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SOME PHYSICAL PROBLEMS OF PSEUDO-HERMITIAN HAMILTONIANS

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Abstract

In this thesis we have discussed on one of the recent topics in physics, in particular in quantum mechanics, which is "the non-Hermitian Hamiltonians", and the conditions that make the spectra of these Hamiltonians real. Initially, the Hermiticity was a necessary and sufficient condition for the reality of the Hamiltonian spectrum. Then a new quantum theory called the " \mathcal{PT} -symmetry" started to emerge, this theory was developed in 1998 by Carl Bender and Stefan Boettcher, where they revealed the existence of a class of non-Hermitian Hamiltonians with real spectra. These Hamiltonians are invariant under the transformation of \mathcal{PT} -symmetry, where \mathcal{P} is the parity operator and \mathcal{T} is the time reversal operator. A few years later, another alternative approach was developed in 2002 by Mostafazadeh who works on pseudo-Hermitian Hamiltonians and he showed that every Hamiltonian with a real spectrum is pseudo-Hermitian. We have found from an application on two examples of a pseudo-Hermitian Hamiltonians "shifted harmonic oscillator" and "cubic anharmonic oscillator" that the energy spectrum of these Hamiltonians are real and positive.

Keywords: Hermiticity, \mathcal{PT} -symmetry, Pseudo-Hermiticity, Quasi-Hermiticity.

Résumé

Dans ce mémoire, nous avons discuté l'un des sujets récents de la physique, notamment en mécanique quantique, qui est "les Hamiltoniens non Hermitiens", et les conditions qui rendent les spectres de ces Hamiltoniens réels. Initialement, l'Hermiticité était une condition nécessaire et suffisante pour la réalité du spectre Hamiltonien. Puis une nouvelle théorie quantique appelée "la symétrie \mathcal{PT} " a commencé à émerger, cette théorie a été développée en 1998 par Carl Bender et Stefan Boettcher, ils ont révélé l'existence d'une classe d'Hamiltoniens non Hermitiens avec des spectres réels. Ces Hamiltoniens sont invariants sous la transformation de la symétrie \mathcal{PT} , où \mathcal{P} est l'opérateur de parité et \mathcal{T} est l'opérateur de renversement du temps. Quelques années plus tard, une autre approche alternative a été développée en 2002 par Mostafazadeh qui travaille sur des Hamiltoniens pseudo-Hermitiens et il a montré que chaque Hamiltonien avec un spectre réel est pseudo-Hermitien. Nous avons trouvé à partir d'une application sur deux exemples d'Hamiltoniens pseudo-Hermitiens "l'oscillateur harmonique décalé" et "l'oscillateur anharmonique cubique" que les spectres d'énergie de ces Hamiltoniens sont réels et positifs.

Mots Clés : Hermiticité, \mathcal{PT} -symétrie, Pseudo-Hermiticité, Quasi-Hermiticité.

ملخص

في هذه الأطروحة، ناقشنا أحد الموضوعات الحديثة في الفيزياء، وخاصة في ميكانيك الكم، وهو مؤثرات هاميلتون الغير هرميتية، والشروط التي تجعل أطياف هته المؤثرات حقيقية. في البداية، كانت الهرميتية شرطاً ضرورياً وكافياً لحقيقية الطيف الهاميلتوني. ثم بدأت نظرية كمومية جديدة في الظهور تسمى تماثل- PT ، وقد تم تطوير هذه النظرية في عام ١٩٩١ من قبل بندر و بوتشر. حيث كشفوا عن وجود فئة من مؤثرات هاميلتون غير هرميتية ذات أطياف حقيقية، هذه المؤثرات ثابتة في ظل تحويل تماثل- PT ، حيث P هو مؤثر التكافؤ و T هو مؤثر انعكاس الزمن. بعد بضع سنوات، تم تطوير نهج بديل آخر في عام ٢٠٠٢ من قبل مصطفى زاده الذي يعمل على مؤثرات هاميلتون هرميتية-زائفة وأظهر أن كل هاميلتوني يملك طيف طاقة حقيقي هو هاميلتون هرميتي زائف. من خلال تطبيق على مثالين من مؤثرات هاميلتون هرميتية-زائفة للمذبذب التوافقي النازح $p^2 + x^2 + i\epsilon x$ و للمذبذب اللاتوافقي المكعب $p^2 + x^2 + i\epsilon x^3$ وجدنا أن طيف الطاقة لهذه المؤثرات حقيقي وإيجابي.

كلمات مفتاحية : الهرميتية، اللاهرمتية، تماثل- PT ، تماثل زائف-هرميتي، تماثل شبه-هرميتي.

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Introduction

Quantum mechanics (QM) is one of the most important achievements of the twentieth century theoretical physics, it was developed by *Heisenerg*, *Pauli*, *Schrödinger*, *Dirac* and many other physicists [1].

Indeed, among the postulates of quantum mechanics which has been the subject of several debates between the physicists and mathematicians of the world, we find that of Hermiticity, the latter states that if a Hamiltonian H is Hermitian, then there eigenvalues are real [2].

However, several years ago, Bessis conjectured on the basis of numerical studies that the spectrum of the Hamiltonian $H = p^2 + x^2 + ix^3$ is real and positive [3], which allowed us to note that the Hermiticity of the Hamiltonian is only a sufficient condition and not necessary for the reality of the spectrum.

The Hamiltonian studied by Bessis is just one example of a huge and remarkable class of non-Hermitian Hamiltonians whose energy levels are real and positive. A more recent attempt generalizing QM , is due to Carl Bender and his collaborators with adopting all its axioms except the one that restricted the Hamiltonian to be Hermitian, where they replaced the latter condition with there requirement that the Hamiltonian must have an exact \mathcal{PT} -symmetry [4, 5].

But the latter was proved insufficient to formulate a valid quantum theory, since the norm of the \mathcal{PT} -inner product is not necessarily positive, hence the probability of presence is not definite positive and therefore it cannot be physically acceptable. To overcome the problem of negative norms, Bender et al constructed a new operator denoted by \mathcal{C} . The latter makes it possible to define a inner product where all the norms are then positive, this inner product is called " \mathcal{CPT} -inner product" [6].

However, in general there are Hermitian Hamiltonians with a real spectrum that are not \mathcal{PT} -symmetric and there are \mathcal{PT} -symmetric Hamiltonians that do not have a real spectrum. Therefore, \mathcal{PT} -symmetry is neither a necessary nor a sufficient condition for a Hamiltonian to have a real spectrum [7, 8, 9]. During the last two decades, several articles have been published and international conferences have been organized annually on the subject.

A few years after Bender's work, Mostafazadeh introduced the notion of pseudo-Hermiticity [10]. He explored the basic structure that is responsible for the spectral reality of non-Hermitian Hamiltonians. He established that all \mathcal{PT} -symmetric Hamiltonians are pseudo-Hermitians. He also showed that a Hamiltonian is pseudo-Hermitian if and only if its eigenvalues are real or there are complex-conjugate pairs of complex eigenvalues. Therefore, pseudo-Hermiticity is a generalization of Hermiticity and \mathcal{PT} -symmetry. So pseudo-Hermiticity is only a necessary condition for the reality of the spectrum, but it's not a sufficient.

Our work is more interested in pseudo-Hermiticity and especially in the way that we calculate the metric operator, we have therefore prepared this master thesis which is composed of an introduction, four chapters and a conclusion.

In the first chapter, we gave the necessary mathematical tools and the postulates of quantum mechanics with a brief history of the non-Hermitian Hamiltonians. In the second chapter, we recalled the essential properties of the parity operator \mathcal{P} and of the time reversal operator \mathcal{T} and their product \mathcal{PT} , then we presented the \mathcal{PT} -symmetric quantum mechanics.

In chapter 3, we will talk about the new quantum theory of pseudo-Hermiticity which has been studied by Ali Mostafazadeh, where we started with a definition and some of its principles, then we presented the action of the metric operator, and finally we introduced the quasi-Hermiticity.

In chapter 4 we made simple applications for a Hamiltonian Pseudo-Hermitian using the perturbation method, then we ended our work with a conclusion.

Chapter 1

Switch from Hermitian to non-Hermitian Hamiltonians

1.1 Introduction

The purpose of this chapter is to show the basis of ordinary quantum mechanics and their necessary components, where any quantum theory would be understood and well established and by virtue of this review the following topics do make sense. The first section will give some mathematical properties of Hilbert space which assigned any quantum theory, the second one reserved to mention the fundamental postulates of quantum mechanics. The last section is about an historical approach of the non-Hermitian Hamiltonians subject, where it became very attractive area of research.

1.2 Mathematical tools of quantum mechanics

One of the axioms of quantum mechanics is that the pure physical states of a quantum system are vectors in the Hilbert space \mathcal{H} . Each vector can be determined from a unique way by an element ψ of \mathcal{H} , the latter is called the state vector. The physical quantities related to a pure state are calculated using the corresponding state vector and the inner product of the Hilbert space.

1.2.1 Inner product

Consider a complex vector space \mathcal{V} and a function $\langle \cdot | \cdot \rangle : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{C}$: that assigns to any pair ψ, ϕ of elements of \mathcal{V} a complex number $\langle \psi | \phi \rangle$ [10]

$$\langle \psi | \phi \rangle = \int_{-\infty}^{+\infty} \psi^*(x) \phi(x) dx. \quad (1.1)$$

Suppose that $\langle \cdot | \cdot \rangle$ is positive-definite, Hermitian, and linear, then $\langle \cdot | \cdot \rangle$ is called an inner product on \mathcal{V} , and the pair $(\mathcal{V}, \langle \cdot | \cdot \rangle)$ is called an inner product space [10]. $\|\psi\| := \sqrt{\langle \psi | \psi \rangle}$ is called the norm of ψ (we can use the norm to define a notion of distance between elements of \mathcal{V}) [10].

1.2.2 Hilbert space

A Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle)$ over \mathbb{C} (or \mathbb{R}) is an inner product space which meets an additional technical condition, namely that its norm defines a complete space. In other words, a Hilbert space is a complete inner product space [10].

1.2.3 Orthonormal basis

A basis (a sequence of vectors) $|V_n\rangle \in \mathcal{H}, n \in \{1, 2, 3, \dots, N\}$, forms an orthonormal basis of the space \mathcal{H} if for all $m, n \in \{1, 2, 3, \dots, N\}$ [10]

$$\langle V_n | V_m \rangle = \delta_{nm}, \quad (1.2)$$

where δ_{nm} denotes the Krönecker delta symbol $\delta_{nm} := 1$ if $n = m$ and $\delta_{nm} := 0$ if $n \neq m$.

Any vector $|\psi\rangle$ decomposes in the form

$$|\psi\rangle = \sum_n c_n |V_n\rangle, \quad (1.3)$$

where the coefficients c_n of the basis ψ are given by

$$c_n = \langle V_n | \psi \rangle, \quad c_n \in \mathbb{C}. \quad (1.4)$$

Furthermore for all $\phi, \psi \in \mathcal{H}$, we have

$$\langle \phi | \psi \rangle = \sum_{n=1}^N \langle \phi | V_n \rangle \langle V_n | \psi \rangle. \quad (1.5)$$

In particular for all $\psi \in \mathcal{H}$, we have

$$\|\psi\|^2 = \sum_{n=1}^N |\langle V_n | \psi \rangle|^2 = \sum_{n=1}^N |c_n|^2. \quad (1.6)$$

Completeness relation

From Eq. (1.3)

$$|\psi\rangle = \sum_n (\langle V_n|\psi\rangle) |V_n\rangle = \left(\sum_n |V_n\rangle\langle V_n| \right) |\psi\rangle. \quad (1.7)$$

As we know, the operator which leaves the vector unchanged is the identity operator

$$\sum_n |V_n\rangle\langle V_n| = \mathbb{1}. \quad (1.8)$$

This expression is called the *completeness relation* [10, 17].

Expression of an operator in a basis

\hat{A} is an operator, we associate its matrix elements in an orthonormal basis $\{V_n\}$ [17]

$$\hat{A}_{nm} = \langle V_n|\hat{A}|V_m\rangle. \quad (1.9)$$

Bi-orthonormal systems

Let $\{\psi_n\}$ be a basis of an N -dimensional separable Hilbert space \mathcal{H} and $\{V_k\}$ be a orthonormal basis, such that for all $n, k \in \{1, 2, 3, \dots, N\}$ [10, 17]

$$|\psi_n\rangle = \sum_{k=1}^N \langle V_k|\psi_n\rangle |V_k\rangle = \sum_{k=1}^N B_{kn}^{-1} |V_k\rangle, \quad (1.10)$$

such that, for all $m \in \{1, 2, 3, \dots, N\}$, the vectors $|\phi_m\rangle$ are defined by

$$|\phi_m\rangle := \sum_{j=1}^N B_{mj}^* |V_j\rangle. \quad (1.11)$$

A sequence (ψ_n, ϕ_n) of ordered pairs of elements of \mathcal{H} for all $m, n \in \{1, 2, 3, \dots, N\}$ satisfy the condition

$$\langle \phi_m|\psi_n\rangle = \delta_{mn}, \quad (1.12)$$

and are called a *bi-orthonormal system* [10, 17].

The generalization of the more familiar completeness relation [10]

$$\sum_{n=1}^N |\psi_n\rangle\langle \phi_n| = \mathbb{1}. \quad (1.13)$$

A bi-orthonormal system satisfying this relation is said to be complete [10].

1.2.4 Operators

In general we call an operator a mathematical object that transforms one element of a set to another element of the same set [14]. Indeed, operators are linear maps of the Hilbert space \mathcal{H} onto itself. If \hat{A} is an operator, then for any $|\psi\rangle$ in \mathcal{H} , $\hat{A}|\psi\rangle$ is another element in \mathcal{H}

$$\hat{A}|\psi\rangle = |\psi'\rangle. \quad (1.14)$$

And the inverse of an operator \hat{A}^{-1} satisfies the following relation

$$|\psi\rangle = \hat{A}^{-1}|\psi'\rangle. \quad (1.15)$$

Linear operators

An operator \hat{A} is called a linear operator if $\forall |\psi\rangle, |\phi\rangle \in \mathcal{H}$, and $\lambda \in \mathbb{C}$, the relation following is verified [10, 14, 17]

$$\hat{A}(\lambda|\psi\rangle) = \lambda\hat{A}|\psi\rangle. \quad (1.16)$$

$$\hat{A}(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1\hat{A}|\psi_1\rangle + \lambda_2\hat{A}|\psi_2\rangle. \quad (1.17)$$

Properties :

An operator \hat{A} is antilinear operator if

$$\hat{A}(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1^*\hat{A}|\psi_1\rangle + \lambda_2^*\hat{A}|\psi_2\rangle. \quad (1.18)$$

If \hat{A}_1, \hat{A}_2 are two linear operators, then $\hat{A}_1\hat{A}_2$ is also linear.

The set of linear operators on \mathcal{H} form a vector space, denoted by $\mathbb{L}(\mathcal{H})$.

Adjoins operators

If \hat{A} is a linear operator, the adjoint operator of \hat{A} is a linear operator, denoted by \hat{A}^\dagger which satisfies [10, 14, 17]

$$\langle \hat{A}\phi|\psi\rangle = \langle \phi|\hat{A}^\dagger\psi\rangle, \forall |\phi\rangle, |\psi\rangle \in \mathcal{H}. \quad (1.19)$$

Properties :

$$\left(\hat{A}^\dagger\right)^\dagger = \hat{A}. \quad (1.20)$$

$$\left(\hat{A}_1\hat{A}_2\right)^\dagger = \hat{A}_2^\dagger\hat{A}_1^\dagger. \quad (1.21)$$

$$\left(\hat{A}_1 + \hat{A}_2\right)^\dagger = \hat{A}_1^\dagger + \hat{A}_2^\dagger. \quad (1.22)$$

$$\left(\hat{A}^n\right)^\dagger = \left(\hat{A}^\dagger\right)^n. \quad (1.23)$$

Hermitian operators

The linear operator \hat{A} is self-adjoint or Hermitian if $\hat{A}^\dagger = \hat{A}$, i.e.

$$\langle \hat{A}\psi_1 | \psi_2 \rangle = \langle \psi_1 | \hat{A}\psi_2 \rangle. \quad (1.24)$$

The adjoint of an operator \hat{A} is the Hermitian conjugate of \hat{A} .

Theorem 1 All the eigenvalues of a Hermitian operator are real [14].

Theorem 2 Two eigenvectors of a Hermitian operator, corresponding to distinct eigenvalues, are orthogonal to each other [14].

Hermitian operators in quantum mechanics are used to represent physical variables, quantities such as energy, momentum, angular momentum, position, The operator representing the energy is the Hamiltonian \hat{H} .

