of non-Hermitian theories are real, and the second amendment can be seen to ensure both the positive-definiteness of imposed Hilbert space inner product and the conservation of norms in time.

Equipped with the knowledge of the postulates of non-Hermitian quantum mechanics and the indication of  $\mathcal{PT}$ -symmetry being an important symmetry of Nature as well as non-Hermitian systems, we introduced the generalised notion of  $\mathcal{PT}$ -symmetry in chapter 4. From defining the  $\mathcal{PT}$  operator as an anti-linear operator which commutes and shares eigenvectors with some operator, it immediately follows that the spectrum of the operator is real. Moreover, we reviewed the properties of pseudo-Hermitian operators and saw how both the  $\mathcal{PT}$ -operator and pseudo-Hermitian maps can be used to construct equivalent inner product structures. Where the construction form  $\mathcal{PT}$  operator required and additional symmetry discrete,  $\mathcal{C}$ , giving the  $\mathcal{CPT}$ -inner product for the inner product structure to be positive semi-definite. More generally, the  $\mathcal{PT}$ -symmetry and pseudo-Hermiticity of operators are in fact equivalent requirements, implying that all pseudo-Hermitian operators are  $\mathcal{PT}$ -symmetric – including all Hermitian operators. Furthermore, finite-dimensional operators with real spectra can be related to Hermitian operators through a similarity transform. Lastly, by requiring the conservation of metric inner products in time it was shown that the pseudo-Hermiticity was a necessary and sufficient condition for unitary evolution of states. In particular the usual time-evolution operator was shown to be unitary with respect to a metric inner product with a pseudo-Hermitian map as the metric, thus implying that  $\mathcal{PT}$ -symmetry is both a necessary and sufficient condition for unitary evolution. It thus follows that the amendments to the Dirac-von Neumann postulates follows from the requirement of unbroken/exact  $\mathcal{PT}$ -symmetry.

In chapter 5 we reviewed two effects of non-Hermitian quantum mechanics. The first, a theorem by [2] which technically do not only apply to non-Hermitian systems but also Hermitian, stating that  $\mathcal{PT}$ -symmetric systems with both gain and loss do not exist. The theorem relates to the fact that processes involving gain does not preserve coherent states. This effect was illustrated through a simple theoretical example of quantum harmonic oscillators coupled to a thermal bath. Moreover, we introduced the notion of exceptional points (EPs), briefly demonstrated some characteristic features and a classification depending on the number,  $n$ , of coalescing eigenvectors. Furthermore, we saw that near EPs non-Hermitian systems exhibit a maximal  $\sqrt[n]{\epsilon}$  dependence in external perturbations  $\epsilon$ , whereas Hermitian systems exhibit a most a linear dependence in  $\epsilon$ .

To illustrate the effect of EPs, an example of EPs in the dynamics of quantum systems in a stochastic environment was constructed in chapter 6. By modelling the effects of the environment on a quantum system as fluctuating system, the master equation for the time-evolution was obtained. Then by an explicit calculation on a qubit system we saw how the EP induced behaviour similar to critical damping and beyond the EPs rapid oscillations. Moreover, we explicitly showed that the decoherence rates and oscillation frequencies of the system exhibits the characteristic square root dependence near the second order EP. Although the example was based on previous system by [109, 111], the analysis was extended beyond two-level systems, the solution technique employed was more general and a novel analysis of the role of EPs in the decoherence was introduced.

Lastly, in chapter 7, we saw that the field of  $\mathcal{PT}$ -symmetric quantum mechanics is a rapidly growing field in physics. We also gave a few examples of theoretical and experimental realisations of  $\mathcal{PT}$ -symmetry and EPs in both classical and quantum

systems. Moreover, we saw that non-Hermitian physics proposes some interesting new opportunities for emerging technologies such as more effective quantum computers using symmetry-protected states and enhanced sensing by utilising the root dependence in external perturbations near EPs.

## Conclusion

We have thus seen that the combined symmetry of the familiar and well motivated parity and time-reversal symmetries can be extended into the generalised notion of  $\mathcal{PT}$ -symmetry. Furthermore, an unbroken  $\mathcal{PT}$ -symmetry of finite-dimensional operators is not only a necessary condition for real eigenspectra, but also a sufficient condition. The existence of an unbroken  $\mathcal{PT}$ -symmetry is equivalent a para-Hermitian map relating non-Hermitian operators to Hermitian counterparts, although the mapping can in general be difficult to find. Moreover, the general  $\mathcal{PT}$ -symmetry, both exact and broken, is both a necessary and sufficient condition for unitary evolution of states. We also note that ordinary quantum mechanics follows from  $\mathcal{PT}$ -symmetric if the pseudo-Hermitian maps are identity maps, at least in finite dimensions.

Although formulation of non-Hermitian quantum mechanics through imposing  $\mathcal{PT}$ -symmetry generalises ordinary quantum mechanics, it does not seem that dynamics of the full universe are truly non-Hermitian. Although this is a slightly dangerous statement to make as no unification of all the fundamental forces of Nature exist. Anyhow, the examples of non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians are typically non-Hermitian because some degrees of freedom have been neglected or simply are not accessible. However, the full Hamiltonian of the Universe should include all degrees of freedom, thus indicating that it should be Hermitian. Although not fundamental, the physical system accessible to us are seldom completely isolated such that degrees of freedom are usually neglected making systems inherently open. The formulation  $\mathcal{PT}$ -symmetric quantum mechanics is thus useful as it allows for a better understanding of a particular group open quantum systems, possibly relatable to a physically manifested symmetries.

## Outlook

Now 25 years after the seminal paper by Bender & Boettcher, [1], most of the fundamentals of  $\mathcal{PT}$ -symmetric quantum mechanics have been properly formulated in a consistent manner. However, there are some unanswered questions regarding the mathematical fundamentals left. To my knowledge has the following problems yet been properly answered:

- For operators of infinite countable or uncountable dimension, is  $\mathcal{PT}$ -symmetry necessary for pseudo-Hermiticity?
- The properties of pseudo-Hermitian operators in Hilbert spaces of infinite uncountable dimension.

Resolving these problems will would further solidify the foundations of  $\mathcal{PT}$ -symmetric quantum mechanics, as well as extending the applicability.

As demonstrated in the previous chapters,  $\mathcal{PT}$ -symmetry has been applied to a large variety of systems and phenomena in both classical and quantum mechanics, and is an active field of research. However, applications of  $\mathcal{PT}$ -symmetry to quantum field theories

(QFTs) is significantly less investigated. Some initial investigations into the role of  $\mathcal{PT}$ -symmetry in QFTs have been made [128–131]. In particular, Bender *et al.* has shown examples of the renormalisation of Hermitian QFTs leading to  $\mathcal{PT}$ -symmetric theories, but also that the  $\mathcal{PT}$ -symmetry can be retained under the functional renormalisation group [130, 131]. Moreover, some discussions regarding the ghosts in the Lee model and applications to beyond standard model theories have also been given [131].  $\mathcal{PT}$ -symmetry could also have applications in conformal field theories and topological quantum field theories [39]. To me, extensions of  $\mathcal{PT}$ -symmetry and pseudo-Hermiticity to field theories is an exciting possibility for further research into the fundamentals of non-Hermitian systems and  $\mathcal{PT}$ -symmetry.

As previously noted, the utilisation of the strong dependence in external perturbation of non-Hermitian systems near EPs provide exciting possibilities for engineering sensors with significantly enhanced sensitivity. As noted in section 7.3 some experimental developments has been made for both classical and quantum systems, however the is relatively new. For reference, the examples provided in section 7.3 were published in 2017 [122] and 2020 [123]. Moreover, utilisations of  $\mathcal{PT}$ -symmetry to control or slow down decoherence in quantum systems, such as qubits, has intriguing possibilities. These effects can be used to enhance control and efficiency in quantum technology such as quantum computers. There also exists a large number of other applications of both  $\mathcal{PT}$ -symmetry and non-Hermitian dynamics [58, 115] in general, opening up a large number of possible applications. If such applications are efficiently realised they could revolutionise both technology and science, however enhancements are bound to be more likely.

Lastly, note that the master equations for the stochastically driven quantum systems given in chapter 6 was derived under the assumption that the Hamiltonians  $H_{\pm}$  were Hermitian. This assumption ensured that the time-evolution operators were unitary, however as seen in section 4.7 the assumption of hermiticity is an overly restrictive condition for conservation of probabilities. A natural extension of the systems considered in chapter 6 is thus to derive the master equations under the requirement of the Hamiltonians being  $\mathcal{PT}$ -symmetric as well and compare the evolutions for simple systems such as qubits. Moreover, the analysis could also be extended to include fluctuators with more than two states as well as multiple fluctuators.