Commutators

The commutator of two operators \hat{A} and \hat{B} is

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \quad (1.25)$$

The Anti-commutator of two operators \hat{A} and \hat{B} is

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}. \quad (1.26)$$

Additional relations:

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}. \quad (1.27)$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}\hat{B}, \hat{C}] + [\hat{C}\hat{A}, \hat{B}]. \quad (1.28)$$

$$[\hat{A}\hat{B}\hat{C}, \hat{D}] = \hat{A}\hat{B}[\hat{C}, \hat{D}] + \hat{A}[\hat{B}, \hat{C}]\hat{D} + [\hat{A}, \hat{D}]\hat{B}\hat{C}. \quad (1.29)$$

Normal operators

A normal operator \hat{A} on a Hilbert space is an operator which commutes with its adjoint

$$\hat{A}^\dagger \hat{A} = \hat{A}\hat{A}^\dagger. \quad (1.30)$$

Unitary operators

An operator \hat{A} is said to be unitary if it satisfies the following relation

$$\hat{A}^\dagger \hat{A} = \hat{A} \hat{A}^\dagger = \mathbb{1}, \quad (1.31)$$

which means that it commutes with its adjoint, therefore, the operator \hat{A} is normal [16].

In this case, the inverse operator \hat{A}^{-1} coincides with the adjoint operator \hat{A}^\dagger . An important property of unitary operators is that they keep invariant the inner product [16]

$$\langle \hat{A}\psi | \hat{A}\phi \rangle = \langle \psi | \phi \rangle. \quad (1.32)$$

Eigenvectors and eigenvalues

Let \hat{A} be a linear operator

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle. \quad (1.33)$$

We say that $|\psi\rangle$ is an eigenvector of operator A and the number λ is called the eigenvalue of v relating to the eigenvector $|\psi\rangle$. The set of eigenvalues of operator \hat{A} constitutes the spectrum of this operator [14].

When the same eigenvalue corresponds to several eigenvectors, we say that the eigenvalue is degenerate, and the number of eigenvectors associated with an eigenvalue is the order of degeneration [14].

1.2.5 Observables

In physics, an observable is a physical quantity that can be measured. Examples include position and momentum. In quantum physics, it is an operator, where the property of the quantum state can be determined by some sequence of operations.

By definition, an operator \hat{A} is said to be observable, if it is Hermitian and diagonalizable, then the eigenvalues of an observable are real [16].

1.3 Postulates of quantum mechanics

It is known in quantum mechanics that it is not possible to determine exactly the trajectory of particles, one however can access the probability of finding system at given point of space. Instead of talking about the position of particles, we introduce a distribution function of their possible position is

called *the wave function* $\psi(x, t)$. This wave function is a probability amplitude which in a way represents the generalization of the notion of wave to material particles.

1.3.1 State of system

Postulate 1

Quantum state at time t would be represented by a state vector $|\psi\rangle$ which belong to a vector space, which is the space of states. This space is a Hilbert space and is built on the field of the set of the complex numbers \mathbb{C} [14].

1.3.2 Operator corresponding to physical quantity

The various physical quantities can be represented by operators. This is the case for example with energy, momentum, . . . , etc. These operators are Hermitians. In quantum mechanics, all physical quantities \mathcal{A} capable of being measured are represented by Hermitian operator \hat{A} .

Postulate 2

To any measurable physical quantity \mathcal{A} , we can match an operator \hat{A} which acts on the state vectors of space \mathcal{H} ; this operator is an *observable* [14].

1.3.3 Measurement of physical quantity

All the results of Measurement of observables are the eigenvalues of the corresponding operator. Each eigenvalue corresponds to one or more eigenfunctions which represent the stationary states of the system.

Postulate 3

The eigenvalue of the observable \hat{A} , corresponding to a physical quantity \mathcal{A} , are the only Measurement values [14].

1.3.4 Schrödinger's equation

For any system, the Schrödinger equation is obtained from the classical expression of the Hamiltonian.

Postulate 4

The Hamiltonian operator \hat{H} of a system is the observable associated with the total energy of this system. The evolution over a time of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation [14].

$$\hat{H}|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle. \quad (1.34)$$

1.3.5 Probability of obtaining an eigenvalue

Consider a system which is in any state described by the normalized vector $|\psi\rangle$. Denote by $|V_n\rangle$ the orthonormal eigenvectors of the Hamiltonian of the system. The vector $|\psi\rangle$ can be written on the basis $\{|V_n\rangle\}_{n \in \mathbb{N}}$

$$|\psi\rangle = \sum_n c_n |V_n\rangle. \quad (1.35)$$

The energy E_n of the system is given by the matrix element of the Hamiltonian \hat{H}

$$E_n = \langle V_n | \hat{H} | V_n \rangle. \quad (1.36)$$

Postulate 5

Let \mathcal{A} be a physical quantity of a quantum system and \hat{A} the corresponding observable whose spectrum contains only non-degenerate eigenvalues a_n associated with orthonormal eigenvectors $|V_n\rangle$. When we measure \mathcal{A} on the system in any state $|\psi\rangle$ with unity norm [14]

$$|\psi\rangle = \sum_n c_n |V_n\rangle. \quad (1.37)$$

The probability $P(a_n)$ of obtaining as a measurement result a_n is giving by [14]

$$P(a_n) = |c_n|^2 = |\langle V_n | \psi \rangle|^2. \quad (1.38)$$

Postulate 6

Let \mathcal{A} be a physical quantity of a system and \hat{A} the corresponding observable; let a_n be an eigenvalue of \hat{A} degenerated g_n times and associated with the orthonormal eigenvectors $|V_n^k\rangle$ (each eigenvalue g_n corresponds to orthonormal eigenvectors $|V_n^k\rangle$, with $k = 1, 2, 3, \dots, g_n$). When we measure \mathcal{A} on the system in the state $|\psi\rangle$ of unity norm [14]

$$|\psi\rangle = \sum_n \sum_{k=1}^{g_n} c_n^k |V_n^k\rangle. \quad (1.39)$$

The probability $P(a_n)$ of obtaining the measurement result a_n is given by [14]

$$P(a_n) = \sum_{k=1}^{g_n} |c_n^k|^2 = \sum_{k=1}^{g_n} |\langle V_n^k | \psi \rangle|^2. \quad (1.40)$$

1.4 Non-Hermitian Hamiltonians

It is known in algebra that if an operator defined on a Hilbert space is Hermitian, then its eigenvalues are all real and the corresponding eigenfunctions form an orthogonal basis. On the other hand, if it's non-Hermitian, its own eigenvalues are not guaranteed to be real, but rather they are generally complex.

In quantum mechanics, the dynamics of a physical system is completely governed by its Hamiltonian operator, such that any physical system must satisfy the following fundamental conditions :

- The Hamiltonian must be Hermitian for his spectrum to be real.
- The inner products of state vectors in Hilbert space must have a positive norm.
- The time evolution operator must be unitary.

As we have already said about the condition of Hermiticity, \hat{H} is said to be Hermitian if it satisfies $\hat{H} = \hat{H}^\dagger$. In the contrary case it is said to be non-Hermitian, and it satisfies the following relation

$$\hat{H} \neq \hat{H}^\dagger. \quad (1.41)$$

The use of non-Hermitian Hamiltonians in physics goes back a long time. One of the earliest use of non-Hermitian Hamiltonians was by Wu in 1959. Wu described the sphere of Bose using a non-Hermitian Hamiltonian, she discovered that the energies of this system are real. In 1967, Wong presented some results on the spectral properties of a class of non-Hermitian Hamiltonians called *physically reasonable*. In 1975, Haydock and Kelly used non-Hermitian Hamiltonians to determine the density of states of chemical pseudo-potentials [15]. In 1980, Caliceti were studying Borel summation of divergent perturbation series arising from classes of anharmonic oscillators, were astonished to find that the eigenvalues of an oscillator having an imaginary cubic self-interaction term are real [5]. In 1981, Faissal and Moloney established a quantum formulation of the process of decline by converting Schrodinger equation for Hermitian Hamiltonians to the non-Hermitians case [15]. In 1992, Hollowood and Scholtz discovered in their own areas of research surprising examples of non-Hermitian Hamiltonians having real spectra [5]. In 1997, Hatano and Nelson justified the use of a complex spectrum to interpret the existence of an imaginary part in the energy of a semiconductor on which an external magnetic field is applied [15].

All this work which uses non-Hermitian Hamiltonians does not belong to any fundamental basis of a non-Hermitian theory. Indeed, the first basis of non-Hermitian quantum theories did not emerge until 1998, when Bender and Boettcher studied the Bessis-Zin Justin conjecture about the reality of the spectrum of the non-Hermitian Hamiltonian $\hat{p}^2 + (i\hat{x})^N$ [3], where N is real. It has been shown that the Hermiticity of a Hamiltonian is not a necessary condition to guarantee a real eigenvalues for the Hamiltonian. There are two other approaches that can be taken. The first has been developed primarily in 1998 by Bender and associates and utilizes space-time reflection symmetry. This is known as \mathcal{PT} -symmetry. Then an alternative approach was developed by Mostafazadeh since 2002, who works with pseudo-Hermitian Hamiltonians.

We will discuss more about these two approaches in the next chapters.

Chapter 2

\mathcal{PT} -symmetric Hamiltonians

2.1 Introduction

The pioneering work of Carl Bender and his student Stefan Boettcher revealed the existence of a class of non-Hermitian Hamiltonians whose eigenvalues are real [3]. These Hamiltonians are invariant under a physical symmetry called (\mathcal{PT} -symmetry), where \mathcal{P} is the parity operator and \mathcal{T} is the time reversal operator [3, 5, 7, 17].

Indeed, in the original article in 1998, C Bender and S Boettcher studied the following Hamiltonian [3]

$$\hat{H} = \hat{p}^2 - (i\hat{x})^N, \quad (2.1)$$

where N is real.

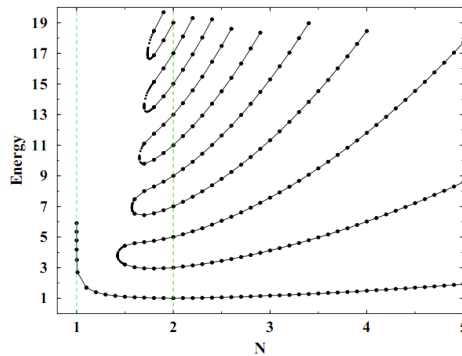


Figure 2.1: Energy levels of the Hamiltonian $\hat{H} = \hat{p}^2 - (i\hat{x})^N$ as a function of the parameter N [3]

In general case, this Hamiltonian is non-Hermitian, the authors showed that :

- For $N \geq 2$, the spectrum is infinite, discrete and entirely real and positive.
- For $1 < N < 2$, there are only finite number of real positive eigenvalues and infinite number of complex conjugate pairs of eigenvalues.
- For $N \leq 1$, there are no real eigenvalues.

In this chapter, we first give a review on discrete symmetries in quantum mechanics, and we'll briefly recall the essential properties of both of parity \mathcal{P} and time reversal \mathcal{T} operators and their product \mathcal{PT} , then we'll present the \mathcal{PT} -symmetric quantum mechanics.

2.2 Some symmetric transformations

In physics, there are several types of transformations, including spatial transformations such as: translation, rotation, parity. And other transformations those involve time such as the time translation or time reversal, when a system is invariant under the effect of a transformation this implies that the system has symmetry [18]. Let \hat{U} be a Hilbert space operator corresponding to a symmetry transformation, ψ and ψ' are the wave functions describing the system before and after the transformation, such that:

$$\psi' = \hat{U}\psi. \quad (2.2)$$

If the mean value of an operator \hat{A} is invariant with respect to this transformation

$$\langle \psi' | \hat{A} | \phi' \rangle = \langle \psi | \hat{U}^\dagger \hat{A} \hat{U} | \phi \rangle = \langle \psi | \hat{A} | \phi \rangle, \quad (2.3)$$

then \hat{A} commutes with \hat{U} , i.e.

$$[\hat{A}, \hat{U}] = 0, \quad (2.4)$$

and the operator \hat{U} is linear and unitary

$$\hat{U}^\dagger = \hat{U}^{-1} \quad \text{and} \quad \hat{U}(\lambda\psi) = \lambda\hat{U}\psi, \quad (2.5)$$

or anti-unitary (anti-linear and unitary)

$$\hat{U}^\dagger = \hat{U}^{-1} \quad \text{and} \quad \hat{U}(\lambda\psi) = \lambda^*\hat{U}\psi. \quad (2.6)$$

If the dynamics of the system described by the Hamiltonian \hat{H} is invariant under the action of this transformation, then \hat{H} commutes with \hat{U}

$$[\hat{H}, \hat{U}] = 0, \quad (2.7)$$

the fact that $\hat{U}^\dagger = \hat{U}^{-1}$, so

$$\hat{H} = \hat{U}\hat{H}\hat{U}^{-1} = \hat{U}\hat{H}\hat{U}^\dagger. \quad (2.8)$$

2.2.1 Parity operator \mathcal{P}

The parity \mathcal{P} is a transformation which corresponds to a reflection in space, that is to say, it is a symmetry with respect to the origin of the coordinates. The action of \mathcal{P} on the position vector $|\mathbf{x}\rangle$ is :

$$\mathcal{P}|\mathbf{x}\rangle = |-\mathbf{x}\rangle. \quad (2.9)$$

and its hermitian conjugate relation gives

$$\langle\mathbf{x}|\mathcal{P}^\dagger = \langle-\mathbf{x}|. \quad (2.10)$$

The action of \mathcal{P}^2 on the position vector $|\mathbf{x}\rangle$ give back to $|\mathbf{x}\rangle$, i.e.

$$\mathcal{P}^2|\mathbf{x}\rangle = \mathcal{P}(\mathcal{P}|\mathbf{x}\rangle) = \mathcal{P}|\mathbf{x}\rangle = |\mathbf{x}\rangle. \quad (2.11)$$

This relation allows us to identify \mathcal{P}^2 as the identity operator (unit operator):

$$\mathcal{P}^2 = \mathbb{1}. \quad (2.12)$$

The parity operator \mathcal{P} change the sign of the position \mathbf{x} and leave the t time unchanged

$$\mathbf{x} \rightarrow \mathbf{x}' = -\mathbf{x}, \quad \text{and} \quad t \rightarrow t' = t. \quad (2.13)$$

This implies that the momentum transforms as follows

$$\mathbf{p} \rightarrow \mathbf{p}' = m \frac{d\mathbf{x}'}{dt'} = -m \frac{d\mathbf{x}}{dt} = -\mathbf{p}. \quad (2.14)$$

The position and momentum operators, and the complex number i transform under the action of the operator \mathcal{P} as follows [3]

$$\mathcal{P}\hat{\mathbf{x}}\mathcal{P} = -\hat{\mathbf{x}}, \quad \mathcal{P}\hat{\mathbf{p}}\mathcal{P} = -\hat{\mathbf{p}}, \quad \mathcal{P}i\mathcal{P} = i. \quad (2.15)$$

And the wave functions transform as follows

$$\psi(x, t) \rightarrow \psi'(x, t) = \mathcal{P}\psi(x, t) = \psi(-x, t). \quad (2.16)$$

If $\psi(x, t)$ is an eigenfunction of \mathcal{P} , i.e.

$$\mathcal{P}\psi(x, t) = \lambda\psi(x, t), \quad (2.17)$$

then after a second reflection from space, the wave function remains unchanged since $\mathcal{P}^2 = I$

$$\mathcal{P}^2\psi(x, t) = \lambda^2\psi(x, t) = \psi(x, t), \quad (2.18)$$

and the eigenvalues of \mathcal{P} can take the following values

$$\begin{cases} \lambda = 1, & \text{if } \psi(x, t) \text{ is even;} \\ \lambda = -1, & \text{if } \psi(x, t) \text{ is odd.} \end{cases} \quad (2.19)$$

We noticed that the parity operator \mathcal{P} is linear, i.e.

$$\mathcal{P}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1\mathcal{P}|\psi_1\rangle + a_2\mathcal{P}|\psi_2\rangle \quad (2.20)$$

2.2.2 Time reversal operator \mathcal{T}

The time direction reversal operator is denoted by \mathcal{T} . The latter changes the sign of the time t and leave the \mathbf{x} position unchanged

$$t \rightarrow t' = -t \quad \text{and} \quad \mathbf{x} \rightarrow \mathbf{x}' = \mathbf{x}. \quad (2.21)$$

This implies that the momentum is transformed in this way

$$\mathbf{p} \rightarrow \mathbf{p}' = m \frac{d\mathbf{x}'}{dt'} = -m \frac{d\mathbf{x}}{dt} = -\mathbf{p}. \quad (2.22)$$

The position and momentum operators, and the complex number i transform under the action of the operator \mathcal{T} as follows [3]

$$\mathcal{T}\hat{\mathbf{x}}\mathcal{T} = \hat{\mathbf{x}}, \quad \mathcal{T}\hat{\mathbf{p}}\mathcal{T} = -\hat{\mathbf{p}}, \quad \mathcal{T}i\mathcal{T} = -i, \quad (2.23)$$

and it leads to:

$$\mathcal{T} [\hat{\mathbf{x}}, \hat{\mathbf{p}}] \mathcal{T} = [\hat{\mathbf{x}}, -\hat{\mathbf{p}}] = -i\hbar. \quad (2.24)$$

The time reversal operator \mathcal{T} can be decomposed into a product of a unitary operator \hat{U} and an anti-linear operator \hat{K} , where \hat{K} is the complex conjugate operator

$$\mathcal{T} = \hat{U}\hat{K}. \quad (2.25)$$

The action of the operator \mathcal{T} on a state $|\psi\rangle$ is written

$$\mathcal{T}|\psi\rangle = \hat{U}\hat{K}|\psi\rangle = \hat{U}|\psi\rangle^*. \quad (2.26)$$

The product of \mathcal{T} by an operator \hat{A} is

$$\mathcal{T}\hat{A} = \hat{U}\hat{K}\hat{A} = \hat{U}\hat{A}^*. \quad (2.27)$$

Indeed

$$\mathcal{T}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1^*\mathcal{T}|\psi_1\rangle + a_2^*\mathcal{T}|\psi_2\rangle. \quad (2.28)$$

The preceding relations imply that the operator \mathcal{T} has an important property which is the anti-unitarity

$$\langle \mathcal{T}\phi | \mathcal{T}\psi \rangle = \langle \phi | \hat{U}^\dagger \hat{U} |\psi\rangle^* = \langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle. \quad (2.29)$$

Since \mathcal{T} is an involution, therefore the double action of \mathcal{T} on a state $|\psi\rangle$ leave the latter unchanged except for a factor phase :

$$\begin{aligned} \mathcal{T}^2|\psi\rangle &= e^{i\phi}|\psi\rangle = \hat{U}\hat{K}\hat{U}\hat{K}|\psi\rangle = \hat{U}\hat{U}^*|\psi\rangle \\ &\Rightarrow e^{i\phi} = \hat{U}\hat{U}^*, \end{aligned} \quad (2.30)$$

$$\begin{aligned} e^{i\phi} &= \hat{U}\hat{U}^* \xrightarrow{\text{Transpose}} e^{i\phi} = \hat{U}^\dagger \hat{U}^T \\ &\Rightarrow \hat{U}e^{i\phi} = \hat{U}\hat{U}^\dagger \hat{U}^T = \hat{U}^T, \end{aligned} \quad (2.31)$$

$$\hat{U}^T = \hat{U}e^{i\phi} \xrightarrow{\text{Transpose}} \hat{U} = \hat{U}^T e^{i\phi} = \left(\hat{U}e^{i\phi}\right) e^{i\phi} = \hat{U}e^{2i\phi}, \quad (2.32)$$

$$e^{2i\phi} = 1 \Rightarrow e^{i\phi} = \pm 1, \quad (2.33)$$

which means

$$\mathcal{T}^2|\psi\rangle = \pm 1|\psi\rangle \Rightarrow \mathcal{T}^2 = \pm 1. \quad (2.34)$$

Note that, $\mathcal{T}^2 = \pm 1$ depending on the spin of the particles, namely

- $\mathcal{T}^2 = +1$ is the case of the reversal symmetry of even time, which corresponds to the integer spin (bosonic case)
- $\mathcal{T}^2 = -1$ is the case of the odd-time reversal symmetry, which corresponds to the half-integer spin (fermionic case).

2.2.3 \mathcal{PT} -Operator

The operator \mathcal{PT} is the composition of the two previous transformations. By combining the previous properties, we can conclude that the operator \mathcal{PT} acts on the operators of the position \mathbf{x} , the momentum \mathbf{p} and on the complex number i as follows [3, 16]

$$(\mathcal{PT}) \hat{\mathbf{x}} (\mathcal{PT}) = -\hat{\mathbf{x}}, \quad (\mathcal{PT}) \hat{\mathbf{p}} (\mathcal{PT}) = \hat{\mathbf{p}}, \quad (\mathcal{PT}) i (\mathcal{PT}) = -i. \quad (2.35)$$

The action of the operator (\mathcal{PT}) and (\mathcal{TP}) on a state $|\psi\rangle$ is written as

$$\mathcal{PT}|\psi\rangle = \lambda U|\psi\rangle^*, \quad \mathcal{TP}|\psi\rangle = U\lambda|\psi\rangle^* = \mathcal{PT}|\psi\rangle, \quad (2.36)$$

and this implies that the operators \mathcal{P} and \mathcal{T} commute, i.e

$$[\mathcal{P}, \mathcal{T}] = 0. \quad (2.37)$$

The \mathcal{PT} operator is an anti-linear operator

$$\begin{aligned} (\mathcal{PT}) (a_1|\psi_1\rangle + a_2|\psi_2\rangle) &= \mathcal{P} (\mathcal{T} (a_1|\psi_1\rangle + a_2|\psi_2\rangle)) \\ &= \mathcal{P} (a_1^*\mathcal{T}|\psi_1\rangle + a_2^*\mathcal{T}|\psi_2\rangle) \\ &= a_1^* (\mathcal{PT}) |\psi_1\rangle + a_2^* (\mathcal{PT}) |\psi_2\rangle. \end{aligned} \quad (2.38)$$

As the operator \mathcal{P} is a unit operator and the operator \mathcal{T} is an anti-unit operator, then the product \mathcal{PT} is an anti-unit operator.

$$\langle \mathcal{PT}\phi | \mathcal{PT}\psi \rangle = \langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle. \quad (2.39)$$

2.3 \mathcal{PT} -Symmetric Hamiltonians

The \mathcal{PT} -symmetric quantum theory introduced by Carl Bender and Stefan Boettcher in 1998, they has offered us a large class of non-Hermitian Hamiltonians which have real spectra [3]. These Hamiltonians are invariant under the transformation of the symmetry \mathcal{PT} .

Definition

A Hamiltonian \hat{H} is said to be \mathcal{PT} symmetric if it satisfies [2, 3, 5, 10]

$$\hat{H} = \hat{H}^{\mathcal{PT}} = \mathcal{PT} \hat{H} \mathcal{PT}. \quad (2.40)$$

Thus, if a Hamiltonian \hat{H} is \mathcal{PT} -symmetric, then it must commute with the discrete product \mathcal{PT} , *i.e.*

$$\left[\hat{H}, \mathcal{PT} \right] = 0. \quad (2.41)$$

In the general case, \hat{H} can be written in the form

$$\hat{H} = \hat{P}^2 + V(\hat{x}), \quad (2.42)$$

where the potential $V(x)$ can be complex.

Therefore, the action of the operator \mathcal{PT} on $V(x)$ is

$$(\mathcal{PT}) V(x) (\mathcal{PT}) = V^*(-x). \quad (2.43)$$

Therefore

$$V(-x) = (\mathcal{PT}) V(-x) (\mathcal{PT}) = V^*(x). \quad (2.44)$$

where x is real.

In the case where $V(x)$ is a real potential, *i.e.* the Hamiltonian \hat{H} is Hermitian, then the condition of \mathcal{PT} -symmetry is equivalent to

$$V(-x) = V(x). \quad (2.45)$$

Which mean that $V(x)$ is an even function.

2.3.1 Broken and unbroken \mathcal{PT} -symmetry

In quantum mechanics, if a linear operator \hat{A} commutes with the Hamiltonian \hat{H} , then the eigenstates of \hat{H} are also eigenstates of \hat{A} [2].

For the case of a \mathcal{PT} -symmetric Hamiltonian, the \mathcal{PT} operator commutes with the Hamiltonian \hat{H} . However, because \mathcal{PT} is not linear \mathcal{PT} -symmetry is more subtle than parity symmetry and the eigenstates of \hat{H} may or may not be eigenstates of \mathcal{PT} [5].

- The first case

We assume that an eigenstate ψ of the Hamiltonian \hat{H} is also an eigenstate of the \mathcal{PT} operator with eigenvalues E and λ .

$$\begin{cases} \hat{H}\psi = E\psi, \\ \text{and} \\ \mathcal{PT}\psi = \lambda\psi, \end{cases} \quad (2.46)$$

multiply the two equations by \mathcal{PT} and use the property that $\mathcal{PT}^2 = \mathbb{1}$, so :

$$\begin{cases} (\mathcal{PT}) \hat{H}\psi = (\mathcal{PT}) E (\mathcal{PT})^2 \psi = (\mathcal{PT}) E (\mathcal{PT}) \lambda\psi, \\ \psi = (\mathcal{PT}) \lambda (\mathcal{PT})^2 \psi = \lambda^* \lambda\psi, \end{cases} \quad (2.47)$$

recalling that \mathcal{PT} commutes with \hat{H} , we get

$$(\mathcal{PT}) \hat{H} \psi = \hat{H} (\mathcal{PT}) \psi = \hat{H} \lambda \psi = (\mathcal{PT}) E (\mathcal{PT}) \lambda \psi, \quad (2.48)$$

finally

$$E \lambda \psi = E^* \lambda \psi. \quad (2.49)$$

Since λ is nonzero, we conclude that the eigenvalue E is real

$$E = E^*. \quad (2.50)$$

- The second case

There are eigenstates of the \mathcal{PT} -symmetric Hamiltonian which are not eigenstates of the \mathcal{PT} operator:

$$\begin{cases} \hat{H} \psi = E \psi, \\ \text{and} \\ \mathcal{PT} \psi \neq \lambda \psi, \end{cases} \quad (2.51)$$

multiply the first equation by \mathcal{PT}

$$(\mathcal{PT}) \hat{H} \psi = (\mathcal{PT}) E \psi, \quad (2.52)$$

we use the property that \mathcal{PT} commutes with \hat{H} and since the \mathcal{PT} operator is anti-linear

$$\hat{H} (\mathcal{PT} \psi) = E^* (\mathcal{PT} \psi). \quad (2.53)$$

which implies that $(\mathcal{PT} \psi)$ is also an eigenfunction of the Hamiltonian \hat{H} with the eigenvalue E^* .

So the spectrum of any \mathcal{PT} -symmetric Hamiltonian consists of pairs of energy complexes conjugated to each other (E, E^*) .

The reality of spectrum

If the \mathcal{PT} -symmetric Hamiltonian has eigenfunctions invariant under the operation of \mathcal{PT} , then the corresponding eigenvalue spectrum is real, we say here that the \mathcal{PT} -symmetry of \hat{H} is unbroken. Conversely, if some of the eigenfunctions of a \mathcal{PT} -symmetric Hamiltonian are not simultaneously eigenfunctions of the \mathcal{PT} operator, the invariance of a non-Hermitian operator \hat{H} under the action of the operator \mathcal{PT} gives a spectrum which consists of pairs of complex energies conjugated to each other, we say here that the \mathcal{PT} symmetry of \hat{H} is broken [5].

Remarks

- In the case where the energy spectrum of a \mathcal{PT} -symmetric Hamiltonian consists of a real part and conjugated complex pairs, the \mathcal{PT} -symmetry is partially broken. On the other hand, if the whole energy spectrum is complex, then the \mathcal{PT} -symmetry is totally broken [16].
- For the Hamiltonian which is studied by Bender and Boettcher (2.1), the \mathcal{PT} -symmetry of H is unbroken for $N \geq 2$, and broken for $N < 2$ [16].

We summarize the role played by \mathcal{PT} -symmetry in figure 2:

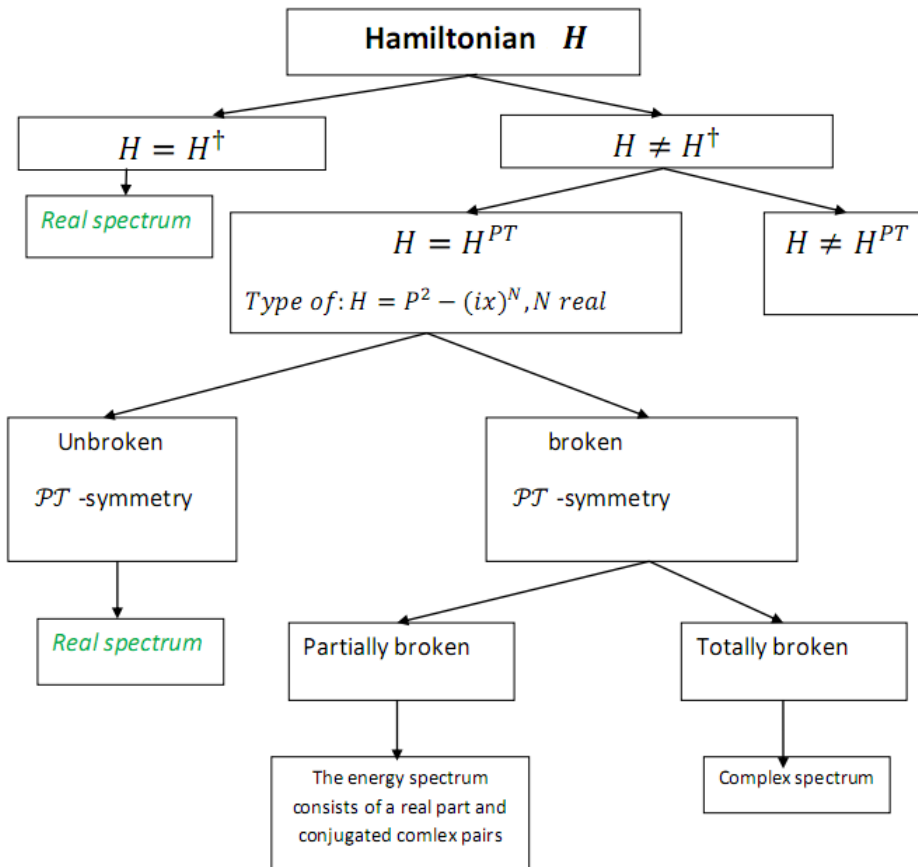


Figure 2.2: \mathcal{PT} -symmetry and real spectrum

2.3.2 \mathcal{PT} -symmetric-inner product

In conventional quantum mechanics, the norm of a vector in Hilbert space must be positive. In addition, the inner product of any two vectors in Hilbert space must be constant over the course of the evolution of time as is the probability (unitarity). These two requirements constitute a fundamental property for quantum theory to be valid. Since the standard Hermitian-inner product ($\hat{H} = \hat{H}^\dagger$) is given by [5, 10]

$$\langle \psi, \phi \rangle = \int dx [\psi(x)]^* \phi(x). \quad (2.54)$$

Bandar is the first who introduced an inner product called " \mathcal{PT} -inner product" associated with \mathcal{PT} -symmetric Hamiltonians, defined by [6, 5]

$$\langle \psi, \phi \rangle_{\mathcal{PT}} = \int_c dx [\psi(x)]^{\mathcal{PT}} \phi(x) = \int_c dx [\psi(-x)]^* \phi(x), \quad (2.55)$$

c is a contour in the complex plane.

The \mathcal{PT} -inner product for the two eigenfunctions $\phi_n(x)$ and $\phi_m(x)$ yields:

$$\begin{aligned} \langle \phi_m, \phi_n \rangle_{\mathcal{PT}} &= \int_c dx [\phi_m(x)]^{\mathcal{PT}} \phi_n(x) \\ &= \int_c dx [\phi_m(-x)]^* \phi_n(x) \\ &= (-1)^n \delta_{mn}. \end{aligned} \quad (2.56)$$

However, when $m = n$, we see that the \mathcal{PT} -norms of the eigenfunctions are not always positive:

$$\langle \phi_n, \phi_n \rangle_{\mathcal{PT}} = \int_c dx [\phi_n(-x)]^* \phi_n(x) = (-1)^n, \quad (2.57)$$

and the completeness relation is written as a function of these eigenfunctions as

$$\sum_n (-1)^n |\phi_n\rangle \langle \phi_n|. \quad (2.58)$$

The norm $(-1)^n$ of a state is not necessarily positive, i.e. the relation defining the \mathcal{PT} -inner product is insufficient to formulate a valid quantum theory, because the \mathcal{PT} -norm of a state is not definite positive.

So it is necessary to build a new inner product where the norm is positive. This prompted Bender to construct a new inner product with a positive norm. It's called the \mathcal{CPT} -inner product.

2.4 The operator \mathcal{C} and the inner-product \mathcal{CPT}

To solve this negative norm problem, and construct an inner product with a positive norm for a complex non-Hermitian Hamiltonian having an *unbroken* \mathcal{PT} -symmetry, Bender introduced another symmetry generated by a new linear operator denoted \mathcal{C} [5], which helps to reconstruct a new inner product which solves the probability violation in the case of \mathcal{PT} -inner product.

2.4.1 \mathcal{C} operator

The use of the symbol \mathcal{C} to represent this new symmetry and the properties of \mathcal{C} are similar to those of the charge conjugation operator in particle physics [6]. \mathcal{C} Operator is an observable, linear, complex and it is represented in coordinate space by a sum of products of the eigenfunctions of the Hamiltonian considered as follows [6]

$$\mathcal{C}(x, y) = \sum_{n=0}^{\infty} \phi_n(x) \phi_n(y), \quad (2.59)$$

where \mathcal{C} commutes with the Hamiltonian \hat{H} and the operator \mathcal{PT} , i.e.

$$[\mathcal{C}, \hat{H}] = [\mathcal{C}, \mathcal{PT}] = 0, \quad (2.60)$$

therefore

$$\mathcal{C}^2 = \mathbb{1}. \quad (2.61)$$

thus the eigenvalues of \mathcal{C} are ± 1 .