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# Appendices



## Appendix A

# More on $\mathcal{PT}$ -Symmetric Quantum Mechanics

Not all proofs and results in chapter 4 are of immediate relevance for the flow of topics given in the thesis. Yet, not all of the results and especially proofs are irrelevant enough to be omitted from the thesis in its entirety. These results will be given in a more or less disconnected manner below. The the content of each of the subsequent sections will be loosely connected, whilst the sections themselves will be connected only by their counterparts in chapter 4.

### A.1 Eigenvectors

*Proof of theorem 4.17.* For a set of normalised left eigenvectors  $|\psi\rangle$  and a set of normalised right eigenvectors  $|\phi\rangle$  of an operator associated with a non-Hermitian system with a common eigenspectrum  $\lambda$  satisfying corollary 4.16, it follows that

$$\langle\psi_m|\left(\hat{O}|\phi_n\rangle\right)=\langle\psi_m|\lambda_n|\phi_n\rangle\quad\text{and}\quad\langle\phi_m|\left(\hat{O}^\dagger|\psi_n\rangle\right)=\langle\phi_m|\lambda_n|\psi_n\rangle.$$

Furthermore, as  $|\phi\rangle\neq|\psi\rangle$  in general by corollary 4.16, then  $\lambda_n\langle\psi_m|\phi_n\rangle=\lambda_n\langle\phi_m|\psi_n\rangle$  and

$$\left(\langle\psi_m|\hat{O}^\dagger\right)|\phi_n\rangle=\lambda_m^*\langle\psi_m|\phi_n\rangle\quad\text{and}\quad\left(\langle\phi_m|\hat{O}\right)|\psi_n\rangle=\lambda_n^*\langle\phi_m|\psi_n\rangle.$$

Then in order for  $\hat{O}$  to be a self-adjoint operator,

$$\langle\psi_m|\left(\hat{O}|\phi_n\rangle\right)=\left(\langle\psi_m|\hat{O}^\dagger\right)|\phi_n\rangle\quad\text{and}\quad\langle\phi_m|\left(\hat{O}^\dagger|\psi_n\rangle\right)=\left(\langle\phi_m|\hat{O}\right)|\psi_n\rangle,$$

implying that

$$\left(\lambda_n-\lambda_m^*\right)\langle\psi_m|\phi_n\rangle=0\quad\text{and}\quad\left(\lambda_m-\lambda_n^*\right)\langle\phi_m|\psi_n\rangle=0.$$

Thus showing that

$$\langle\psi_m|\phi_n\rangle=\langle\phi_m|\psi_n\rangle=0\quad\text{if }m\neq n,$$

and by the first relation above

$$\langle\psi_m|\phi_n\rangle=\langle\phi_m|\psi_n\rangle=1\quad\text{if }m=n,$$

i.e.,

$$\langle \psi_m | \phi_n \rangle = \langle \phi_m | \psi_n \rangle = \delta_{m,n}.$$

Furthermore, using this relation it follows that

$$\langle \psi_m | \left( \sum_{\ell} |\phi_{\ell}\rangle\langle\psi_{\ell}| \right) | \phi_n \rangle = \sum_{\ell} \langle \psi_m | \phi_{\ell} \rangle \langle \psi_{\ell} | \phi_n \rangle = \sum_{\ell} \delta_{m,\ell} \delta_{\ell,n} = \delta_{m,n} = \langle \psi_m | \phi_n \rangle.$$

Thus showing that the action of  $\sum_{\ell} |\phi_{\ell}\rangle\langle\psi_{\ell}|$  is identical to that of the identity operator  $\mathbb{1}$ , and by a similar calculation for  $\sum_{\ell} |\psi_{\ell}\rangle\langle\phi_{\ell}|$  it follows that

$$\sum_{\ell} |\psi_{\ell}\rangle\langle\phi_{\ell}| = \sum_{\ell} |\phi_{\ell}\rangle\langle\psi_{\ell}| = \mathbb{1}.$$

Then  $|\psi\rangle$  and  $|\phi\rangle$  satisfies the necessary requirements for forming a biorthogonal basis.  $\square$

## A.2 The Inversion Operators

### A.2.1 The $\mathcal{T}$ -Operator

As noted in section 1.2 the time-inversion operator must be an anti-linear operator. In particular, as noted by Wigner symmetry operators involving time-inversion are anti-unitary [81]. The  $\mathcal{PT}$ -operator is thus one such operator. Moreover, due to the non-linear nature of time-inversion operator it does not admit a matrix representation.

*Proof of theorem 4.4.* From [81] it follows that if the operator  $\tau$  is the operation of complex conjugation, then any anti-unitary operator  $A$  can be decomposes as

$$A = U\tau$$

where  $U$  is a unitary operator [81]. It thus follows from corollary 4.3 that the  $\mathcal{PT}$  operator can be decomposed as

$$\mathcal{PT} = VA = VU\tau$$

where  $V$  is a unitary operator as the product of two unitary operators is a unitary operator:

$$(VU)(VU)^{\dagger} = VUU^{\dagger}V^{\dagger} = VV^{\dagger} = \mathbb{1}.$$

Thus let the the anti-linear part, possibly up to some linear unitary operator  $U$  be associated with the time-inversion operator in order for it to reduce to the familiar operator for a physical  $\mathcal{PT}$ -symmetry. The  $\mathcal{T}$  operator can thus be represented as the anti-unitary operator  $\mathcal{T} = U\tau$ , and the remaining unitary part be associated with the parity operator ( $\mathcal{P} = V$ ). It is thus clear that  $\mathcal{P}$  satisfies eq. (1.8) trivially and

$$\mathcal{T}^2 = U\tau U\tau = UU^*,$$

such that in order for  $\mathcal{T}$  to reduce to the physical time-inversion operator it is by eq. (1.8) required to be an involution. Hence, the operator  $U$  is required to satisfy  $UU^* = \mathbb{1}$ , where  $*$  denotes the complex conjugate and not and not the Hermitian adjoint.

Furthermore,

$$\mathcal{T}\mathcal{T}^{\dagger} = U\tau\tau U^{\dagger} = UU^{\dagger} = \mathbb{1}$$

as two subsequent complex conjugations leaves a quantity unchanged. It is thus clear that  $\mathcal{T}^{\dagger} = \mathcal{T}^{-1}$ .  $\square$

### A.2.2 The $\mathcal{P}$ -Operator

From the above proof of theorem 4.4, we can give the following remark on the  $\mathcal{P}$  in general:

*Remark A.1.* The parity operator  $\mathcal{P}$  is canonically defined as the as a linear operator, hence it is a unitary operator.

*Proof of theorem 4.18.* Given a non-Hermitian operator with two eigenvectors,  $|\tilde{\psi}\rangle, |\tilde{\phi}\rangle \in \mathcal{H}$ , orthogonal under a  $\mathcal{PT}$ -inner product, then it follows that

$$\delta_{m,n} = \langle \tilde{\psi}_m | \tilde{\phi}_n \rangle_{\mathcal{PT}} = \langle \tilde{\psi}_m | \mathcal{P}^T | \tilde{\phi}_n \rangle = \langle \psi_m | \tilde{\phi}_n \rangle = \delta_{m,n},$$

where  $|\psi_m\rangle = \mathcal{P} |\tilde{\psi}_m\rangle$ . It thus follows by theorem 4.17 that  $\{|\psi_m\rangle, |\tilde{\phi}_n\rangle\}$  generates a biorthogonal basis, and that

$$\langle \tilde{\phi}_n | \psi_m \rangle = \langle \psi_m | \tilde{\phi}_n \rangle = \delta_{m,n} \Rightarrow \langle \tilde{\psi}_m | \mathcal{P}^T | \tilde{\phi}_m \rangle = \langle \tilde{\phi}_m | \mathcal{P} | \tilde{\phi}_m \rangle.$$

Thus showing that the operator  $\mathcal{P}$  is symmetric, i.e.  $\mathcal{P} = \mathcal{P}^T$ , and that

$$\langle \tilde{\psi}_m | \tilde{\psi}_n \rangle_{\mathcal{PT}} = \langle \mathcal{P}\psi_m | \mathcal{P}\psi_n \rangle_{\mathcal{PT}} = \langle \psi_m | \mathcal{P}^T \mathcal{P}^2 | \psi_n \rangle = \delta_{m,n}.$$

Such that  $\langle \psi_m | \psi_n \rangle_{\mathcal{PT}} = \delta_{m,n}$  and  $\mathcal{P}$  is an involution, i.e.  $\mathcal{P}^2 = \mathbf{1}$ . Furthermore, it follows from theorem 4.17 and the above results that

$$\hat{H}^\dagger |\psi\rangle = \mathcal{P} \hat{H} \mathcal{P} |\psi\rangle = \lambda |\psi\rangle \Rightarrow \hat{H} \mathcal{P} |\psi\rangle = \lambda \mathcal{P} |\psi\rangle,$$

which is equivalent with the action of the right eigenvectors. Thus showing that  $\mathcal{P} |\psi\rangle = c |\phi\rangle$ , for some constants  $c \in \mathbb{C}$ . Moreover,

$$c = c \langle \psi | \phi \rangle = \langle \psi | \mathcal{P} \psi \rangle = \langle \mathcal{P} \psi | \psi \rangle = c^* \langle \phi | \psi \rangle = c^*,$$

showing that  $c \in \mathbb{R}$ . Lastly

$$[\langle \psi | c^* \rangle c |\psi\rangle = \langle \phi | \mathcal{P}^2 | \phi \rangle \Rightarrow c^2 = \frac{\langle \phi | \phi \rangle}{\langle \psi | \psi \rangle},$$

and from theorem 4.17 it is clear that rescaling of the eigenvectors,

$$|\psi\rangle \rightarrow \frac{1}{\alpha} |\psi\rangle \text{ and } |\phi\rangle \rightarrow \alpha |\phi\rangle, \forall \alpha \in \mathbb{C},$$

leaves the construction unchanged [80]. Thus for all constructions,  $\alpha$  can be chosen such that  $c^2 = |\alpha|^4 = 1$ , implying that  $s = \pm 1$  and proving theorem 4.18.  $\square$

### A.2.3 The $\mathcal{C}$ -Operator

Before giving a proof of the properties of the  $\mathcal{C}$  operator given in theorem 4.19, let us introduce a more general result from [79]. Due to the generalised structure of the  $\mathcal{PT}$  operator given by definition 4.1, the  $\mathcal{C}$  operator can also be given in a basis-independent manner. However, realising the need for the  $\mathcal{C}$  operator to complete the inner product becomes less clear, hence the discussion was omitted from section 4.4.2.

From [79], let us state without proof:

**Theorem A.2.** *Let  $O \in \mathcal{B}(H)$  be a diagonalisable  $\mathcal{PT}$ -symmetric operator. Then there exists a nonempty set  $\mathcal{C}$  of operators  $C$  that nontrivially obey  $[C, O]$  and  $C^2$ . If **every** such operator commutes with the  $\mathcal{PT}$  operator,*

$$[\mathcal{PT}, C] = 0 \quad \forall C \in \mathcal{C},$$

*then the spectrum  $\sigma(O)$  is entirely real. If at least one  $C \in \mathcal{C}$  does not commute with the  $\mathcal{PT}$  operator, then  $\sigma(O)$  must contain at least one complex-conjugate pair of eigenvalues.*

The theorem is identical to [79, Theorem 2]

Theorem A.2 thus guarantees the existence of the  $\mathcal{CPT}$  inner product, at least for diagonalisable operators. It does not however, guarantee the existence of  $\mathcal{C}$  operators on the form of theorem 4.19. Moreover, it should be noted that although theorem A.2 is a strong requirement, finding the entire set  $\mathcal{C}$  of operators is in general a difficult task [79]. Hence, the theorem is not extremely useful for determining the spectrum of an operator.

Furthermore, let us show the properties of  $\mathcal{C}$  operators as described by theorem 4.19.

*Proof of theorem 4.19.* Given an operator  $\mathcal{C} \equiv \sum_n s_n |\psi_n\rangle\langle\phi_n|$ , constructed from a biorthogonal basis  $\{|\psi\rangle, |\phi\rangle\} \in \mathcal{H}$  associated with a Hamiltonian. Then it follows from theorem 4.17 that

$$\mathcal{C}^2 = \sum_m \sum_n s_m s_n |\psi_m\rangle\langle\phi_m| |\psi_n\rangle\langle\phi_n| = \sum_m \sum_n s_m s_n \delta_{m,n} |\psi_n\rangle\langle\phi_m| = \sum_n s_n^2 |\psi_n\rangle\langle\phi_n| = \mathbf{1},$$

thus showing that the operator  $\mathcal{C}$  is an involution.

Furthermore, using property ii) of definition 4.1 it follows that left eigenvectors of the Hamiltonian also are left eigenvectors of the  $\mathcal{PT}$  operator and similarly for the right eigenvectors, such that

$$\langle\phi_m| \mathcal{CPT} |\psi_m\rangle = e^{i\theta} \langle\phi_m| \mathcal{P} |\psi_m\rangle = e^{i\theta} \sum_n s_n \langle\phi_m|\psi_n\rangle \langle\phi_n|\psi_m\rangle = s_m e^{i\theta_m},$$

and

$$\langle\phi_m| \mathcal{PTC} |\psi_m\rangle = e^{i\varphi} \langle\phi_m| \mathcal{P} |\psi_m\rangle = e^{i\varphi} \sum_n s_n \langle\phi_m|\psi_n\rangle \langle\phi_n|\psi_m\rangle = s_m e^{i\varphi_m}.$$

Then by theorem 4.17 it follows that  $\phi_m = \varphi_m$  if the vectors are to form a biorthnormal basis, such that

$$\langle\phi_m| \mathcal{CPT} |\psi_m\rangle - \langle\phi_m| \mathcal{PTC} |\psi_m\rangle = \langle\phi_m| [\mathcal{PT}, \mathcal{C}] |\psi_m\rangle = 0 \Rightarrow [\mathcal{PT}, \mathcal{C}] = 0.$$

This would also follow from the fact that both  $\mathcal{P}$  and  $\mathcal{PT}$  are involutions, and that two involutions commute.

Lastly, by requiring that the Hamiltonian is self-adjoint under the  $\mathcal{CPT}$ -inner product, i.e.

$$\langle\psi|\hat{H}\psi\rangle_{\mathcal{CPT}} = \langle\hat{H}\psi|\psi\rangle_{\mathcal{CPT}},$$

it is clear that  $[\hat{H}, \mathcal{CPT}] = 0$ . Then it follows that

$$\begin{aligned} \hat{H}\mathcal{CPT} - \mathcal{CPT}\hat{H} &= \hat{H}\mathcal{CPT} - \mathcal{C} \left( -[\hat{H}, \mathcal{PT}] + \hat{H}\mathcal{PT} \right) \\ &= (\hat{H}\mathcal{C} - \mathcal{C}\hat{H}) \mathcal{PT} \\ &= [\hat{H}, \mathcal{C}] \mathcal{PT} = 0, \end{aligned}$$

thus implying that  $[\hat{H}, \mathcal{C}] = 0$  because  $\mathcal{PT} \neq 0$  by definition 4.1.  $\square$

### A.3 Characteristics of Pseudo-Hermitian Operators

#### A.4 Unitary Evolution

*Proof of corollary 4.28.* Immediately, we note that eq. (4.14a) follows immediately from the proof of eq. (4.13a). Furthermore, it is clear that

$$-\frac{i}{\hbar} \int_t^{t'} d\tau \hat{H}(\tau) - \frac{i}{\hbar} \int_{t'}^{t''} d\tau \hat{H}(\tau) = -\frac{i}{\hbar} \int_t^{t''} d\tau \hat{H}(\tau)$$

if  $t < t' < t''$ . Then form the BCH formula [92]

$$\exp\left\{-\frac{i}{\hbar} \int_t^{t'} d\tau \hat{H}(\tau)\right\} \exp\left\{-\frac{i}{\hbar} \int_{t'}^{t''} d\tau \hat{H}(\tau)\right\} = \exp\left\{-\frac{i}{\hbar} \int_t^{t''} d\tau \hat{H}(\tau)\right\},$$

because the Hamiltonian always commutes with itself, thus proving eq. (4.14b). Lastly it is clear that because the integral in the exponent of eq. (4.13a) evaluated over a vanishing domain must tend to zero, then eq. (4.14c) must be true.  $\square$