The action of \mathcal{C} on the eigenfunctions of \hat{H} is given by

$$\mathcal{C}\phi_n(x) = (-1)^n \phi_n(x). \quad (2.62)$$

The parity operator \mathcal{P} can be constructed in terms of the eigenfunctions of \hat{H} , the linear operator \mathcal{P} is represented in coordinate space by

$$\mathcal{P}(x, y) = \delta(x + y) = \sum_{n \geq 0} (-1)^n \phi_n(x) \phi_n(y). \quad (2.63)$$

As the operator \mathcal{C} , the square of the parity operator is also unity, $\mathcal{P}^2 = 1$ and $\mathcal{C}^2 = 1$, but \mathcal{P} and \mathcal{C} are not identical. Indeed, the parity operator \mathcal{P} is real, while \mathcal{C} is complex ($\mathcal{P} \neq \mathcal{C}$), furthermore, these two operators do not commute [6]; specifically, in the position representation

$$(\mathcal{CP})(x, y) = \sum_n \phi_n(x) \phi_n(-y), \quad (2.64)$$

whereas

$$(\mathcal{PC})(x, y) = \sum_n \phi_n(-x) \phi_n(y), \quad (2.65)$$

which shows that

$$(\mathcal{CP}) = (\mathcal{PC})^*. \quad (2.66)$$

Hence \mathcal{C} commutes with the operator \mathcal{PT} , which means that the linear operator \mathcal{CPT} solves the problem of negative norm.

2.4.2 \mathcal{CPT} -inner product

Finally, by having obtained the operator \mathcal{C} , we can define a new inner product structure having positive definite norm [6]

$$\langle \psi, \phi \rangle_{\mathcal{CPT}} = \int_c dx [\psi(x)]^{\mathcal{CPT}} \phi(x) = \int_c dx [\mathcal{CPT}\psi(x)] \phi(x), \quad (2.67)$$

where

$$\mathcal{CPT}\psi(x) = \int_c dy [\mathcal{CPT}\psi(x, y)] \phi^*(-y). \quad (2.68)$$

The \mathcal{CPT} -inner product for the two eigenfunctions $\phi_n(x)$ and $\phi_m(x)$ is

$$\langle \phi_m, \phi_n \rangle_{\mathcal{CPT}} = \int_c dx [\mathcal{CPT}\phi_m(x)] \phi_n(x) = \delta_{mn}. \quad (2.69)$$

And this \mathcal{CPT} -inner product is definite positive.

2.5 Conclusion

We have seen that there exists a class of non-Hermitian Hamiltonians whose eigenvalues are real [3]. These Hamiltonians are invariant under \mathcal{PT} -symmetry, if only if the latter is unbroken. Indeed, the \mathcal{PT} -symmetric Hamiltonians are invariant under the action of the operator \mathcal{C} which is solved the problem of the negativity of the norm of the \mathcal{PT} -inner product.

However in general, there are Hermitian Hamiltonians with a real spectrum that are not \mathcal{PT} -symmetric and there are \mathcal{PT} -symmetric Hamiltonians that do not have a real spectrum. Therefore, \mathcal{PT} -symmetry is neither a necessary nor a sufficient condition for a Hamiltonian to have a real spectrum [7]. We will see in the next chapter a more general theory than \mathcal{PT} -symmetry, which is the notion of pseudo-Hermiticity.

Chapter 3

Pseudo-Hermitian Hamiltonians

3.1 Introduction

The notion of pseudo-Hermiticity was born in the forties thanks to Dirac and Pauli, then it was targeted in value by Lee and Sudarshan [10], in quantification in electrodynamics and lots of quantum theories of field.

In 2002, Mostafazadeh revolutionized the concept of pseudo-Hermiticity and he published three first articles, in which he presented an alternative theory to conventional quantum mechanics and the \mathcal{PT} -symmetric quantum theory, for non-Hermitian Hamiltonians whose spectrum is real. This theory is called pseudo-Hermitian quantum theory. He showed that every real-spectrum Hamiltonian is pseudo-Hermitian [10].

In this chapter we will introduce the main definitions and properties of the pseudo-Hermitian Hamiltonians.

3.2 Pseudo-Hermiticity

Let $\hat{H} : \mathcal{H} \rightarrow \mathcal{H}$ be a linear operator acting in a Hilbert space \mathcal{H} and $\eta : \mathcal{H} \rightarrow \mathcal{H}$ be a linear Hermitian automorphism (invertible transformation). Then, the η -pseudo-Hermitian adjoint of \hat{H} is defined by

$$\hat{H}^\# := \eta^{-1} \hat{H}^\dagger \eta. \quad (3.1)$$

\hat{H} is said to be pseudo-Hermitian with respect to η or simply η -pseudo-Hermitian if $\hat{H}^\# = \hat{H}$.

\hat{H} is said to be pseudo-Hermitian if it is pseudo-Hermitian with respect to all linear Hermitian automorphism η [7].

3.2.1 Fundamental theorems of pseudo-Hermiticity

Let \hat{H} be a non-Hermitian Hamiltonian having a discrete spectrum and admitting a complete bi-orthonormal basis. \hat{H} is Pseudo-Hermitian if and only if one of the following conditions is verified [17].

- The eigenvalues of \hat{H} are real.
- The eigenvalues of \hat{H} consist of pairs of complex.

To understand these two conditions, we will explain in the following subsection.

3.2.2 Spectral properties of pseudo-Hermitian Hamiltonians

Let \hat{H} be a pseudo-Hermitian Hamiltonian with discrete spectrum. According to the last theorems, the eigenvalues of \hat{H} are real or consist of pairs of complex eigenvalues conjugated to each other with the same multiplicity. From the equations $\hat{H}^\dagger = \eta \hat{H} \eta^{-1}$, we have

$$\hat{H} (\eta^{-1} |\phi_{n,a}\rangle) = \eta^{-1} \hat{H}^\dagger |\phi_{n,a}\rangle = E_n^* (\eta^{-1} |\phi_{n,a}\rangle). \quad (3.2)$$

The operator η^{-1} is invertible, $\eta^{-1} |\phi_{n,a}\rangle$ is an eigenvector of \hat{H} with eigenvalue E_n^* , so E_n and E_n^* have the same multiplicity. We can represent the Hamiltonian \hat{H} spectrally as follows [10].

$$\begin{aligned} \hat{H} = & \sum_{n_0} \sum_{a=1}^{d_{n_0}} E_{n_0} |\psi_{n_0,a}\rangle \langle \phi_{n_0,a}| \\ & + \sum_{n_+, n_-} \sum_{\alpha=1}^{d_{n_+}} (E_{n_+} |\psi_{n_+, \alpha}\rangle \langle \phi_{n_+, \alpha}| + E_{n_+}^* |\psi_{n_-, \alpha}\rangle \langle \phi_{n_-, \alpha}|). \end{aligned} \quad (3.3)$$

Note that, we use the notation n_0 for real eigenvalues and the corresponding eigenstates and the notation n_\pm for complex eigenvalues with an imaginary part \pm and the associated eigenstates.

In this case, the eigenvectors of \hat{H}^\dagger are related to the eigenvectors of \hat{H} by the following relations

$$|\phi_{n_0,a}\rangle = \eta |\psi_{n_0,a}\rangle, \quad |\phi_{n_\pm, \alpha}\rangle = \eta |\psi_{n_\pm, \alpha}\rangle. \quad (3.4)$$

Then, we have the relations of the metric operator η and its inverse η^{-1} as follows

$$\eta = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\phi_{n_0,a}\rangle \langle \phi_{n_0,a}| + \sum_{n_+,n_-} \sum_{\alpha=1}^{d_{n_+}} (|\phi_{n_-, \alpha}\rangle \langle \phi_{n_+, \alpha}| + |\phi_{n_+, \alpha}\rangle \langle \phi_{n_-, \alpha}|) \quad (3.5)$$

$$\eta^{-1} = \sum_{n_0} \sum_{a=1}^{d_{n_0}} |\psi_{n_0,a}\rangle \langle \psi_{n_0,a}| + \sum_{n_+,n_-} \sum_{\alpha=1}^{d_{n_+}} (|\psi_{n_-, \alpha}\rangle \langle \psi_{n_+, \alpha}| + |\psi_{n_+, \alpha}\rangle \langle \psi_{n_-, \alpha}|) \quad (3.6)$$

3.2.3 Pseudo-Hermitian Hamiltonians with a complete biorthonormal eigenbasis

Let \hat{H} be an η -pseudo-Hermitian Hamiltonian with a complete bi-orthonormal eigenbasis $\{|\psi_n, a\rangle, |\phi_n, a\rangle\}$ and a discrete spectrum. Then, by definition

$$\hat{H} |\psi_n, a\rangle = E_n |\psi_n, a\rangle, \quad \hat{H}^\dagger |\phi_n, a\rangle = E_n^* |\phi_n, a\rangle \quad (3.7)$$

$$\langle \phi_m, b | \psi_n, a \rangle = \delta_{mn} \delta_{ab} \quad (3.8)$$

$$\sum_n \sum_{a=1}^{d_n} |\phi_n, a\rangle \langle \psi_n, a| = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle \langle \phi_n, a| = \mathbb{1} \quad (3.9)$$

where d_n is the multiplicity (degree of degeneracy) of the eigenvalue E_n , and a and b are degeneracy labels [7].

3.3 Mapping from pseudo-Hermitian Hamiltonian to Hermitian Hamiltonian

The notion of pseudo-Hermiticity is based on the Hermiticity of the Hamiltonian equivalent of the pseudo-Hermitian Hamiltonian of the physical system under study, because every pseudo-Hermitian Hamiltonian with associated positive metric operation has an equivalent Hermitian Hamiltonian and both of them have the same energy spectrum, *i.e.* they are iso-spectrale. So we can derive an equivalent pseudo-Hermitian Hamiltonian \hat{H} from a Hermitian Hamiltonian \hat{h} by the relation

$$\hat{h} = \rho \hat{H} \rho^{-1}. \quad (3.10)$$

where ρ is a linear invertible and Hermitian operator.

The Hermitian Hamiltonian \hat{h} is diagonalizable (symmetric) and preserve the inner product.

$$\langle \varphi_n | \varphi_m \rangle = \delta_{nm}, \quad (3.11)$$

and the eigenvectors of \hat{h} satisfy the following relation

$$\langle \varphi_n | h\varphi_m \rangle = \varepsilon_m \langle \varphi_n | \varphi_m \rangle, \quad (3.12)$$

$$\langle \hat{h}\varphi_n | \varphi_m \rangle = \varepsilon_n \langle \varphi_n | \varphi_m \rangle. \quad (3.13)$$

The new inner product of the pseudo-Hermitian Hamiltonian is defined by

$$\langle \phi_n | \phi_m \rangle_\eta = \langle \phi_n | \eta\phi_m \rangle, \quad (3.14)$$

When $\rho^2 = \eta$, we get the relation $\phi = \rho^{-1}\varphi$ if ϕ and φ are the eigenvectors of \hat{H} and \hat{h} respectively. Then

$$\begin{aligned} \langle \phi_n | \phi_m \rangle_\eta &= \langle \phi_n | \eta\phi_m \rangle = \langle \rho^{-1}\varphi_n | \rho\varphi_m \rangle \\ &= \langle \varphi_n | \varphi_m \rangle. \end{aligned} \quad (3.15)$$

As \hat{h} is Hermitian, so

$$\hat{h} = \rho\hat{H}\rho^{-1} = \hat{h}^\dagger = \rho^{-1}\hat{H}^\dagger\rho, \quad (3.16)$$

it is given that $\rho\hat{H}\rho^{-1} = \rho^{-1}\hat{H}^\dagger\rho$. Therefore

$$\hat{H}^\dagger = \rho^2\hat{H}(\rho^{-1})^2 = \eta\hat{H}\eta^{-1}. \quad (3.17)$$

This relation is nothing than but the pseudo-Hermitian relation that we mentioned in (3,1) [20].

3.4 Pseudo-metric operator

A pseudo-Hermitian quantum system is defined by a (Quasi-Hermitian) Hamiltonian operator and an associated metric operator η . This makes the construction of η the central problem in pseudo-Hermitian quantum mechanics. And that is why there are various methods of calculating a metric operator [12].

In this section, we talk about the definition of the metric operator and one of its method of calculation.

3.4.1 Metric operator

There is a metric operator η who can makes \hat{H} to a pseudo-Hermitian Hamiltonian. This metric operator has the following properties :

- Defined positive if all its eigenvalues are positive. If the last one is not, realized the metric operator will be undefined positive.
- Hermitian $\eta^\dagger = \eta$.
- Invertible.
- Linear.
- Not unique.

3.4.2 Different methods to calculate the metric operator

There are different methods to find the final result, we can find :

- Perturbation theory.
- Spectral method.
- Differential representation of pseudo-Hermiticity.
- Lie algebraic method.

We select one method to use it in the next section which is the perturbation method [11].

3.4.3 Perturbation method

Consider a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \epsilon \hat{H}_1, \quad (3.18)$$

where ϵ is a real perturbation parameter and \hat{H}_0 and \hat{H}_1 are respectively Hermitian and anti-Hermitian. ϵ independent operator, Suppose that for sufficiently small values of ϵ , the Hamiltonian \hat{H} has a real spectrum and a complete set of eigenvectors, so that a positive definite metric operator η_+ exists such an operator has a well defined Hermitian logarithm we shall let $Q = -\ln \eta_+$, or alternatively

$$\eta_+ = e^{-Q}. \quad (3.19)$$

And employ the pseudo-Hermiticity relation $\hat{H}^\dagger = \eta \hat{H} \eta^{-1}$, to obtain a perturbative expansion for Q in the form:

$$Q = \sum_{i=0}^{\infty} Q_i \epsilon^i. \quad (3.20)$$

where Q_i is ϵ -independent Hermitian operator that we can calculate it by using the Baker-Campbell-Hausdorff formula, i.e.

$$e^{-Q} H e^Q = H + \sum_{n=1}^{\infty} \frac{1}{n!} [H, Q]^n = H + [H, Q] + \frac{1}{2!} [[H, Q], Q] + \frac{1}{3!} [[H, Q], [H, Q], Q] + \dots \quad (3.21)$$

and n : is the number of copies of Q .

Then we have for more explicitly the result of each commutator

$$[H_0, Q_1] = -2H_1. \quad (3.22)$$

$$[H_0, Q_2] = 0. \quad (3.23)$$

$$[H_0, Q_3] = \frac{1}{6} [[H_1, Q_1], Q_1]. \quad (3.24)$$

$$[H_0, Q_4] = \frac{-1}{6} ([[H_1, Q_1], Q_2] + [[H_1, Q_2], Q_1]). \quad (3.25)$$

Remarks :

- Note that if the operator η is equal to the identity operator $\mathbb{1}$ than $\hat{H}^\dagger = \hat{H}$. The pseudo-Hermiticity reduce to Hermiticity.
- If the operator η is equal to the parity operator \mathcal{P} then the condition $\hat{H}^\dagger = \eta \hat{H} \eta^{-1}$ reduces to $\hat{H}^\dagger = \mathcal{P} \hat{H} \mathcal{P}^{-1}$ on the pseudo-Hermiticity reduce to the \mathcal{PT} symmetry that we have discussed about it in the first chapter.
- In the case of a positive deduced metric, there exists an operator ρ such that $\eta = \rho^2$, where ρ is a Hermitian linear operator and invertible.

Then \hat{H} admits a corresponding Hermitian Hamiltonian \hat{h} which satisfies the similarity relation $\hat{h} = \rho \hat{H} \rho^{-1}$. In this case, we say that \hat{H} is said to be a quasi-Hermitian that we will discuss now.

3.5 Quasi-Hermitian Hamiltonian

Schooltz were probably the first physicist who discovered that whenever the standard quantization happen to produce a probability complicated version of a realistic Hamiltonian operator $\hat{H} = \hat{H}^\dagger$ in usual Hilbert space it still possible. To try to simplify the equation by make a mapping into another space and we can go to the quasi-Hermitian Hamiltonian by written in the right notation with

$$\rho = \eta^{\frac{1}{2}}. \quad (3.26)$$

3.5.1 Definition of quasi-Hermitian Hamiltonian

\hat{H} it is a linear operator $\hat{H} : \mathcal{H} \rightarrow \mathcal{H}$ is said to be quasi-Hermitian if there exist an invertible bounded self-adjoint positive operator $\eta^{\frac{1}{2}} : \mathcal{H} \rightarrow \mathcal{H}$ satisfying [19]

$$\hat{H}^\dagger = \eta^{\frac{1}{2}} \hat{H} \eta^{-\frac{1}{2}}. \quad (3.27)$$

3.5.2 Fundamental theorem of quasi-Hermitian

Let \hat{H} be non-Hermitian Hamiltonian having a discrete spectrum and admitting a basis complete bi-orthonormal \hat{H} is quasi-Hermitian if and only if one of the condition following is verified [17].

- \hat{H} is pseudo-Hermitian with a metric operator of the form $\eta = \rho^2$, where ρ is a linear invertible and Hermitian operator.
- \hat{H} admit a real spectrum.
- \hat{H} admit a corresponding Hermitian Hamiltonian \hat{h} via the similarity relation $\hat{h} = \rho \hat{H} \rho^{-1}$ and $\hat{h}^\dagger = \eta^{\frac{1}{2}} \hat{H} \eta^{-\frac{1}{2}}$, such that \hat{H} and \hat{h} are isospectral.

3.6 Conclusion

After knowing the pseudo-Hermitian and mentioning some of its properties, we see that the relation between it and the concept of \mathcal{PT} -symmetry is that any \mathcal{PT} -symmetric Hamiltonian implies the pre-presence of the pseudo-Hermiticity, because the \mathcal{PT} -symmetry is an anti-linear symmetry knowing that the \mathcal{PT} -symmetry is a physical condition contrary to the pseudo-Hermitian which is a mathematical condition. The metric operator allows us to treat in a simple way the quasi-Hermiticity, which is the result of the mapping of the pseudo-Hermiticity.

Chapter 4

Applications

4.1 Introduction

As we said in the previous chapter, Mostafazadeh observed that the square root of the positive operator $\rho = \eta^{1/2}$ can be used to construct a similarity transformation $\hat{h} = \rho \hat{H} \rho^{-1} = \eta^{1/2} \hat{H} \eta^{-1/2}$ that maps a non-Hermitian Hamiltonian \hat{H} to an equivalent Hermitian Hamiltonian \hat{h} , and both have the same spectral energy [5, 10, 11].

The classical Hamiltonian is obtained by expressing \hat{h} in terms of \hat{x} and \hat{p} and replacing the latter with the classical position \hat{x}_c and momentum \hat{p}_c observables. The classical Hamiltonian \hat{H}_c is then obtained by evaluating this expression in the limit $\hbar \rightarrow 0$, i.e., assuming that this limit exists [13],

$$\hat{H}_c(\hat{x}_c, \hat{p}_c) := \lim_{\hbar=0} \hat{h}(\hat{x}_c, \hat{p}_c) \quad (4.1)$$

The aim of this chapter is to calculate the operator η of each of the following two Hamiltonians to determine the new Hermitian Hamiltonian \hat{h} and The classical Hamiltonian \hat{H}_c , then to calculate its energy which is the same energy of \hat{H} by using the Maple-soft application

- The shifted harmonic oscillator

$$\hat{H} = \hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}. \quad (4.2)$$

- The cubic anharmonic oscillator

$$\hat{H} = \hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3. \quad (4.3)$$

4.2 The shifted harmonic oscillator

We have the following Hamiltonian

$$\hat{H} = \hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}. \quad (4.4)$$

According to the perturbation method we assume that

$$\eta = e^{-Q}, \quad Q = \sum_{j=1}^{\infty} \epsilon^j Q_j. \quad (4.5)$$

$$\hat{H}^\dagger = e^{-Q} H e^Q = H + [H, Q] + \frac{1}{2} [[H, Q], Q] + \dots. \quad (4.6)$$

$$\hat{p}^2 + \hat{x}^2 - i\epsilon\hat{x} = p^2 + \hat{x}^2 + i\epsilon\hat{x} + [\hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}, Q] + \dots. \quad (4.7)$$

$$-2i\epsilon\hat{x} = [\hat{p}^2, Q] + [\hat{x}^2, Q] + i\epsilon[\hat{x}, Q] + \dots. \quad (4.8)$$

$$\begin{aligned} -2i\epsilon\hat{x} &= [\hat{p}^2, \epsilon Q_1 + \epsilon^2 Q_2 + \dots] + [\hat{x}^2, \epsilon Q_1 + \epsilon^2 Q_2 + \dots] \\ &\quad + i\epsilon[\hat{x}, \epsilon Q_1 + \epsilon^2 Q_2 + \dots] + \dots. \end{aligned} \quad (4.9)$$

We will eliminate the formulas which contain ϵ^j with $j \geq 2$. The previous relations will be:

$$-2i\epsilon\hat{x} = \epsilon[\hat{p}^2, Q_1] + \epsilon[\hat{x}^2, Q_1], \quad (4.10)$$

we pose that $Q_1 = \alpha\hat{x} + \gamma\hat{p}$, then

$$\begin{aligned} -2i\hat{x} &= [\hat{p}^2, \alpha\hat{x} + \gamma\hat{p}] + [\hat{x}^2, \alpha\hat{x} + \gamma\hat{p}], \\ -2i\hat{x} &= \alpha[\hat{p}^2, \hat{x}] + \gamma[\hat{p}^2, \hat{p}] + \alpha[\hat{x}^2, \hat{x}] + \gamma[\hat{x}^2, \hat{p}]. \end{aligned} \quad (4.11)$$

By using the following results

$$[\hat{p}^2, \hat{p}] = [\hat{x}^2, \hat{x}] = 0, \quad (4.12)$$

$$[\hat{p}^2, \hat{x}] = \hat{p}[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}]\hat{p} = -2i\hbar\hat{p}, \quad (4.13)$$

$$[\hat{x}^2, \hat{p}] = \hat{x}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{x} = 2i\hbar\hat{x}, \quad (4.14)$$

then the equation (4.7) will be

$$-2i\hat{x} = -2i\alpha\hbar\hat{p} + 2i\gamma\hbar\hat{x}, \quad (4.15)$$

therefore

$$\begin{cases} \alpha = 0, \\ \text{and} \\ \gamma = -\frac{1}{\hbar}, \end{cases} \quad (4.16)$$

and the operator Q the metric operator η will be

$$\begin{cases} Q = \epsilon Q_1 = -\frac{\epsilon \hat{p}}{\hbar}, \\ \eta = e^{-Q} = e^{\frac{\epsilon \hat{p}}{\hbar}}. \end{cases} \quad (4.17)$$

There exist a Hermitian Hamiltonian \hat{h} which can be mapped from \hat{H} and satisfies similarity relation

$$\hat{h}^\dagger = \hat{h} = \eta^{1/2} \hat{H} \eta^{-1/2}, \quad (4.18)$$

by substituting \hat{H} into the expression of \hat{h} , we get

$$\hat{h} = e^{\frac{\epsilon \hat{p}}{2\hbar}} (\hat{p}^2 + \hat{x}^2 + i\epsilon \hat{x}) e^{-\frac{\epsilon \hat{p}}{2\hbar}}, \quad (4.19)$$

by simplification \hat{h} becomes

$$\hat{h} = \hat{p}^2 + \hat{x}^2 - \epsilon \hbar \hat{p} + \frac{\epsilon^2}{2}. \quad (4.20)$$

Using the Maple-soft application, we find that the corresponding energy spectrum (details are on Appendix A)

$$E_n = 2n + 1 + \frac{\epsilon^2}{2}. \quad (4.21)$$

Having calculated the Hermitian operator \hat{h} we can determine the classical Hamiltonian \hat{H}_c for this system using Eq. (4.1) (details are on Appendix A)

$$\hat{H}_c(\hat{x}_c, \hat{p}_c) := \lim_{\hbar=0} \hat{h}(\hat{x}_c, \hat{p}_c) = \hat{p}^2 + \hat{x}^2 + \frac{\epsilon^2}{2}. \quad (4.22)$$

4.3 The cubic anharmonic oscillator

We have the following cubic Hamiltonian

$$\hat{H} = \hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3. \quad (4.23)$$

From the perturbation method and using the formula of Baker-Campbell-Hausdorff, we assume that

$$\hat{H}^\dagger = e^{-Q} H e^Q = H + [H, Q] + \frac{1}{2} [[H, Q], Q] + \dots, \quad (4.24)$$

$$\begin{aligned} \hat{p}^2 + \hat{x}^2 - i\epsilon\hat{x}^3 &= \hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3 + [\hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3, Q] \\ &+ \frac{1}{2} [[\hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3, Q], Q] \dots \end{aligned} \quad (4.25)$$

We replace Q by its expression, $Q = \epsilon Q_1 + \epsilon^2 Q_2 + \epsilon^3 Q_3 \dots$, the previous equation will be

$$\begin{aligned} -2i\epsilon\hat{x}^3 &= [\hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3, \epsilon Q_1 + \epsilon^2 Q_2 + \epsilon^3 Q_3 \dots] \\ &+ \frac{1}{2} [[\hat{p}^2 + \hat{x}^2 + i\epsilon\hat{x}^3, \epsilon Q_1 + \epsilon^2 Q_2 + \epsilon^3 Q_3 \dots], \epsilon Q_1 + \epsilon^2 Q_2 + \epsilon^3 Q_3 \dots] \dots \end{aligned} \quad (4.26)$$

We will calculate the operator Q_j for $j = 1, 2, 3$, from the following relations

$$\begin{cases} Q_{2i} = 0, \\ Q_{2i+1} = \sum_{j,k=0}^{i+1} c_{ijk} \{\hat{x}^{2j}, \hat{p}^{2k+1}\}, \end{cases} \quad (4.27)$$

and

$$\begin{cases} [H_0, Q_1] = -2H_1, \\ [H_0, Q_2] = 0, \\ [H_0, Q_3] = -\frac{1}{6} [[H_1, Q_1], Q_1]. \end{cases} \quad (4.28)$$

Using the Maple-soft application (details are on Appendix B), we find that

$$\begin{cases} Q_1 = -\frac{2\hat{p}^3}{3\hbar} - \frac{\{\hat{x}^2, \hat{p}\}}{2\hbar}, \\ Q_2 = 0, \\ Q_3 = \hbar\hat{p} + \frac{16}{15\hbar}\hat{p}^5 + \frac{5}{6\hbar}\{\hat{x}^2, \hat{p}^3\} + \frac{1}{2\hbar}\{\hat{x}^4, \hat{p}\}, \end{cases} \quad (4.29)$$

and the operator $Q(\hat{x}, \hat{p})$ will be

$$Q(\hat{x}, \hat{p}) = \epsilon \left(-\frac{2\hat{p}^3}{3\hbar} - \frac{\{\hat{x}^2, \hat{p}\}}{2\hbar} \right) + \epsilon^2 \left(\hbar\hat{p} + \frac{16}{15\hbar}\hat{p}^5 + \frac{5}{6\hbar}\{\hat{x}^2, \hat{p}^3\} + \frac{1}{2\hbar}\{\hat{x}^4, \hat{p}\} \right). \quad (4.30)$$

Substituting $Q(\hat{x}, \hat{p})$ in $\eta = e^{-Q(\hat{x}, \hat{p})}$ we get

$$\eta = \exp \left[\epsilon \left(\frac{2\hat{p}^3}{3\hbar} + \frac{\{\hat{x}^2, \hat{p}\}}{2\hbar} \right) - \epsilon^2 \left(\hbar\hat{p} + \frac{16}{15\hbar}\hat{p}^5 + \frac{5}{6\hbar}\{\hat{x}^2, \hat{p}^3\} + \frac{1}{2\hbar}\{\hat{x}^4, \hat{p}\} \right) \right], \quad (4.31)$$

such that

$$\begin{cases} \{\hat{x}^2, \hat{p}\} = 2\hat{x}\hat{p}\hat{x}, \\ \{\hat{x}^2, \hat{p}^3\} = 2\hat{x}\hat{p}^3\hat{x} - 6\hat{p}, \\ \{\hat{x}^4, \hat{p}\} = 2\hat{x}^2\hat{p}\hat{x}^2. \end{cases} \quad (4.32)$$

The mapped Hermitian Hamiltonian \hat{h} is gotten by similarity relation.

$$\hat{h}^\dagger = \hat{h} = \eta^{1/2} \hat{H} \eta^{-1/2}, \quad (4.33)$$

and by substituting \hat{h} (details are on Appendix B), it becomes

$$\begin{aligned} \hat{h} &= \hat{p}^2 + \hat{x}^2 + (-3\hbar\hat{x}^2\hat{p} + 3i\hbar^2\hat{x}) \epsilon \\ &+ \left(-2\hbar^2 - 6i\hbar\hat{x}\hat{p} + 3\hat{x}^2\hat{p}^2 - 9\hbar^2\hat{p}^2 + \frac{3\hat{x}^4}{2} - 6i\hbar\hat{x}\hat{p}^3 \right) \epsilon^2 + o(\epsilon^3) \end{aligned} \quad (4.34)$$

Using the Maple-soft application, we find that the corresponding energy spectrum (details are on Appendix B)

$$E_n = 2n + 1 + \left(\frac{30n^2 + (-72\hbar^2 + 72\hbar + 30)n - 52\hbar + 60\hbar + 3}{8} \right) \epsilon^2. \quad (4.35)$$

If $\hbar = 1$ we find

$$E_n = 2n + 1 + \left(\frac{11}{8} + \frac{15}{4}n + \frac{15}{4}n^2 \right) \epsilon^2. \quad (4.36)$$

Having calculated the Hermitian operator \hat{h} we can determine the classical Hamiltonian \hat{H}_c for this system using Eq. (4.1)

$$\hat{H}_c(\hat{x}_c, \hat{p}_c) := \lim_{\hbar=0} \hat{h}(\hat{x}_c, \hat{p}_c) = \hat{p}_c^2 + \hat{x}_c^2 + \left(3\hat{x}_c^2\hat{p}_c^2 + \frac{3\hat{x}_c^4}{2} \right) \epsilon^2. \quad (4.37)$$

Conclusion

This master thesis is devoted to the study of quantum systems described by non-Hermitian Hamiltonians having real spectra.

We recalled in the first chapter the mathematical tools and the postulates of quantum mechanics and a brief history on the non-Hermitian Hamiltonians.

Then, in the second chapter, we presented the \mathcal{PT} -symmetric quantum mechanics introduced by Carl Bender and Stefan Boettcher in 1998 for non-Hermitian Hamiltonians invariants under the action of the transformation of the \mathcal{PT} -symmetry, if the latter is not broken then these Hamiltonians have real spectra.

In the third chapter, we presented pseudo-Hermitian quantum theory for non-Hermitian Hamiltonians whose spectrum is real and which is a generalization of \mathcal{PT} -symmetric quantum mechanics. This quantum theory introduced by Ali Mostafazadeh in 2002, states that all real spectrum Hamiltonians are pseudo-Hermitians. In particular, all \mathcal{PT} -symmetric Hamiltonians belong to the class of pseudo-Hermitian Hamiltonians.

In the last part, we made an application of the perturbation method to calculate the metric operator for two non-Hermitian Hamiltonian systems "The shifted harmonic oscillator" $\hat{H} = p^2 + \hat{x}^2 + i\epsilon\hat{x}$ and " The cubic anharmonic oscillator " $\hat{H} = p^2 + \hat{x}^2 + i\epsilon\hat{x}^3$. In all these applications, we looked for the Hermitian Hamiltonians equivalent to the Hermitian pseudo-Hamiltonians $\hat{h} = \eta^{1/2}\hat{H}\eta^{-1/2}$ which has the same energy spectrum of \hat{H} , and we have proved that the spectra of these two examples are real.