*Proof of theorem 4.31.* Similarly to the time-independent states of section 4.3, let us assume that the eigenstates  $|\psi(t)\rangle$  of the time-dependent non-Hermitian Hamiltonian and the corresponding states  $|\phi(t)\rangle$  of the time-dependent Hermitian Hamiltonian relates as

$$|\phi(t)\rangle = \eta(t) |\psi(t)\rangle.$$

Then from the Schrödinger equation with  $\hat{h}(t)$  as the generator of time-evolution,

$$\hat{h}(t) |\phi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\phi(t)\rangle,$$

it follows from insertion that

$$\hat{h}(t)\eta(t) |\psi(t)\rangle = i\hbar \frac{\partial \eta(t)}{\partial t} |\psi(t)\rangle + i\hbar \eta(t) \frac{\partial |\psi(t)\rangle}{\partial t}.$$

Furthermore, the last derivative in the above expression allows us to insert the right-hand side of the Schrödinger equation for  $\hat{H}(t)$ . Thus

$$\hat{h}(t)\eta(t) |\psi(t)\rangle = i\hbar \frac{\partial \eta(t)}{\partial t} |\psi(t)\rangle + \eta(t) \hat{H}(t) |\psi(t)\rangle \Rightarrow \hat{h}(t) = i\hbar \frac{\partial \eta(t)}{\partial t} \eta^{-1}(t) + \eta(t) \hat{H}(t) \eta^{-1}(t).$$

$\square$





## Appendix B

# Quantum Harmonic Oscillator

In the following appendix, the calculations of the example given to illustrate theorem 5.1 in section 5.1 are given. As stated in section 5.1.1, the system in question is that of a quantum harmonic oscillator coupled to a thermal bath. The system exhibit a constant gain with a rate given by the parameter  $\gamma$  when  $\hat{a}^\dagger$  is the Lindblad operator. As the gain is independent on the energy in the system, it is analogous to a system in contact with a thermal bath of infinite temperature. Hence, the system with  $L = \hat{a}^\dagger$  is said to be at  $T = \infty$ . The calculations accompanying this example system is found in appendix B.1.

To compare the roles of loss and gain, a quantum harmonic oscillator with a constant loss can also be constructed. As stated in section 5.1.1, if the system is coupled to a thermal bath with the  $L = \hat{a}$  as the Lindblad operator, then it will experience a constant loss at a rate given by  $\gamma$ . The system is thus analogous to a system in contact with a thermal bath at absolute zero temperature, hence the system will be referred to as a quantum harmonic oscillator at  $T = 0$ . The calculations accompanying this example system is found in appendix B.2.

### B.1 Quantum Harmonic Oscillator at $T = \infty$

Let us consider a simple system described by the Hermitian Hamiltonian  $H = \hbar\omega\hat{a}^\dagger\hat{a}$  where  $\hat{a}$  and  $\hat{a}^\dagger$  are the usual harmonic oscillator ladder operators. Let the be open, i.e. let the oscillator be connected to a reservoir such that the dynamics of system is described by the Lindblad equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{\gamma}{2} \left( \left\{ \hat{a}\hat{a}^\dagger, \rho \right\} - 2\hat{a}^\dagger\rho\hat{a} \right), \quad (\text{B.1})$$

where  $\rho(t)$  is the density operator.

#### B.1.1 Energy States

Let us first assume an energy eigenbasis in terms of the regular energy eigenstates of the QHO. Let  $|m\rangle$  and  $|n\rangle$  be two such states, it then follows that

$$\langle m | [H, \rho] | n \rangle = \rho_{m,n}(E_m - E_n).$$

Similarly, using that  $\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$  and  $\hat{a} |n\rangle = \sqrt{n} |n-1\rangle$ , we find that

$$\langle m | \left( \left\{ \hat{a}^\dagger\hat{a}, \rho \right\} - 2\hat{a}^\dagger\rho\hat{a} \right) | n \rangle = (m+n+2)\rho_{m,n} - 2\sqrt{mn}\rho_{m-1,n-1}.$$

Thus if we consider the average excitation of the oscillator,  $N = \langle \hat{a}^\dagger \hat{a} \rangle$ . It follows from the Lindblad equation, eq. (B.1), that

$$\begin{aligned} \frac{dN}{dt} &= \frac{d}{dt} \text{Tr} [\hat{a}^\dagger \hat{a} \rho] = \sum_m \left\langle m \left| \hat{a}^\dagger \hat{a} \frac{d\rho}{dt} \right| m \right\rangle \\ &= \gamma \sum_m \rho_{m,m} = +\gamma N. \end{aligned} \quad (\text{B.2})$$

Thus implying that

$$N(t) \propto e^{+\gamma t}. \quad (\text{B.3})$$

Hence, the average number of excitations is expected to grow exponentially in time. Of course, this is expected as energy is constantly being added to the system.

Keeping to representation of the system in terms of energy eigenstates. Let us prepare the system in an energy eigenstate  $|n\rangle$  such that

$$\rho_{i,j}(t=0) = \begin{cases} 1, & i = j = n \\ 0 & \text{else} \end{cases}.$$

Furthermore, the probability  $P_m$  of finding the system in an energy state  $|m\rangle$  at a time  $t$  is  $P_m(t) = \rho_{m,m}(t)$ . The Lindblad equation, eq. (B.1), then reduces to

$$\frac{dP_m}{dt} = -\frac{\gamma}{2}(2m+1)P_m + \gamma m P_{m-1}. \quad (\text{B.4})$$

Then by writing out the first few equations for a given initial state  $|n\rangle$  it seems that the probability of finding the system in a state  $|m\rangle$  at a time  $t$  is

$$P_m(t) \propto e^{-(m+\frac{1}{2})\gamma t} (e^{\gamma t} - 1)^\chi. \quad (\text{B.5})$$

Where  $\chi = m - n \geq 0$  and  $P_m(t) = 0$  for  $m < n$ . Here, the last statement follows directly from eq. (B.4) as probabilities for energy states below  $|n\rangle$  are untouched by the difference equation.

From eq. (B.5) it is clear that as  $\gamma t \gg 1$ , the probability of finding the system in high-energy states becomes large whilst becoming low for the low-energy states compared to the initial probability. It is also clear that the system does not seem to converge to a particular state, but rather the probability distribution becomes smeared towards high energies.

Having considered the evolution in terms of the energy basis let us now turn to another case of interest, namely the evolution of coherent states.

### B.1.2 Evolution of Coherent State

Let us assume the initial state of the system to be a coherent state. Then in order to ease calculations, let us define the following transformation of the density operator:

$$C(\lambda, \lambda^*, t) \equiv \text{Tr} \left[ \rho e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right]. \quad (\text{B.6})$$

Furthermore, we identify the partial derivatives of the transform,

$$\frac{\partial C}{\partial \lambda} = \text{Tr} \left[ \rho \hat{a}^\dagger e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] \text{ and } \frac{\partial C}{\partial \lambda^*} = \text{Tr} \left[ \rho \hat{a} e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right].$$

And using eq. (B.1) we find that

$$\frac{\partial C}{\partial t} = -i\omega \operatorname{Tr} \left[ \left[ \hat{a}^\dagger \hat{a}, \rho \right] e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] - \frac{\gamma}{2} \operatorname{Tr} \left[ \left( \left\{ \hat{a}^\dagger \hat{a}, \rho \right\} - 2\hat{a}^\dagger \rho \hat{a} \right) e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right]. \quad (\text{B.7})$$

Then using a special case of the Baker–Campbell–Hausdorff [92] formula (BCH) we obtain the following relations

$$\left. \begin{aligned} e^{-\lambda \hat{a}^\dagger} \hat{a} e^{\lambda \hat{a}^\dagger} &= \hat{a} + \lambda \\ e^{\lambda^* \hat{a}} \hat{a}^\dagger e^{-\lambda^* \hat{a}} &= \hat{a}^\dagger + \lambda^* \end{aligned} \right\} \Rightarrow \begin{aligned} \hat{a} e^{\lambda \hat{a}^\dagger} &= e^{\lambda \hat{a}^\dagger} (\hat{a} + \lambda) \\ \hat{a}^\dagger e^{-\lambda^* \hat{a}} &= e^{-\lambda^* \hat{a}} (\hat{a}^\dagger + \lambda^*) \end{aligned}$$