Appendix A

The shifted harmonic oscillator

<pre>> with(Physics); ['*', '\', Annihilation, AntiCommutator, Bra, Bracket, Check, Commutator, Coordinates, Creation, Dagger, Define, Dgamma, FeynmanDiagrams, Fundiff, Intc, Inverse, Ket, \delta, LeviCivita, Parameters, Projector, Psigma, Setup, Simplify, SpaceTimeVector, Trace, Vectors, '^', dAlembertian, d_, diff, g_]</pre>	(1)
<pre>> Setup(Math = true); * Partial match of 'Math' against keyword 'mathematicalnotation' [mathematicalnotation = true]</pre>	(2)
<pre>> Setup(Hermitian = {x, p}, %Commutator(x, p) = I \hbar); * Partial match of 'Hermitian' against keyword 'hermitianoperators' [algebrarules = { [x, p]_ = I \hbar }, hermitianoperators = { p, x }]</pre>	(3)
<pre>> Setup(redo, algebra = {%Commutator(x, p^m) = I \cdot m \cdot \hbar \cdot p^{m-1}}); * Partial match of 'algebra' against keyword 'algebrarules' [algebrarules = { [x, p^m]_ = I m \hbar p^{m-1} }]</pre>	(4)
<pre>> a := Annihilation(\phi, 1);</pre>	(5)
<pre>> b := Creation(\phi, 1);</pre>	(6)
<pre>> a.Ket(\phi, n);</pre>	(7)
<pre>> Bra(\phi, n).b;</pre>	(8)
<pre>> b.Ket(\phi, n);</pre>	(9)
<pre>> Bra(\phi, n).b^2;</pre>	(10)
<pre>> Commutator(a, b);</pre>	(11)
<pre>> Q(1) := \sum_{j=0}^1 \sum_{k=0}^1 C_{0,j,k} \cdot AntiCommutator(x^{2j}, p^{2k+1}); Q(1) := 2 C_{0,0,0} p + 2 C_{0,0,1} p^3 + C_{0,1,0} [x^2, p]_+ + C_{0,1,1} [x^2, p^3]_+</pre>	(12)
<pre>> Commutator(p^2 + x^2, Q(1)) = -2 I x C_{0,1,0} [p^2, [x^2, p]_+]_+ + C_{0,1,1} [p^2, [x^2, p^3]_+]_+ + 4 I C_{0,0,0} x \hbar + 6 I C_{0,0,1} \hbar (2 I \hbar p + 2 p^2 x) + C_{0,1,0} [x^2, [x^2, p]_+]_+ + C_{0,1,1} [x^2, [x^2, p^3]_+]_+ = -2 I x</pre>	(13)
<pre>> simplify((13)) 4 \hbar (9 C_{0,1,1} \hbar x^2 p + 3 I C_{0,1,1} x^3 p^2 + I C_{0,1,0} x^3 - 4 C_{0,1,1} \hbar p^3 + 3 C_{0,0,1} \hbar p</pre>	(14)

$$\begin{aligned}
& -2IC_{0,1,0}xp^2 + IC_{0,0,0}x - 2IC_{0,1,1}xp^4 - 2C_{0,1,0}\hbar p + 3IC_{0,0,1}xp^2 \\
& - 6IC_{0,1,1}\hbar^2x) = -2Ix \\
> \text{eval}((14), [C[0,0,1]=0, C[0,1,0]=0, C[0,1,1]=0]) \\
& \quad 4IC_{0,0,0}x\hbar = -2Ix \tag{15} \\
> \text{solve}(\{(15)\}, [C[0,0,0]]) \\
& \quad \left[\left[C_{0,0,0} = -\frac{1}{2\hbar} \right] \right] \tag{16} \\
> Q(1) := -\frac{1}{\hbar}p \\
& \quad Q(1) := -\frac{p}{\hbar} \tag{17} \\
> Q := \varepsilon \cdot Q(1) \\
& \quad Q := -\frac{\varepsilon p}{\hbar} \tag{18} \\
> h := p^2 + x^2 + I \cdot \varepsilon x + \text{Commutator}\left(p^2 + x^2 + I \cdot \varepsilon x, \frac{Q}{2}\right) + \frac{1}{2} \text{Commutator}\left(p^2 + x^2 + I \cdot \varepsilon x^3, \right. \\
& \quad \left. \text{Commutator}\left(p^2 + x^2 + I \cdot \varepsilon x, \frac{Q}{2}\right)\right) \\
& \quad h := p^2 + x^2 + I \varepsilon x - \frac{\varepsilon(2Ix\hbar - \varepsilon\hbar)}{2\hbar} - \varepsilon\hbar p \tag{19} \\
> \text{simplify}((19)) \\
& \quad p^2 + x^2 + \frac{1}{2}\varepsilon^2 - \varepsilon\hbar p \tag{20} \\
> h := p^2 + x^2 + \frac{1}{2}\varepsilon^2 - \varepsilon\hbar p \\
& \quad h := p^2 + x^2 + \frac{1}{2}\varepsilon^2 - \varepsilon\hbar p \tag{21} \\
> \text{subs}\left(p = \frac{I}{\sqrt{2}}(b-a), x = \frac{1}{\sqrt{2}}(a+b), h\right); \\
& \quad \left(\frac{1}{2}\sqrt{2}(a+-a-)\right)^2 + \left(\frac{\sqrt{2}(a-+a+)}{2}\right)^2 + \frac{\varepsilon^2}{2} - \frac{I\varepsilon\hbar\sqrt{2}(a+-a-)}{2} \tag{22} \\
> h := \left(\frac{1}{2}\sqrt{2}(b-a)\right)^2 + \left(\frac{\sqrt{2}(b+a)}{2}\right)^2 + \frac{\varepsilon^2}{2} - \frac{I\varepsilon\hbar\sqrt{2}(b-a)}{2} \\
& \quad \hbar := -\frac{(a+-a-)^2}{2} + \frac{(a-+a+)^2}{2} + \frac{\varepsilon^2}{2} - \frac{I\varepsilon\hbar\sqrt{2}(a+-a-)}{2} \tag{23} \\
> E[n] := \text{Bra}(\varphi, n) \cdot h \cdot \text{Ket}(\varphi, n); \\
& \quad E_n := 2n + 1 + \frac{\varepsilon^2}{2} \tag{24} \\
> \\
> \text{subs}(p = p_c, x = x_c, h) \tag{25}
\end{aligned}$$

$$\left[\begin{array}{l}
 & p_c^2 + x_c^2 + \frac{1}{2} \epsilon^2 - \epsilon \hbar p_c & (25) \\
 > h_c := p_c^2 + x_c^2 + \frac{1}{2} \epsilon^2 - \epsilon \hbar p_c \\
 & h_c := p_c^2 + x_c^2 + \frac{1}{2} \epsilon^2 - \epsilon \hbar p_c & (26) \\
 > eval((26), [\hbar=0]) \\
 & p_c^2 + x_c^2 + \frac{\epsilon^2}{2} & (27) \\
 > H_c := p_c^2 + x_c^2 + \frac{\epsilon^2}{2}
 \end{array} \right.$$

Appendix B

Cubic anharmonic oscillator

```

> with(Physics);
[ '*', '\ ', Annihilation, AntiCommutator, Bra, Bracket, Check, Commutator, Coordinates,
  Creation, Dagger, Define, Dgamma, FeynmanDiagrams, Fundiff, Intc, Inverse, Ket, \alpha,
  LeviCivita, Parameters, Projector, Psigma, Setup, Simplify, SpaceTimeVector, Trace,
  Vectors, '^', dAlembertian, d_, diff, g_]
(1)
> Setup(Math = true);
* Partial match of 'Math' against keyword 'mathematicalnotation'
[mathematicalnotation = true]
(2)
> Setup(Hermitian = {x, p}, %Commutator(x, p) = I \hbar);
* Partial match of 'Hermitian' against keyword 'hermitianoperators'
[algebrarules = {[x, p]_ = I \hbar, [x, p^m]_ = I m \hbar p^{m-1}, [a-, a+]_ = 1}, hermitianoperators
  = {p, x}]
(3)
> Setup(redo, algebra = {%Commutator(x, p^m) = I \cdot m \cdot \hbar \cdot p^{m-1}});
* Partial match of 'algebra' against keyword 'algebrarules'
[algebrarules = {[x, p^m]_ = I m \hbar p^{m-1}}]
(4)
> a := Annihilation(\phi, 1);
a := a-
(5)
> b := Creation(\phi, 1);
b := a+
(6)
> a.Ket(\phi, n);
\sqrt{n} | \phi_{n-1} \rangle
(7)
> Bra(\phi, n).b;
\sqrt{n} \langle \phi_{n-1} |
(8)
> b.Ket(\phi, n);
\sqrt{n+1} | \phi_{n+1} \rangle
(9)
> Bra(\phi, n).b^2;
\sqrt{n} \sqrt{n-1} \langle \phi_{n-2} |
(10)
> Commutator(a, b);
0
(11)
> QI := \sum_{j=0}^1 \sum_{k=0}^1 C_{0,j,k} \cdot AntiCommutator(x^{2j}, p^{2k+1});
QI := 2 C_{0,0,0} p + 2 C_{0,0,1} p^3 + C_{0,1,0} [x^2, p]_+ + C_{0,1,1} [x^2, p^3]_+
(12)
> Commutator(p^2 + x^2, QI) = - 2 I x^3
C_{0,1,0} [p^2, [x^2, p]_+]_ + C_{0,1,1} [p^2, [x^2, p^3]_+]_ + 4 I C_{0,0,0} x \hbar + 6 I C_{0,0,1} \hbar (2 I \hbar p
  + 2 p^2 x) + C_{0,1,0} [x^2, [x^2, p]_+]_ + C_{0,1,1} [x^2, [x^2, p^3]_+]_ = - 2 I x^3
(13)
> simplify( (13) )
(14)

```

$$4 \hbar \left(-2 C_{0,1,0} \hbar p - 4 C_{0,1,1} \hbar p^3 - 6 I C_{0,1,1} \hbar^2 x + 9 C_{0,1,1} \hbar x^2 p + 3 I C_{0,1,1} x^3 p^2 \right. \\ \left. + 3 I C_{0,0,1} x p^2 - 2 I C_{0,1,1} x p^4 + 3 C_{0,0,1} \hbar p + I C_{0,0,0} x - 2 I C_{0,1,0} x p^2 + I C_{0,1,0} x^3 \right) \\ = -2 I x^3 \quad (14)$$

$$\text{eval}(\text{(14)}, [C[0,0,0]=0, C[0,1,1]=0]) \\ 4 \hbar \left(3 I C_{0,0,1} x p^2 - 2 I C_{0,1,0} x p^2 - 2 C_{0,1,0} \hbar p + 3 C_{0,0,1} \hbar p + I C_{0,1,0} x^3 \right) = -2 I x^3 \quad (15)$$

$$X := 4 \hbar \left(3 I C_{0,0,1} x p^2 + 3 C_{0,0,1} \hbar p - 2 C_{0,1,0} \hbar p + I C_{0,1,0} x^3 - 2 I C_{0,1,0} x p^2 \right) \\ X := 4 \hbar \left(3 I C_{0,0,1} x p^2 - 2 I C_{0,1,0} x p^2 - 2 C_{0,1,0} \hbar p + 3 C_{0,0,1} \hbar p + I C_{0,1,0} x^3 \right) \quad (16)$$

$$\text{subs}\left(C_{0,1,0} = -\frac{1}{2\hbar}, X\right); \\ 4 \hbar \left(3 I C_{0,0,1} x p^2 + \frac{I x p^2}{\hbar} + p + 3 C_{0,0,1} \hbar p - \frac{I x^3}{2\hbar} \right) \quad (17)$$

$$4 \hbar \left(3 I C_{0,0,1} x p^2 + 3 C_{0,0,1} \hbar p + p - \frac{I x^3}{2\hbar} + \frac{I x p^2}{\hbar} \right) = -2 I x^3 \\ 4 \hbar \left(3 I C_{0,0,1} x p^2 + \frac{I x p^2}{\hbar} + p + 3 C_{0,0,1} \hbar p - \frac{I x^3}{2\hbar} \right) = -2 I x^3 \quad (18)$$

$$\text{solve}(\{ \text{(18)} \}, [C[0,0,1]]) \\ \left[\left[C_{0,0,1} = -\frac{1}{3\hbar} \right] \right] \quad (19)$$

$$Q1 := -\frac{2}{3\hbar} p^3 - \frac{1}{2\hbar} [x^2, p]_+ \\ Q1 := -\frac{2p^3}{3\hbar} - \frac{[x^2, p]_+}{2\hbar} \quad (20)$$

$$-\frac{1}{6} \text{Commutator}(Q1, (\text{Commutator}(Q1, I x^3))); \\ -\frac{1}{6} \left(-\frac{1}{3\hbar} \left(2 \left(\right. \right. \right) \quad (21)$$

$$\frac{2 \left(-3 I \hbar p [p^3, [p, x^2]_+] - 3 I \hbar (-2 I \hbar p (I \hbar + 2 p x) - 2 I \hbar x p^2) p^2 \right)}{3 \hbar} \\ - \frac{[p^3, [[x^2, p]_+, x^3]_-]}{2 \hbar} \left. \right) - \frac{1}{2 \hbar} \left(\right. \\ \frac{2 \left(-3 I \hbar [[x^2, p]_+, p]_- [p, x^2]_+ - 3 I \hbar (x^2 [[x^2, p]_+, p^2]_- + [[x^2, p]_+, x^2]_- p^2) \right)}{3 \hbar} \\ \left. - \frac{[[x^2, p]_+, [[x^2, p]_+, x^3]_-]}{2 \hbar} \right) \right)$$

$$\text{simplify}(\text{(21)}) \\ 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4 \quad (22)$$

$$\begin{aligned}
&> Q3 := \sum_{j=0}^2 \sum_{k=0}^2 B_{0,j,k} \text{AntiCommutator}(x^{2j}, p^{2k+1}); \\
Q3 &:= 2 B_{0,0,0} p + 2 B_{0,0,1} p^3 + 2 B_{0,0,2} p^5 + B_{0,1,0} [x^2, p]_+ + B_{0,1,1} [x^2, p^3]_+ + B_{0,1,2} [x^2, \\
& p^5]_+ + B_{0,2,0} [x^4, p]_+ + B_{0,2,1} [x^4, p^3]_+ + B_{0,2,2} [x^4, p^5]_+ \quad (23)
\end{aligned}$$

$$\begin{aligned}
&> \text{Commutator}(p^2 + x^2, Q3) = 6 \hbar x^2 p + 2 I x^3 p^2 - 6 I \hbar^2 x + 2 I x^5 + 4 I x p^4 + 8 \hbar p^3 \\
B_{0,1,0} [p^2, [x^2, p]_+]_- + B_{0,1,1} [p^2, [x^2, p^3]_+]_- + B_{0,1,2} [p^2, [x^2, p^5]_+]_- + B_{0,2,0} [p^2, [x^4, p]_+]_- \\
& + B_{0,2,1} [p^2, [x^4, p^3]_+]_- + B_{0,2,2} [p^2, [x^4, p^5]_+]_- + 4 I B_{0,0,0} x \hbar \\
& + 6 I B_{0,0,1} \hbar (2 I \hbar p + 2 p^2 x) + 10 I B_{0,0,2} \hbar (4 I \hbar p^3 + 2 p^4 x) + B_{0,1,0} [x^2, [x^2, p]_+]_- \\
& + B_{0,1,1} [x^2, [x^2, p^3]_+]_- + B_{0,1,2} [x^2, [x^2, p^5]_+]_- + B_{0,2,0} [x^2, [x^4, p]_+]_- \\
& + B_{0,2,1} [x^2, [x^4, p^3]_+]_- + B_{0,2,2} [x^2, [x^4, p^5]_+]_- = 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 \\
& - 6 I \hbar^2 x + 4 I x p^4 \quad (24)
\end{aligned}$$

$$\begin{aligned}
&> \text{simplify}((24)) \\
-4 \hbar (-54 I B_{0,2,1} \hbar^2 x p^2 + 60 I B_{0,1,2} \hbar^2 x p^2 - 150 I B_{0,2,2} \hbar^2 x p^4 + 240 I B_{0,2,2} \hbar^2 x^3 p^2 \\
& + 24 I B_{0,2,1} \hbar^2 x^3 - 3 B_{0,0,1} \hbar p + 2 B_{0,1,0} \hbar p + 30 B_{0,1,2} \hbar^3 p - 30 B_{0,2,1} \hbar^3 p \\
& - I B_{0,0,0} x + 6 I B_{0,1,1} \hbar^2 x - 180 I B_{0,2,2} \hbar^4 x - 6 I B_{0,2,0} \hbar^2 x + 12 B_{0,2,0} \hbar x^2 p \\
& + 4 B_{0,1,1} \hbar p^3 + 36 B_{0,2,2} \hbar x^2 p^5 + 6 B_{0,1,2} \hbar p^5 - 15 B_{0,2,1} \hbar x^4 p - 180 B_{0,2,2} \hbar^3 p^3 \\
& - 50 B_{0,2,2} \hbar x^4 p^3 + 420 B_{0,2,2} \hbar^3 x^2 p - 30 B_{0,1,2} \hbar x^2 p^3 - 5 I B_{0,1,2} x^3 p^4 \\
& + 4 I B_{0,2,1} x^3 p^4 - I B_{0,1,0} x^3 + 4 I B_{0,2,2} x^3 p^6 + 4 I B_{0,2,0} x^3 p^2 - 5 I B_{0,0,2} x p^4 \\
& - 3 I B_{0,0,1} x p^2 - 5 I B_{0,2,2} x^5 p^4 + 2 I B_{0,1,1} x p^4 - I B_{0,2,0} x^5 - 3 I B_{0,2,1} x^5 p^2 \\
& + 2 I B_{0,1,0} x p^2 + 2 I B_{0,1,2} x p^6 - 3 I B_{0,1,1} x^3 p^2 - 10 B_{0,0,2} \hbar p^3 - 9 B_{0,1,1} \hbar x^2 p \\
& + 24 B_{0,2,1} \hbar x^2 p^3) = 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4 \quad (25)
\end{aligned}$$