Moreover, using these relations we find that

$$\operatorname{Tr} \left[ \hat{a}^\dagger \hat{a} \rho e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] = \operatorname{Tr} \left[ \hat{a} \rho \hat{a}^\dagger e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] + \lambda^* \frac{\partial C}{\partial \lambda^*}, \quad (\text{B.8a})$$

$$\operatorname{Tr} \left[ \rho \hat{a}^\dagger \hat{a} e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] = \operatorname{Tr} \left[ \hat{a} \rho \hat{a}^\dagger e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] + \lambda \frac{\partial C}{\partial \lambda}, \quad (\text{B.8b})$$

$$\operatorname{Tr} \left[ \hat{a} \hat{a}^\dagger \rho e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] = \operatorname{Tr} \left[ \hat{a}^\dagger \rho e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] - \lambda \frac{\partial C}{\partial \lambda} + \lambda \lambda^* C, \quad (\text{B.8c})$$

$$\operatorname{Tr} \left[ \rho \hat{a} \hat{a}^\dagger e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] = \operatorname{Tr} \left[ \hat{a}^\dagger \rho e^{\lambda \hat{a}^\dagger} e^{-\lambda^* \hat{a}} \right] - \lambda^* \frac{\partial C}{\partial \lambda^*} + \lambda \lambda^* C. \quad (\text{B.8d})$$

Then by inserting eqs. (B.8a) to (B.8d) into eq. (B.7) we find the transformed Lindblad equation of the system

$$\frac{\partial}{\partial t} C = \left( \frac{\gamma}{2} + i\omega \right) \lambda \frac{\partial C}{\partial \lambda} + \left( \frac{\gamma}{2} - i\omega \right) \lambda^* \frac{\partial C}{\partial \lambda^*} - \gamma |\lambda|^2 C. \quad (\text{B.9})$$

Furthermore, we recognise that eq. (B.9) takes form similar to that of a total derivative. The transformed Lindblad equation may thus be solved by the method of characteristics [101, Chapter 18] to obtain

$$C(\lambda, \lambda^*, t) = C_0 \left( \lambda e^{\left(\frac{\gamma}{2} + i\omega\right)t}, \lambda^* e^{\left(\frac{\gamma}{2} - i\omega\right)t} \right) e^{(1 - e^{\gamma t}) |\lambda|^2}. \quad (\text{B.10})$$

Note here that the transformation parameter  $\lambda$  is still formally a function of time such that  $C_0$  is a purely static object thus allowing us to omit its explicit time parameterisation. It thus follows that

$$\lambda(t) = \lambda_0 e^{-\left(\frac{\gamma}{2} + i\omega\right)t}.$$

From looking directly at eq. (B.10) it is not immediately clear how system will evolve. Let us thus assume that at  $t = 0$ , the system is in a coherent state  $|z_0\rangle$ . It thus follows immediately from eq. (B.6) that

$$C(\lambda_0, \lambda_0^*, t = 0) = e^{\lambda_0 z_0^* - \lambda_0^* z_0},$$

where  $\hat{a}|z_0\rangle = z_0|z_0\rangle$  as  $|z_0\rangle$  is a coherent state. Then by insertion into eq. (B.10), we find that the transformed function takes the form

$$C(\lambda, \lambda^*, t) = e^{\lambda(t)z^*(t) - \lambda^*(t)z(t)} e^{|\lambda(t)|^2 (1 - e^{\gamma t})}. \quad (\text{B.11})$$

Where we now have that  $z(t) = z_0 e^{\left(\frac{\gamma}{2} - i\omega\right)t}$  and have the time-evolution of the transformation function. Thus let us now attempt to invert the transformation in order to retrieve the time-evolution of the density operator.

In order to invert the transformation, let us look for a function,  $f(\zeta, \zeta^*, t)$ , such that

$$\rho(t) = \int d\zeta d\zeta^* f(\zeta, \zeta^*, t) |\zeta\rangle\langle\zeta|. \quad (\text{B.12})$$

The transformation thus takes the form

$$C(\lambda, \lambda^*, t) = \text{Tr} \left[ \int d\zeta d\zeta^* f(\zeta, \zeta^*, t) |\zeta\rangle\langle\zeta| e^{\lambda \hat{a}^\dagger - \lambda^* \hat{a}} \right],$$

which reduces to

$$C(\lambda, \lambda^*, t) = \int d\zeta d\zeta^* f(\zeta, \zeta^*, t) e^{\lambda \zeta^* - \lambda^* \zeta}, \quad (\text{B.13})$$

if  $|\zeta\rangle$  is chosen to be a coherent basis. Furthermore, by solving the integral, we see that eq. (B.13) reduces to eq. (B.11) when  $f(\zeta, \zeta^*, t)$  is a Gaussian function in the parameter  $\zeta$ . The calculation also allows us to identify the correct normalisation of the Gaussian. By explicit calculation, it is clear that eq. (B.13) reduces to eq. (B.11) if the transformation function takes the form

$$f(\zeta, \zeta^*, t) = \frac{1}{\pi(e^{\gamma t} - 1)} e^{-\frac{|\zeta - z(t)|^2}{e^{\gamma t} - 1}}.$$

Equipped with this reverse transformation, we find that the amplitude of the system being in a coherent state  $|z\rangle$  is

$$\langle z|\rho|z\rangle = \int d\zeta d\zeta^* \underbrace{\frac{1}{\pi(e^{\gamma t} - 1)} e^{-\frac{|\zeta - z(t)|^2}{e^{\gamma t} - 1}}}_{F(z(t), \zeta)}. \quad (\text{B.14})$$

Where we have used the relation that  $|\langle z|\zeta\rangle|^2 = e^{-|\zeta - z(t)|^2}$  for coherent states. By identifying the integrand as the amplitude distribution,  $F(z(t), \zeta)$ , we can now visualise how the amplitude distribution evolves in time. Figure 5.2 then shows the evolution of the amplitude over approximately one rotation in the complex plane. From the figure it is clear that the initial distribution closely resembles a delta function located at  $\zeta = 1 + i0$ , which was our chosen initial state. As the time evolves, the peak of the distribution rotates counter clockwise in the complex plane with an increasing broadening of the peak. This entails that the system will not remain in a coherent state.

To further illustrate the non-coherent evolution of the system, fig. 5.3a shows the evolution maximal amplitude of the distribution in time. Note the logarithmic y-axis in fig. 5.3a, showing that the amplitude decay away very quickly at early times. In fact, for  $t/\gamma \lesssim 1$  the decay is much larger than that of an exponential with a linear exponent, whereas for greater times the decay appears linear in the exponent. Similarly, fig. 5.3b shows the associated standard deviation, which is shown to grow rapidly for small times.

## B.2 Quantum Harmonic Oscillator at $T = 0$

This example, including some explicit calculations can be found in [132, Section 6].

By utilising almost exactly the same procedure as for appendix B.1, the problem can be reversed to describe a lossy system. By interchanging the Lindblad operators, i.e.  $L \rightarrow L^\dagger$  and  $L^\dagger \rightarrow L$ , the system will be an open quantum system where energy is

constantly removed at a fixed rate. The Lindblad operator is thus  $L = \hat{a}$ , the harmonic oscillator annihilation operator. Then classically we would have expected the evolutions described by these two systems to be opposite processes, e.i. the Hamiltonian, eq. (B.1), to be the reverse process given by eq. (B.15). However, as the solution below shows, they are not. Demonstrating a significant difference between our expectations from classical processes and the behaviour of quantum systems.

The time-evolution of the system will thus be given by the Liouville-von Neumann equation,

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{\gamma}{2} \left( \left\{ \hat{a}^\dagger \hat{a}, \rho \right\} - 2\hat{a}\rho\hat{a}^\dagger \right). \quad (\text{B.15})$$

Then following the same procedure as appendix B.1, the calculation becomes essentially the same.

### B.2.1 Energy States

Equivalently to eq. (B.2) it is clear that the average number of excitations in this case evolves as

$$\frac{dN}{dt} = -\gamma N \Rightarrow N(t) \propto e^{-\gamma t}.$$

The average number of excitations are thus exponentially decaying in time. In a similar manner to the QHO at  $T = \infty$ , an analysis in terms of the evolution of the probabilities of energy eigenstates can be conducted. As such, a similar expression to that of eq. (B.4) can be obtained. However, by inspecting the asymmetric nature of the associated Lindblad equations, eqs. (B.1) and (B.15), and the subsequent relations to the probabilities it is clear that the equivalent differential equation will force the system into an energy eigenstate in time. This is however exactly what the construction of the system, eq. (B.15), was designed to do. This thus only confirms our interpretation of the constructed system.

### B.2.2 Evolution of Coherent State

Furthermore, by assuming that the state at a time  $t = 0$  is in a coherent state  $|z\rangle$  the transformation of the density operator, eq. (B.6), used on the QHO at  $T = \infty$  still applies. Using this transformation on this variant of the system, we find a similar to eq. (B.11):

$$C(\lambda, \lambda^*, t) = e^{\lambda z^*(t) - \lambda^* z(t)} \text{ where } z(t) = z_0 e^{-(\frac{\gamma}{2} + i\omega)t}.$$

From this it is immediately clear that  $z(t) \rightarrow z_0, \forall \gamma \geq 0$ . The system will thus always decay into a coherent state when starting in a coherent state, i.e. a coherent state remains coherent. This is contrary to the equivalent expression for the QHO at  $T = \infty$  which appears to grow in an oscillating manner, where the oscillations have the opposite direction. It should thus be clear at this point that we expect the general behaviour of the coherent states of the system to be different from the  $T = \infty$ -case.

Furthermore, in a similar manner to the calculation of eq. (B.14), the coherent amplitude distribution can be obtained. If we assume the function  $f(\zeta, \zeta^*, t)$  to be a Gaussian in this case as well, we find that it must be a Gaussian with zero width. It is thus clear that the function  $f(\zeta, \zeta^*, t)$  must be a delta function, forcing the density matrix, eq. (B.12), to remain in the coherent state. That is

$$\langle z|\rho|z\rangle = \int d\zeta d\zeta^* \delta(z(t) - \zeta). \quad (\text{B.16})$$

Thus for comparison the amplitude distribution is

$$F(z(t), \zeta) = \delta(z(t) - \zeta) \tag{B.17}$$

for the quantum harmonic oscillator at zero temperature.

## Appendix C

# Quantum System in Stochastic Environment

The following appendix contains calculations omitted from chapter 6. The sections below should be read as a supplement to the corresponding sections in chapter 6 and as such, they do not necessarily define all quantities. Quantities relevant for the calculation steps below will be redefined and/or referred to when necessary.

### C.1 The Master Equations

The main steps of the calculation of the master equations of the quantum system in a stochastic environment can be found in section 6.2. There are however some steps that were omitted for sake brevity. Let us begin by explaining the steps from eqs. (6.6) and (6.8) to eqs. (6.9a) and (6.9b) in some more detail.

#### C.1.1 The Master Equations of Probability

Starting from the probability equations, eqs. (6.6) and (6.8), let us rewrite them here for consistency

$$p_+(t + \epsilon, \rho) = \alpha p_\pm \left( t, \rho - U_\pm(\epsilon) \rho U_\pm^\dagger(\epsilon) \right) + \beta p_\mp \left( t, \rho - U_\mp(\epsilon) \rho U_\mp^\dagger(\epsilon) \right), \quad (\text{C.1a})$$

$$p_-(t + \epsilon, \rho) = \beta p_\pm \left( t, \rho - U_\pm(\epsilon) \rho U_\pm^\dagger(\epsilon) \right) + \alpha p_\mp \left( t, \rho - U_\mp(\epsilon) \rho U_\mp^\dagger(\epsilon) \right). \quad (\text{C.1b})$$

From section 6.2, remember that to first order in  $\epsilon$ ,  $\alpha \approx 1 - \gamma\epsilon + \mathcal{O}(\epsilon^2)$  and  $\beta \approx \gamma\epsilon + \mathcal{O}(\epsilon^2)$ . Note that the coefficients  $\alpha$  and  $\beta$  have been

Furthermore, assuming that the rate of change of  $H_\pm(t)$  is small compared to  $\epsilon \ll 1$ , we find that the unitary time-evolution operator is

$$U(\epsilon) = \mathbb{1} - \frac{i}{\hbar} H_\pm \epsilon + \mathcal{O}(\epsilon^2).$$

Then expanding the first term in eqs. (6.6) and (6.8) to first order in  $\epsilon$ , we find that

$$\begin{aligned} p_\pm \left( t, U_\pm(\epsilon) \rho U_\pm^\dagger(\epsilon) \right) &= p_\pm + \left( \rho - \mathbb{1} \rho \mathbb{1} + \frac{i}{\hbar} H_\pm \rho \mathbb{1} \epsilon - \frac{i}{\hbar} \mathbb{1} \rho H_\pm \epsilon \right) \cdot \nabla p_\pm + \mathcal{O}(\epsilon^2) \\ &= p_\pm + \frac{i}{\hbar} [H_\pm, \rho] \cdot \nabla p_\pm \epsilon + \mathcal{O}(\epsilon^2). \end{aligned}$$

Here,  $p_{\pm} = p_{\pm}(\rho, t)$  unless otherwise stated and we let  $\nabla p_{\pm}$  denote the gradient of  $p_{\pm}$  with respect to  $\rho$ , i.e.

$$\nabla = \frac{\partial}{\partial r_i} \tau_i, \quad \forall \tau_i \in \mathfrak{su}(N) \quad \text{where} \quad \rho = \frac{1}{N} \left( \mathbf{1} + \sum_i^N r_i \tau_i \right).$$

Note the commutator is an operator of the same dimension as its entries, then in a similar fashion as eq. (6.11) it can be represented as

$$[H_{\pm}, \rho] \cdot \nabla p_{\pm} = A = a_0 \mathbf{1} + \mathbf{a} \cdot \vec{\tau}.$$

The inner product,  $\cdot$ , with  $\nabla p_{\pm}$  is thus formally

$$[H_{\pm}, \rho] \cdot \nabla p_{\pm} = A_{\pm} \cdot \nabla p_{\pm} = \sum_i^N a_i \frac{\partial p_{\pm}}{\partial r_i},$$

which is a scalar quantity. The inner product  $\cdot$  between the operators can thus be interpreted as a scalar product between the vector representations of the operators  $[H_{\pm}, \rho]$  and  $\nabla p_{\pm}$ .

Furthermore, by expanding  $p_{\pm}$  in time as well. We find that

$$p_{\pm}(t + \epsilon, \rho) = p_{\pm}(t, \rho) + \dot{p}_{\pm}(t, \rho) \epsilon + \mathcal{O}(\epsilon^2).$$

By inserting these expansions into eq. (C.1a), we obtain

$$p_+ + \dot{p}_+ \epsilon = (1 - \gamma \epsilon) \left( p_+ + \frac{i}{\hbar} [H_+, \rho] \cdot \nabla p_+ \epsilon \right) + \gamma \epsilon \left( p_- + \frac{i}{\hbar} [H_-, \rho] \cdot \nabla p_- \epsilon \right) + \mathcal{O}(\epsilon^2),$$

which simplifies to

$$\dot{p}_+ = -\gamma p_+ + \gamma p_- + \frac{i}{\hbar} [H_+, \rho] \cdot \nabla p_+ + \mathcal{O}(\epsilon^2).$$

By a similar insertion into eq. (C.1b), we obtain the other probability as well:

$$\dot{p}_- = \gamma p_+ - \gamma p_- + \frac{i}{\hbar} [H_-, \rho] \cdot \nabla p_- + \mathcal{O}(\epsilon^2).$$

We have thus obtained the master equations eqs. (6.9a) and (6.9b). The above master equations can be written in the compact form

$$\dot{p}_{\pm} = \mp \gamma (p_+ - p_-) + \frac{i}{\hbar} [H_{\pm}, \rho] \cdot \nabla p_{\pm} + \mathcal{O}(\epsilon^2). \quad (\text{C.2})$$

Then equipped with eq. (C.2), we can further simplify the problem by obtaining a representation of  $\rho$  in terms of averaged vectors.

### C.1.2 The Averaged Master Equations

Using the definition of the expectation values  $\mathbf{m}_{\pm}$ , eq. (6.10), and writing  $\rho$  and  $H_{\pm}$  in terms of the generators of  $\mathfrak{su}(N)$ , eq. (C.2) can be written as

$$\dot{\mathbf{m}}^{\pm} = \mp \gamma (\mathbf{m}^+ - \mathbf{m}^-) + \frac{i}{\hbar} \int d^N r d_i^{\pm} r_j [\tau_i, \tau_j] \cdot \nabla p_{\pm} \mathbf{r}$$



by multiplying by  $\mathbf{r}$  and integrating over the whole domain of  $\mathbf{r}$ , i.e. the entire domain of  $\rho$ .