$$\begin{aligned}
&> \text{simplify}((25), 'size') \\
-4 \hbar (-54 I B_{0,2,1} \hbar^2 x p^2 + 60 I B_{0,1,2} \hbar^2 x p^2 - 150 I B_{0,2,2} \hbar^2 x p^4 + 240 I B_{0,2,2} \hbar^2 x^3 p^2 \\
& + 24 I B_{0,2,1} \hbar^2 x^3 - 3 B_{0,0,1} \hbar p + 2 B_{0,1,0} \hbar p + 30 B_{0,1,2} \hbar^3 p - 30 B_{0,2,1} \hbar^3 p \\
& - I B_{0,0,0} x + 6 I B_{0,1,1} \hbar^2 x - 180 I B_{0,2,2} \hbar^4 x - 6 I B_{0,2,0} \hbar^2 x + 12 B_{0,2,0} \hbar x^2 p \\
& + 4 B_{0,1,1} \hbar p^3 + 36 B_{0,2,2} \hbar x^2 p^5 + 6 B_{0,1,2} \hbar p^5 - 15 B_{0,2,1} \hbar x^4 p - 180 B_{0,2,2} \hbar^3 p^3 \\
& - 50 B_{0,2,2} \hbar x^4 p^3 + 420 B_{0,2,2} \hbar^3 x^2 p - 30 B_{0,1,2} \hbar x^2 p^3 - 5 I B_{0,1,2} x^3 p^4 \\
& + 4 I B_{0,2,1} x^3 p^4 - I B_{0,1,0} x^3 + 4 I B_{0,2,2} x^3 p^6 + 4 I B_{0,2,0} x^3 p^2 - 5 I B_{0,0,2} x p^4 \\
& - 3 I B_{0,0,1} x p^2 - 5 I B_{0,2,2} x^5 p^4 + 2 I B_{0,1,1} x p^4 - I B_{0,2,0} x^5 - 3 I B_{0,2,1} x^5 p^2 \\
& + 2 I B_{0,1,0} x p^2 + 2 I B_{0,1,2} x p^6 - 3 I B_{0,1,1} x^3 p^2 - 10 B_{0,0,2} \hbar p^3 - 9 B_{0,1,1} \hbar x^2 p \\
& + 24 B_{0,2,1} \hbar x^2 p^3) = 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4 \quad (26)
\end{aligned}$$

$$\begin{aligned}
&> \text{eval}(\text{(26)}, [B[0, 0, 1]=0, B[0, 1, 0]=0, B[0, 1, 2]=0, B[0, 2, 2]=0, B[0, 2, 1]=0]) \\
&-4 \hbar \left(-3 I B_{0,1,1} x^3 p^2 - 9 B_{0,1,1} \hbar x^2 p - 10 B_{0,0,2} \hbar p^3 + 12 B_{0,2,0} \hbar x^2 p + 4 B_{0,1,1} \hbar p^3 \right. \\
&\quad + 4 I B_{0,2,0} x^3 p^2 - 5 I B_{0,0,2} x p^4 + 2 I B_{0,1,1} x p^4 - I B_{0,0,0} x - I B_{0,2,0} x^5 + 6 I B_{0,1,1} \hbar^2 x \\
&\quad \left. - 6 I B_{0,2,0} \hbar^2 x \right) = 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4
\end{aligned} \tag{27}$$

$$\begin{aligned}
&> 4 I \cdot \hbar \cdot B_{0,2,0} x^5 = 2 I x^5 \\
&\qquad\qquad\qquad 4 I B_{0,2,0} \hbar x^5 = 2 I x^5
\end{aligned} \tag{28}$$

$$\begin{aligned}
&> \text{solve}(\text{(28)}, [B[0, 2, 0]]) \\
&\qquad\qquad\qquad \left[\left[B_{0,2,0} = \frac{1}{2 \hbar} \right] \right]
\end{aligned} \tag{29}$$

$$\begin{aligned}
&> -4 \hbar \left(-3 I B_{0,1,1} x^3 p^2 - 9 B_{0,1,1} \hbar x^2 p - 10 B_{0,0,2} \hbar p^3 + 12 B_{0,2,0} \hbar x^2 p + 4 B_{0,1,1} \hbar p^3 \right. \\
&\quad + 4 I B_{0,2,0} x^3 p^2 - 5 I B_{0,0,2} x p^4 + 2 I B_{0,1,1} x p^4 - I B_{0,0,0} x - I B_{0,2,0} x^5 + 6 I B_{0,1,1} \hbar^2 x \\
&\quad \left. - 6 I B_{0,2,0} \hbar^2 x \right) = 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4 \\
&-4 \hbar \left(-3 I B_{0,1,1} x^3 p^2 - 9 B_{0,1,1} \hbar x^2 p - 10 B_{0,0,2} \hbar p^3 + 12 B_{0,2,0} \hbar x^2 p + 4 B_{0,1,1} \hbar p^3 \right. \\
&\quad + 4 I B_{0,2,0} x^3 p^2 - 5 I B_{0,0,2} x p^4 + 2 I B_{0,1,1} x p^4 - I B_{0,0,0} x - I B_{0,2,0} x^5 + 6 I B_{0,1,1} \hbar^2 x \\
&\quad \left. - 6 I B_{0,2,0} \hbar^2 x \right) = 8 \hbar p^3 + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4
\end{aligned} \tag{30}$$

$$\begin{aligned}
&> \text{eval}\left(\text{(30)}, \left[B[0, 2, 0] = \frac{1}{2 \hbar} \right] \right) \\
&-4 \hbar \left(-3 I B_{0,1,1} x^3 p^2 - 9 B_{0,1,1} \hbar x^2 p - 10 B_{0,0,2} \hbar p^3 + 6 x^2 p + 4 B_{0,1,1} \hbar p^3 + \frac{2 I x^3 p^2}{\hbar} \right. \\
&\quad \left. - 5 I B_{0,0,2} x p^4 + 2 I B_{0,1,1} x p^4 - I B_{0,0,0} x - \frac{I x^5}{2 \hbar} + 6 I B_{0,1,1} \hbar^2 x - 3 I \hbar x \right) = 8 \hbar p^3 \\
&\quad + 6 \hbar x^2 p + 2 I x^3 p^2 + 2 I x^5 - 6 I \hbar^2 x + 4 I x p^4
\end{aligned} \tag{31}$$

$$\begin{aligned}
&> -4 \hbar \left(\frac{2 I x^3 p^2}{\hbar} \right) + 4 \hbar \cdot (3 I B_{0,1,1} x^3 p^2) = 2 I x^3 p^2 \\
&\qquad\qquad\qquad -8 I x^3 p^2 + 12 I B_{0,1,1} \hbar x^3 p^2 = 2 I x^3 p^2
\end{aligned} \tag{32}$$

$$\begin{aligned}
&> \text{solve}(\text{(32)}, [B[0, 1, 1]]) \\
&\qquad\qquad\qquad \left[\left[B_{0,1,1} = \frac{5}{6 \hbar} \right] \right]
\end{aligned} \tag{33}$$

$$\begin{aligned}
&> 4 \hbar \left(10 B_{0,0,2} \hbar p^3 - 4 B_{0,1,1} \hbar p^3 - 6 x^2 p + 9 B_{0,1,1} \hbar x^2 p + I B_{0,0,0} x - 2 I B_{0,1,1} x p^4 \right. \\
&\quad \left. - \frac{2 I x^3 p^2}{\hbar} + 3 I B_{0,1,1} x^3 p^2 + 5 I B_{0,0,2} x p^4 + \frac{I x^5}{2 \hbar} - 6 I B_{0,1,1} \hbar^2 x + 3 I \hbar x \right) = -6 I \hbar^2 x \\
&\quad + 2 I x^3 p^2 + 6 \hbar x^2 p + 2 I x^5 + 8 \hbar p^3 + 4 I x p^4 \\
&4 \hbar \left(10 B_{0,0,2} \hbar p^3 - 4 B_{0,1,1} \hbar p^3 - 6 x^2 p + 9 B_{0,1,1} \hbar x^2 p + I B_{0,0,0} x - 2 I B_{0,1,1} x p^4 \right.
\end{aligned} \tag{34}$$

$$\begin{aligned}
& -\frac{2Ix^3p^2}{\hbar} + 3IB_{0,1,1}x^3p^2 + 5IB_{0,0,2}xp^4 + \frac{Ix^5}{2\hbar} - 6IB_{0,1,1}\hbar^2x + 3I\hbar x \Big) = 8\hbar p^3 \\
& + 6\hbar x^2p + 2Ix^3p^2 + 2Ix^5 - 6I\hbar^2x + 4Ix p^4 \\
& > \text{eval} \left((34), \left[B[0,1,1] = \frac{5}{6\hbar} \right] \right) \\
& 4\hbar \left(10B_{0,0,2}\hbar p^3 - \frac{10p^3}{3} + \frac{3x^2p}{2} + IB_{0,0,0}x - \frac{5Ix p^4}{3\hbar} + \frac{Ix^3p^2}{2\hbar} + 5IB_{0,0,2}xp^4 \right. \\
& \quad \left. + \frac{Ix^5}{2\hbar} - 2I\hbar x \right) = 8\hbar p^3 + 6\hbar x^2p + 2Ix^3p^2 + 2Ix^5 - 6I\hbar^2x + 4Ix p^4 \quad (35) \\
& > 4\hbar \left(10B_{0,0,2}\hbar p^3 - \frac{10p^3}{3} \right) = 8\hbar p^3 \\
& \quad 4\hbar \left(10B_{0,0,2}\hbar p^3 - \frac{10}{3}p^3 \right) = 8\hbar p^3 \quad (36) \\
& > \text{solve} \left(\{ (36) \}, [B[0,0,2]] \right) \\
& \quad \left[\left[B_{0,0,2} = \frac{8}{15\hbar} \right] \right] \quad (37) \\
& > 4\hbar \left(10B_{0,0,2}\hbar p^3 - \frac{10p^3}{3} + \frac{3x^2p}{2} + IB_{0,0,0}x - \frac{5Ix p^4}{3\hbar} + \frac{Ix^3p^2}{2\hbar} + 5IB_{0,0,2}xp^4 \right. \\
& \quad \left. + \frac{Ix^5}{2\hbar} - 2I\hbar x \right) = -6I\hbar^2x + 2Ix^3p^2 + 6\hbar x^2p + 2Ix^5 + 8\hbar p^3 + 4Ix p^4 \\
& 4\hbar \left(10B_{0,0,2}\hbar p^3 - \frac{10p^3}{3} + \frac{3x^2p}{2} + IB_{0,0,0}x - \frac{5Ix p^4}{3\hbar} + \frac{Ix^3p^2}{2\hbar} + 5IB_{0,0,2}xp^4 \right. \\
& \quad \left. + \frac{Ix^5}{2\hbar} - 2I\hbar x \right) = 8\hbar p^3 + 6\hbar x^2p + 2Ix^3p^2 + 2Ix^5 - 6I\hbar^2x + 4Ix p^4 \quad (38) \\
& > \text{simplify} \left((38), 'size' \right) \\
& 2Ix^3p^2 + \frac{(-20I + 60IB_{0,0,2}\hbar)xp^4}{3} + 6\hbar x^2p + \frac{(-40\hbar + 120B_{0,0,2}\hbar^2)p^3}{3} - 8I\hbar^2x \\
& \quad + 4IB_{0,0,0}x\hbar + 2Ix^5 = 8\hbar p^3 + 6\hbar x^2p + 2Ix^3p^2 + 2Ix^5 - 6I\hbar^2x + 4Ix p^4 \quad (39) \\
& > \text{eval} \left((38), \left[B[0,0,2] = \frac{8}{15\hbar} \right] \right) \\
& 4\hbar \left(2p^3 + \frac{3x^2p}{2} + IB_{0,0,0}x + \frac{Ix p^4}{\hbar} + \frac{Ix^3p^2}{2\hbar} + \frac{Ix^5}{2\hbar} - 2I\hbar x \right) = 8\hbar p^3 + 6\hbar x^2p \\
& \quad + 2Ix^3p^2 + 2Ix^5 - 6I\hbar^2x + 4Ix p^4 \quad (40) \\
& > \text{simplify} \left((40) \right) \\
& 8\hbar p^3 + 6\hbar x^2p + 4IB_{0,0,0}x\hbar + 4Ix p^4 + 2Ix^3p^2 + 2Ix^5 - 8I\hbar^2x = 8\hbar p^3 + 6\hbar x^2p \\
& \quad + 2Ix^3p^2 + 2Ix^5 - 6I\hbar^2x + 4Ix p^4 \quad (41) \\
& > 4IB_{0,0,0}x\hbar - 8I\hbar^2x = -6I\hbar^2x \\
& \quad 4IB_{0,0,0}x\hbar - 8I\hbar^2x = -6I\hbar^2x \quad (42) \\
& > \text{solve} \left(\{ (42) \}, [B[0,0,0]] \right)
\end{aligned}$$

$$\left[\left[B_{0,0,0} = \frac{\hbar}{2} \right] \right] \quad (43)$$

$$\begin{aligned} > Q3 := 2B_{0,0,0}p + 2B_{0,0,1}p^3 + 2B_{0,0,2}p^5 + B_{0,1,0}[x^2, p]_+ + B_{0,1,1}[x^2, p^3]_+ + B_{0,1,2}[x^2, \\ & p^5]_+ + B_{0,2,0}[x^4, p]_+ + B_{0,2,1}[x^4, p^3]_+ + B_{0,2,2}[x^4, p^5]_+ \\ Q3 := 2B_{0,0,0}p + 2B_{0,0,1}p^3 + 2B_{0,0,2}p^5 + B_{0,1,0}[x^2, p]_+ + B_{0,1,1}[x^2, p^3]_+ + B_{0,1,2}[x^2, \\ & p^5]_+ + B_{0,2,0}[x^4, p]_+ + B_{0,2,1}[x^4, p^3]_+ + B_{0,2,2}[x^4, p^5]_+ \end{aligned} \quad (44)$$

$$\begin{aligned} > \text{eval}((44), [B[0,0,0]=1/2\hbar, B[0,0,1]=0, B[0,0,2]=8/(15\hbar), B[0,1,0]=0, B[0,1,1]=5 \\ / (6\hbar), B[0,1,2]=0, B[0,2,0]=1/(2\hbar), B[0,2,1]=0, B[0,2,2]=0]) \\ \hbar p + \frac{16p^5}{15\hbar} + \frac{5[x^2, p^3]_+}{6\hbar} + \frac{[x^4, p]_+}{2\hbar} \end{aligned} \quad (45)$$

$$\begin{aligned} > Q1 := -\frac{2}{3\hbar}p^3 - \frac{1}{2\hbar}[x^2, p]_+ \\ Q1 := -\frac{2p^3}{3\hbar} - \frac{[x^2, p]_+}{2\hbar} \end{aligned} \quad (46)$$

$$\begin{aligned} > Q3 := \hbar p + \frac{16p^5}{15\hbar} + \frac{5[x^2, p^3]_+}{6\hbar} + \frac{[x^4, p]_+}{2\hbar} \\ Q3 := \hbar p + \frac{16p^5}{15\hbar} + \frac{5[x^2, p^3]_+}{6\hbar} + \frac{[x^4, p]_+}{2\hbar} \end{aligned} \quad (47)$$

$$\begin{aligned} > Q := \varepsilon \cdot Q1 + \varepsilon^3 \cdot Q3; \\ Q := \varepsilon \left(-\frac{2p^3}{3\hbar} - \frac{[x^2, p]_+}{2\hbar} \right) + \varepsilon^3 \left(\hbar p + \frac{16p^5}{15\hbar} + \frac{5[x^2, p^3]_+}{6\hbar} + \frac{[x^4, p]_+}{2\hbar} \right) \end{aligned} \quad (48)$$

$$\begin{aligned} > h := p^2 + x^2 + I \cdot \varepsilon x^3 + \text{Commutator} \left(p^2 + x^2 + I \cdot \varepsilon x^3, \frac{Q}{2} \right) + \frac{1}{2} \text{Commutator} \left(p^2 + x^2 + I \cdot \varepsilon \right. \\ & \left. x^3, \left(\text{Commutator} \left(p^2 + x^2 + I \cdot \varepsilon x^3, \frac{Q}{2} \right) \right) \right) \end{aligned}$$

$$\begin{aligned} h := p^2 + x^2 + \frac{1}{2} \left(I \varepsilon \left(\frac{1}{2} \left(\varepsilon \left(\right. \right. \right. \right. \\ \left. \left. \left. \frac{2(3I\hbar(-4I\hbar xp^3 - 2I\hbar p(2I\hbar p + 2p^2x)) + 6\hbar^2 p^2(I\hbar + 2px))}{3\hbar} \right. \right. \right. \right. \\ \left. \left. \left. - \frac{[p^2, [x^3, [x^2, p]_+]_-]_-}{2\hbar} \right) \right) + \frac{1}{2} \left(\varepsilon^3 \left(6\hbar^3(I\hbar + 2px) \right. \right. \right. \\ \left. \left. \left. + \frac{16(5I\hbar(-4I\hbar xp^5 - 2I\hbar p(4I\hbar p^3 + 2p^4x)) + 10\hbar^2 p^4(I\hbar + 2px))}{15\hbar} \right. \right. \right. \\ \left. \left. \left. + \frac{5[p^2, [x^3, [x^2, p^3]_+]_-]_-}{6\hbar} + \frac{[p^2, [x^3, [x^4, p]_+]_-]_-}{2\hbar} \right) \right) \right) - \frac{\varepsilon[p^2, [x^2, p]_+]_-}{4\hbar} \end{aligned} \quad (49)$$