Let us take a closer look at the last term in this expression. Rewriting the last term as

$$[\tau_i, \tau_j] \tau_k \int d^N r d_i^\pm r_j \frac{\partial p_\pm}{\partial r_k} \mathbf{r},$$

it is clear that by writing the integral in component form and using integration by parts

$$d_i^\pm \int d\mathbf{r} r_j r_a \frac{\partial p_\pm}{\partial r_k} = d_i^\pm \left( r_j r_a p_\pm \delta_{k,a} \Big|_{-\infty}^{\infty} - \int d\mathbf{r} \frac{\partial r_j r_a}{\partial r_k} p_\pm \right).$$

Furthermore, we require that the probability vanishes at the boundary of the domain of  $\rho$ . Hence the first term must vanish. Moreover, because the commutator of two  $\mathfrak{su}(N)$  commutators is defined as

$$[\tau_i, \tau_j] = i f_{i,j,\ell} \tau_\ell,$$

where  $f_{i,j,\ell}$  is the structure constants of the Lie algebra. Then using that  $f_{i,j,\ell}$  is antisymmetric in all indices, we find that

$$d_i^\pm \int d\mathbf{r} r_j r_a \frac{\partial p_\pm}{\partial r_k} = -d_i^\pm \int d\mathbf{r} r_j \frac{\partial r_a}{\partial r_k} p_\pm = -d_i^\pm \int d\mathbf{r} r_j p_\pm \delta_{k,a}.$$

We have thus shown that

$$\frac{i}{\hbar} \int d^N r d_i^\pm r_j [\tau_i, \tau_j] \cdot \nabla p_\pm \mathbf{r} = -\frac{i}{\hbar} \int d^N r d_i^\pm [\tau_i, \tau_j] r_j p_\pm.$$

The master equations of the expectation values are thus

$$\dot{m}_i^\pm = \mp \gamma (m_i^+ - m_i^-) + \frac{1}{\hbar} d_j^\pm m_k^\pm f_{i,j,k}, \quad (\text{C.3})$$

by eq. (6.10) and we have shown eq. (6.12).

Furthermore, let us define

$$\begin{aligned} \rho_\pm &= \frac{1}{N} \left( \mathbb{1} + \sum_i^N m_i^\pm \tau_i \right) \\ &= \int d\rho p_\pm(t, \rho) \rho. \end{aligned} \quad (\text{C.4})$$

It is thus clear that eq. (C.3) can be rewritten in the compact form

$$\dot{\rho}_\pm = \mp \gamma (\rho_+ - \rho_-) - \frac{i}{\hbar} [H_\pm, \rho_\pm] \quad (\text{C.5})$$

in terms of the purely auxiliary quantities  $\rho_\pm$

## C.2 Two-Level Systems

There are a couple of steps in the calculations in section 6.3 that were omitted for the sake of brevity. For the completeness of the calculation, they can be found below.

### C.2.1 Transformed Master Equation

There are several ways of transforming the master equations into a simpler form. These will of course depend on the specifics of the system, of these the straightforward diagonalisation as done in section 6.3 is one. That is however not necessarily a feasible solution method if the Hamiltonians  $H_{\pm}$  are time dependent. Let us thus consider an avenue more feasible for time-dependent systems.

Let  $P$  and  $S$  diagonalise  $\alpha$  and  $\beta$  in eq. (6.16) respectively, i.e.  $\alpha = S_+ J_+ S_+^{-1}$  and  $\beta = S_- J_- S_-^{-1}$ , where  $\alpha$  and  $\beta$  are diagonalisable as long as  $|\mathbf{d}^{\pm}| \neq 0$ . However,  $|\mathbf{d}^{\pm}| = 0$  should not be a problem as it would correspond to a zero Hamiltonian.

The matrix  $A$  can be rewritten as

$$A = \begin{pmatrix} S_+ & 0 \\ 0 & S_- \end{pmatrix} \begin{pmatrix} J_+ & S_+^{-1} S_- \\ S_-^{-1} S_+ & J_- \end{pmatrix} \begin{pmatrix} S_+^{-1} & 0 \\ 0 & S_-^{-1} \end{pmatrix} = V B V^{-1}.$$

From this we immediately see that  $V V^{-1} = \mathbf{1}$  and that in the event that  $S_+$  and  $S_-$  are similar,  $S_+^{-1} S_-$  should be a sparse matrix. Then although  $V$  does not diagonalise  $A$ , it simplifies the problem. Furthermore, because  $S_-^{-1} S_+ = (S_+^{-1} S_-)^{-1}$  further simplifies the problem as it limits the possible number of free parameters. As both  $D$  and  $J$  are diagonal, the number of unrelated, non-zero entries can at most be  $3 + 3 + 3 \times 3 = 15$ . Comparing this to  $A$  which has 18 non-zero entries, it is a possible improvement in diagonalising  $A$ .

Let us define

$$\mathbf{p}(t) = V^{-1} \mathbf{m}(t),$$

where  $V$  in principle can be time-dependent. Then eq. (6.16) can be written as

$$\dot{\mathbf{m}} = \gamma V B V^{-1} \mathbf{m}.$$

Furthermore, if we define  $\mathbf{p}(t) = V^{-1} \mathbf{m}(t)$ , then

$$\frac{\partial}{\partial t} \mathbf{p}(t) = \frac{\partial V^{-1}}{\partial t} \mathbf{m} + V^{-1} \frac{\partial \mathbf{m}}{\partial t},$$

as  $V$  is generally time-dependent due to the possible time-dependence on the Hamiltonians  $H_{\pm}(t)$ . Furthermore, by the differentiation identity [22]

$$\frac{\partial V^{-1}}{\partial t} = -V^{-1} \frac{\partial V}{\partial t} V^{-1},$$

the time derivative of  $\mathbf{n}$  may be rewritten as

$$\dot{\mathbf{m}} = V \dot{\mathbf{p}} - \frac{\partial V}{\partial t} \mathbf{p}.$$

Using this, eq. (6.16) can be rewritten in terms of the transformed vector  $\mathbf{n}$  as

$$V \dot{\mathbf{p}} - \frac{\partial V}{\partial t} \mathbf{p} = \gamma V B \mathbf{p}.$$

It is thus clear that the transformed master equation takes the form

$$\dot{\mathbf{p}} = \left( \gamma B - V^{-1} \frac{\partial V}{\partial t} \right) \mathbf{p}. \quad (\text{C.6})$$

Where the transformation holds as long as  $V$  exists and is invertible.

Furthermore, note that due to the block-diagonal structure of  $V$ , the last term in eq. (C.6) can be written as

$$V^{-1} \frac{\partial V}{\partial t} = \begin{pmatrix} S_+^{-1} \frac{\partial S_+}{\partial t} & 0 \\ 0 & S_-^{-1} \frac{\partial S_-}{\partial t} \end{pmatrix}.$$

Thus solving eq. (6.16) is the problem of diagonalising  $\gamma B - V^{-1} \frac{\partial V}{\partial t}$ , which in general does not seem an easy task. However, for certain systems  $\gamma B - V^{-1} \frac{\partial V}{\partial t}$  hopefully takes on a simpler and possibly time-independent form. A possible application of this transformed master equation is perhaps systems of the form given in [111].

### C.2.2 Representations of Two-Level Systems

Let us consider a general Hermitian Hamiltonian of a two-level system at a time  $t$ . Represented as a Bloch vector  $\mathbf{b}$  along with the contribution from the fluctuator along a general direction  $\pm \mathbf{v}$ , the fluctuator Hamiltonians can be represented as

$$H_{\pm} = (\mathbf{b} \pm \mathbf{v}) \cdot \vec{\sigma}, \quad (\text{C.7})$$

up to some arbitrary constant for  $\mathbf{b}, \mathbf{v} \in \mathbb{R}^3$ .

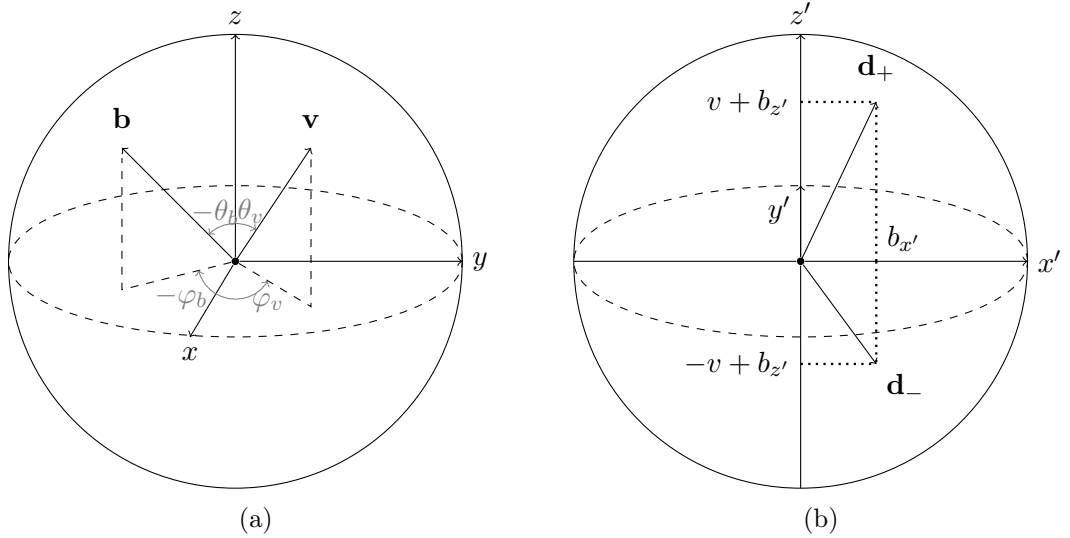


Figure C.1: The Hamiltonians  $H_{\pm}$  of a two-level system represented in terms of the vectors generic vectors  $\mathbf{b}$  and  $\mathbf{v}$  (left) and coordinates with minimal set of parameters  $\mathbf{d}_{\pm} = (g, 0, \Delta \pm g)$  (right).

Then in arbitrary coordinate system the vectors  $\mathbf{b}$  and  $\mathbf{v}$  can be expressed in terms of spherical coordinates,

$$\mathbf{b} = \begin{pmatrix} b \sin \theta_b \cos \varphi_b \\ b \sin \theta_b \sin \varphi_b \\ b \cos \theta_b \end{pmatrix} \quad \text{and} \quad \mathbf{v} = \begin{pmatrix} v \sin \theta_v \cos \varphi_v \\ v \sin \theta_v \sin \varphi_v \\ v \cos \theta_v \end{pmatrix},$$

as shown by fig. C.1a. Let us thus choose a new set of coordinates such that  $\mathbf{v}$  only has a component along the  $z'$ -axis. That is choosing a coordinate system in which  $\cos \theta_v = 1$ , or  $\theta_v = 0$ , such that the polar angle of the vector  $\mathbf{b}$  is shifted to  $\theta_b - \theta_v$  in going from  $z$  to  $z'$ . We thus note that in this choice the angle  $\varphi_v$  will not be of physical significance and is a redundant parameter. Furthermore, in changing the coordinates let us choose the  $y'$ -axis such that the vector  $\mathbf{b}$  has a vanishing  $y'$ -component. That is a coordinate system in which  $\sin \varphi_b = 0$ , or  $\varphi_b = \pm\pi/2$ , where we for simplicity choose  $\varphi_b$  such that the  $x'$ -component of  $\mathbf{b}$  is positive. The general Hamiltonian, eq. (C.7), can thus be expressed in a coordinate system such that

$$\mathbf{d}_{\pm} = \mathbf{b} \pm \mathbf{v} = \begin{pmatrix} b \sin(\theta_b - \theta_v) \\ 0 \\ b \cos(\theta_b - \theta_v) \pm v \end{pmatrix} \quad (\text{C.8})$$

as shown by fig. C.1b. Thus showing that three real parameters are needed to represent eq. (C.7) and that eq. (6.17) can describe any system with two anti-parallel fluctuator states.

Furthermore, we note that in doing such a coordinate transformation we perform a unitary transformation from one representation of the two-level system to another. It is thus a transformation from one set of  $SU(2)$  generators  $\sigma_i$  to another  $\sigma'_i$ . We find that for the particular coordinate transformation above, the representations are related as

$$\begin{pmatrix} \sigma'_x \\ \sigma'_y \\ \sigma'_z \end{pmatrix} = \begin{pmatrix} \cos \theta_v \cos \varphi_b & \cos \theta_v \sin \varphi_b & \sin \theta_v \\ \sin \theta_v \cos \varphi_b & \sin \theta_v \sin \varphi_b & \cos \theta_v \\ \sin \theta_v \cos \varphi_b & \sin \theta_v \sin \varphi_b & \cos \theta_v \end{pmatrix} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}. \quad (\text{C.9})$$

The angles  $\theta_v$  and  $\varphi_b$  here refer to the angles shown in fig. C.1b. Equation (C.9) allows us to in principle relate the two coordinates, however, for theoretical purposes this will not be necessary to do in practice.

Moreover, note that this coordinate transformation will also hold for generally time-dependent Hamiltonians. The procedure is thus exactly the same, whoever the angles will thus be time-dependent. This can in principle induce a coordinate transformation to a rotating frame of reference. However, the transformation from a stationary to a rotating frame does not change the dynamics of the physical system as they are equivalent frames, only the interpretation of the states.

### C.2.3 Simplified Two-Level System

From the diagonalisation,  $S$ , of  $A$ , eq. (6.24), we can readily calculate the explicit form of  $\mathbf{m}_{\pm}$  remembering that

$$[\mathbf{m}_+(t), \mathbf{m}_-(t)] = \mathbf{m}(t) = S\mathbf{n}(t) = Se^{\gamma Ct}\mathbf{n}_0,$$

where for reference

$$S = \begin{pmatrix} 0 & 0 & -\tilde{v} - i\mu & -\tilde{v} - i\mu & -\tilde{v} + i\mu & -\tilde{v} + i\mu \\ 0 & 0 & -i\tilde{v} + \mu & i\tilde{v} - \mu & -i\tilde{v} - \mu & i\tilde{v} + \mu \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & i & -i & i \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

For simplicity let us define

$$a \equiv \tilde{v} + i\mu = \frac{v + \sqrt{v^2 - \gamma^2 \hbar^2}}{\gamma \hbar} \quad \text{and} \quad b \equiv \tilde{v} - i\mu = \frac{v - \sqrt{v^2 - \gamma^2 \hbar^2}}{\gamma \hbar},$$

such that eq. (6.24) simplifies to

$$S = \begin{pmatrix} 0 & 0 & -a & -a & -b & -b \\ 0 & 0 & -ia & ia & -ib & ib \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & i & -i & i \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Then expressed in terms of  $n_i(t)$ , we find that

$$m_1^+ = -a(n_3 + n_4) - b(n_5 + n_6), \quad (\text{C.10a})$$

$$m_2^+ = ia(n_4 - n_3) + ib(n_6 - n_5), \quad (\text{C.10b})$$

$$m_3^+ = -n_1 + n_2, \quad (\text{C.10c})$$

$$m_1^- = i(n_4 - n_3 + n_6 - n_5), \quad (\text{C.10d})$$

$$m_2^- = n_3 + n_4 + n_5 + n_6, \quad (\text{C.10e})$$

$$m_3^- = n_1 + n_2. \quad (\text{C.10f})$$

Which can be combined as  $m_i^+ + m_i^-$  to form the averaged Bloch vector components

$$r_1(t) = -(i + a)n_3(t) + (i - a)n_4(t) - (i + b)n_5(t) + (i - b)n_6(t), \quad (\text{C.11a})$$

$$r_2(t) = (1 - ia)n_3(t) + (1 + ia)n_4(t) + (1 - ib)n_5(t) + (1 + ib)n_6(t), \quad (\text{C.11b})$$

$$r_3(t) = 2n_2(0). \quad (\text{C.11c})$$

It is thus immediately clear that  $r_3(t)$  is constant in time, as we would expect as there is no component in the Hamiltonian coupling the third block vector to the plane. On average, the fluctuator does not affect the component parallel to the flipping, this would also follow directly from the cross-product in eq. (6.14). Furthermore, it is clear that the initial condition  $r_3(0)$  fully fixes  $n_2(0)$  whilst  $n_1(0)$  as an arbitrary free parameter that do not appear in any of the physical solutions, but eventually will decay away as it is associated with the constant decoherence rate  $T_0^-$ . Furthermore, it becomes clear that the initial conditions  $r_1(0)$  and  $r_2(0)$  does not fully fix the remaining  $n_i(0)$ .