$$\begin{aligned}
& + \frac{\varepsilon^3 \left(\frac{5 [p^2, [x^2, p^3]_+]_-}{6 \hbar} + \frac{[p^2, [x^4, p]_+]_-}{2 \hbar} \right)}{2} \\
& + \frac{\varepsilon \left(-2I(2I\hbar p + 2p^2 x) - \frac{[x^2, [x^2, p]_+]_-}{2 \hbar} \right)}{2} \\
& + \frac{\varepsilon^3 \left(2I\hbar^2 x + \frac{16I(4I\hbar p^3 + 2p^4 x)}{3} + \frac{5 [x^2, [x^2, p^3]_+]_-}{6 \hbar} + \frac{[x^2, [x^4, p]_+]_-}{2 \hbar} \right)}{2} \\
& + \frac{1}{2} \left(I\varepsilon \left(-\frac{\varepsilon(3I\hbar x(-4\hbar^2 x + 4I\hbar(I\hbar + 2px)x) - 6\hbar^2(I\hbar + 2px)x^2)}{3 \hbar} \right. \right. \\
& + \frac{1}{2} \left(\varepsilon^3 \left(\frac{1}{15 \hbar} (16(5I\hbar x(-24I\hbar^3 p - 24\hbar^2 p^2 x + 8I\hbar(3I\hbar p^2 + 2p^3 x)x) \right. \right. \right. \\
& \left. \left. \left. - 20\hbar^2(3I\hbar p^2 + 2p^3 x)x^2) + \frac{5 [x^2, [x^3, [x^2, p^3]_+]_-]_-}{6 \hbar} \right) \right) \right) \\
& - \frac{\varepsilon [p^2, [p^2, [x^2, p]_+]_-]_-}{8 \hbar} \\
& + \frac{\varepsilon^3 \left(\frac{5 [p^2, [p^2, [x^2, p^3]_+]_-]_-}{6 \hbar} + \frac{[p^2, [p^2, [x^4, p]_+]_-]_-}{2 \hbar} \right)}{4} \\
& + \frac{\varepsilon \left(-8 \hbar p^3 - \frac{[p^2, [x^2, [x^2, p]_+]_-]_-}{2 \hbar} \right)}{4} \\
& + \frac{\varepsilon^3 \left(4 \hbar^3 p + \frac{64 \hbar p^5}{3} + \frac{5 [p^2, [x^2, [x^2, p^3]_+]_-]_-}{6 \hbar} + \frac{[p^2, [x^2, [x^4, p]_+]_-]_-}{2 \hbar} \right)}{4} \\
& + \frac{1}{2} \left(I\varepsilon \left(-\frac{\varepsilon [x^3, [p^2, [x^2, p]_+]_-]_-}{4 \hbar} \right. \right. \\
& + \frac{\varepsilon^3 \left(\frac{5 [x^3, [p^2, [x^2, p^3]_+]_-]_-}{6 \hbar} + \frac{[x^3, [p^2, [x^4, p]_+]_-]_-}{2 \hbar} \right)}{2} - I\varepsilon(-6\hbar^2 x^2 \\
& \left. \left. + 2(2I\hbar x(I\hbar + 2px) + 2I\hbar px^2)x \right) \right)
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \left(\epsilon^3 \left(\frac{1}{3} (16I(4I\hbar(3I\hbar x(2I\hbar p + 2p^2 x) + 3I\hbar p^2 x^2) + 2(4I\hbar x(3I\hbar p^2 \right. \right. \\
& \left. \left. + 2p^3 x) + 4I\hbar p^3 x^2) x) + \frac{5[x^3, [x^2, [x^2, p^3]_+]_-]_-}{6\hbar} \right) \right) + I\epsilon \left(\right. \\
& \left. - \frac{1}{3\hbar} (\epsilon(3I\hbar x(-6\hbar^2 x^2 + 2(2I\hbar x(I\hbar + 2px) + 2I\hbar p x^2) x) + 3I\hbar(2I\hbar x(I\hbar \right. \right. \\
& \left. \left. + 2px) + 2I\hbar p x^2) x^2) + \frac{1}{2} \left(\epsilon^3 \left(\frac{1}{15\hbar} (16(5I\hbar x(-12\hbar^2 x(2I\hbar p \right. \right. \right. \\
& \left. \left. + 2p^2 x) - 12\hbar^2 p^2 x^2 + 2(4I\hbar x(3I\hbar p^2 + 2p^3 x) + 4I\hbar p^3 x^2) x) \right. \right. \right. \\
& \left. \left. \left. + 5I\hbar(4I\hbar x(3I\hbar p^2 + 2p^3 x) + 4I\hbar p^3 x^2) x^2) + \frac{5[x^3, [x^3, [x^2, p^3]_+]_-]_-}{6\hbar} \right) \right) \right) \right) \\
& - \frac{\epsilon[x^2, [p^2, [x^2, p]_+]_-]_-}{8\hbar} \\
& + \frac{\epsilon^3 \left(\frac{5[x^2, [p^2, [x^2, p^3]_+]_-]_-}{6\hbar} + \frac{[x^2, [p^2, [x^4, p]_+]_-]_-}{2\hbar} \right)}{4} \\
& + I\epsilon \left(\frac{\epsilon \left(-\frac{2(3I\hbar x(2I\hbar p + 2p^2 x) + 3I\hbar p^2 x^2)}{3\hbar} - \frac{[x^3, [x^2, p]_+]_-}{2\hbar} \right)}{2} \right) \\
& + \frac{1}{2} \left(\epsilon^3 \left(3I\hbar^2 x^2 + \frac{16(5I\hbar x(4I\hbar p^3 + 2p^4 x) + 5I\hbar p^4 x^2)}{15\hbar} + \frac{5[x^3, [x^2, p^3]_+]_-}{6\hbar} \right. \right. \\
& \left. \left. + \frac{[x^3, [x^4, p]_+]_-}{2\hbar} \right) \right) \\
& + \frac{1}{4} \left(\epsilon^3 \left(\frac{16I(-12\hbar^2(2I\hbar p + 2p^2 x) + 8I\hbar(3I\hbar p^2 + 2p^3 x) x)}{3} \right. \right. \\
& \left. \left. + \frac{5[x^2, [x^2, [x^2, p^3]_+]_-]_-}{6\hbar} \right) \right) + I\epsilon x^3 - \frac{I\epsilon(-4\hbar^2 x + 4I\hbar(I\hbar + 2px) x)}{2}
\end{aligned}$$

> simplify((49))

$$\begin{aligned}
& I\epsilon^3 x^5 + 2\epsilon^3 \hbar p^5 + I\epsilon^3 x^3 p^2 + 26\epsilon^4 \hbar^2 x^2 - 3\hbar \epsilon x^2 p + 2I\epsilon^3 x p^4 + 32\hbar^2 \epsilon^4 p^2 + \frac{45\hbar \epsilon^5 x^6 p}{2} \quad (50) \\
& + 3\hbar \epsilon^3 x^2 p - \frac{45\hbar^2 \epsilon^4 x^4}{2} - 5\hbar \epsilon^3 x^2 p^3 - 6\epsilon^3 \hbar x^4 p + 48\epsilon^5 \hbar x^4 p^3 - 9\epsilon^2 \hbar^2 p^2
\end{aligned}$$

$$\begin{aligned}
& -480 \epsilon^5 \hbar^3 x^2 p + 40 \epsilon^4 \hbar^2 p^4 + 4 \epsilon^3 \hbar p^3 - 63 \epsilon^4 \hbar^2 x^2 p^2 + 192 I \hbar^4 \epsilon^5 x - 6 I \hbar \epsilon^2 x p \\
& - 6 I \hbar \epsilon^2 x p^3 + 15 I \hbar^2 \epsilon^3 x p^2 - 14 I \hbar \epsilon^4 x^3 p^3 + 16 I \hbar \epsilon^4 x p^5 - 9 I \hbar \epsilon^4 x^5 p \\
& - \frac{135 I \hbar^2 \epsilon^5 x^5}{2} + 32 I \hbar \epsilon^4 x p^3 + 12 I \epsilon^3 \hbar^2 x^3 - 288 I \hbar^2 \epsilon^5 x^3 p^2 + 30 I \hbar \epsilon^4 x^3 p - 2 \hbar^2 \epsilon^2 \\
& + 6 \epsilon^3 \hbar^3 p + p^2 + x^2 + 18 \epsilon^4 \hbar^4 - \frac{3 \epsilon^4 x^6}{2} + 3 \epsilon^2 x^2 p^2 + \frac{3 \epsilon^2 x^4}{2} - 8 \epsilon^4 x^2 p^4 \\
& - \frac{15 \epsilon^4 x^4 p^2}{2} + 78 I \hbar^3 \epsilon^4 x p + 3 I \hbar^2 \epsilon x - 3 I \epsilon^3 \hbar^2 x
\end{aligned}$$

> series((50), \epsilon, 5)

$$\begin{aligned}
& p^2 + x^2 + (-3 \hbar x^2 p + 3 I \hbar^2 x) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x p + 3 x^2 p^2 - 9 \hbar^2 p^2 + \frac{3 x^4}{2} \right. \\
& \left. - 6 I \hbar x p^3 \right) \epsilon^2 + (I x^3 p^2 + 4 \hbar p^3 + I x^5 + 6 \hbar^3 p - 6 \hbar x^4 p + 2 \hbar p^5 + 3 \hbar x^2 p + 12 I \hbar^2 x^3 \\
& + 15 I \hbar^2 x p^2 - 3 I \hbar^2 x - 5 \hbar x^2 p^3 + 2 I x p^4) \epsilon^3 + \left(26 \hbar^2 x^2 + 18 \hbar^4 + 16 I \hbar x p^5 \right. \\
& + 32 \hbar^2 p^2 - 14 I \hbar x^3 p^3 - \frac{3 x^6}{2} + 32 I \hbar x p^3 + 78 I \hbar^3 x p - \frac{15 x^4 p^2}{2} + 40 \hbar^2 p^4 \\
& \left. - 9 I \hbar x^5 p + 30 I \hbar x^3 p - \frac{45 \hbar^2 x^4}{2} - 8 x^2 p^4 - 63 \hbar^2 x^2 p^2 \right) \epsilon^4 + O(\epsilon^5)
\end{aligned} \tag{51}$$

> series((51), \epsilon, 3)

$$\begin{aligned}
& p^2 + x^2 + (-3 \hbar x^2 p + 3 I \hbar^2 x) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x p + 3 x^2 p^2 - 9 \hbar^2 p^2 + \frac{3 x^4}{2} \right. \\
& \left. - 6 I \hbar x p^3 \right) \epsilon^2 + O(\epsilon^3)
\end{aligned} \tag{52}$$

$$\begin{aligned}
& h := p^2 + x^2 + (-3 \hbar x^2 p + 3 I \hbar^2 x) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x p + 3 x^2 p^2 - 9 \hbar^2 p^2 + \frac{3 x^4}{2} \right. \\
& \left. - 6 I \hbar x p^3 \right) \epsilon^2 + O(\epsilon^3)
\end{aligned}$$

$$\begin{aligned}
& h := p^2 + x^2 + (-3 \hbar x^2 p + 3 I \hbar^2 x) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x p + 3 x^2 p^2 - 9 \hbar^2 p^2 + \frac{3 x^4}{2} \right. \\
& \left. - 6 I \hbar x p^3 \right) \epsilon^2 + O(\epsilon^3)
\end{aligned} \tag{53}$$

> subs(p = \frac{I}{\sqrt{2}} \cdot (b - a), x = \frac{1}{\sqrt{2}} (a + b), h);

$$\begin{aligned}
& \left(\frac{I}{2} \sqrt{2} (a + -a) \right)^2 + \left(\frac{\sqrt{2} (a + a +)}{2} \right)^2 + \left(-3 \hbar \left(\frac{\sqrt{2} (a + a +)}{2} \right) \right)^2 \frac{I}{2} \sqrt{2} (a + \\
& - a) + \frac{3 I \hbar^2 \sqrt{2} (a + a +)}{2} \epsilon + \left(-2 \hbar^2 - 6 I \hbar \frac{\sqrt{2} (a + a +)}{2} \frac{I}{2} \sqrt{2} (a + -a) \right)
\end{aligned} \tag{54}$$

$$+ 3 \left(\frac{\sqrt{2} (a-+a+)}{2} \right)^2 \left(\frac{1}{2} \sqrt{2} (a+-a-) \right)^2 - 9 \hbar^2 \left(\frac{1}{2} \sqrt{2} (a+-a-) \right)^2$$

$$+ \frac{3 \left(\frac{\sqrt{2} (a-+a+)}{2} \right)^4}{2} - 6 I \hbar \frac{\sqrt{2} (a-+a+)}{2} \left(\frac{1}{2} \sqrt{2} (a+-a-) \right)^3 \Big) \varepsilon^2 + O(\varepsilon^3)$$

> series((54), \hbar, 3)

$$- \frac{(a+-a-)^2}{2} + \frac{(a-+a+)^2}{2} + O(\varepsilon^3) + \left(\frac{3(a-+a+)^4}{8} - \frac{3(a-+a+)^2(a+-a-)^2}{4} \right) \varepsilon^2 \quad (55)$$

$$+ \left(- \frac{3I(a-+a+)^2 \sqrt{2} (a+-a-) \varepsilon}{4} + \left(3(a-+a+) (a+-a-) \right. \right.$$

$$\left. \left. - \frac{3(a-+a+) (a+-a-)^3}{2} \right) \varepsilon^2 \right) \hbar + \left(\left(\frac{9(a+-a-)^2}{2} - 2 \right) \varepsilon^2 \right.$$

$$\left. + \frac{3I\sqrt{2} (a-+a+) \varepsilon}{2} \right) \hbar^2$$

$$> h := - \frac{(b-a)^2}{2} + \frac{(a+b)^2}{2} + \left(- \frac{3(a+b)^2(b-a)^2}{4} + \frac{3(a+b)^4}{8} \right) \cdot \varepsilon^2 + \left(\right.$$

$$\left. - \frac{3I\sqrt{2} (a+b)^2(b-a) \varepsilon}{4} + \left(3(a+b)(b-a) - \frac{3(a+b)(b-a)^3}{2} \right) \cdot \varepsilon^2 \right) \cdot \hbar$$

$$+ \left(\left(\frac{9(b-a)^2}{2} - 2 \right) \cdot \varepsilon^2 + \frac{3I\sqrt{2} (a+b) \varepsilon}{2} \right) \cdot \hbar^2$$

$$h := - \frac{(a+-a-)^2}{2} + \frac{(a-+a+)^2}{2} + \left(- \frac{3(a-+a+)^2(a+-a-)^2}{4} + \frac{3(a-+a+)^4}{8} \right) \varepsilon^2 \quad (56)$$

$$+ \left(- \frac{3I\sqrt{2} \varepsilon (a-+a+)^2 (a+-a-)}{4} + \left((3a+3a+) (a+-a-) \right. \right.$$

$$\left. \left. - \frac{(3a+3a+) (a+-a-)^3}{2} \right) \varepsilon^2 \right) \hbar + \left(\left(\frac{9(a+-a-)^2}{2} - 2 \right) \varepsilon^2 \right.$$

$$\left. + \frac{3I\sqrt{2} (a-+a+) \varepsilon}{2} \right) \hbar^2$$

> E[n] := Bra(\varphi, n).h.Ket(\varphi, n)

$$E_n := \frac{(30n^2 + (-72\hbar^2 + 72\hbar + 30)n - 52\hbar^2 + 60\hbar + 3) \varepsilon^2}{8} + 2n + 1 \quad (57)$$

> eval((57), [\hbar=1])

$$\left(\frac{15}{4} n^2 + \frac{15}{4} n + \frac{11}{8} \right) \varepsilon^2 + 2n + 1 \quad (58)$$

$$> h := p^2 + x^2 + (-3\hbar x^2 p + 3I\hbar^2 x) \varepsilon + \left(-2\hbar^2 - 6I\hbar x p + 3x^2 p^2 - 9\hbar^2 p^2 + \frac{3x^4}{2} \right.$$

$$\left. - 6I\hbar x p^3 \right) \varepsilon^2 + O(\varepsilon^3)$$

$$h := p^2 + x^2 + (-3 \hbar x^2 p + 3 I \hbar^2 x) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x p + 3 x^2 p^2 - 9 \hbar^2 p^2 + \frac{3 x^4}{2} - 6 I \hbar x p^3 \right) \epsilon^2 + O(\epsilon^3) \quad (59)$$

> subs(p=p_c, x=x_c, h)

$$p_c^2 + x_c^2 + (-3 \hbar x_c^2 p_c + 3 I \hbar^2 x_c) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x_c p_c + 3 x_c^2 p_c^2 - 9 \hbar^2 p_c^2 + \frac{3 x_c^4}{2} - 6 I \hbar x_c p_c^3 \right) \epsilon^2 + O(\epsilon^3) \quad (60)$$

$$h_c := p_c^2 + x_c^2 + (-3 \hbar x_c^2 p_c + 3 I \hbar^2 x_c) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x_c p_c + 3 x_c^2 p_c^2 - 9 \hbar^2 p_c^2 + \frac{3 x_c^4}{2} - 6 I \hbar x_c p_c^3 \right) \epsilon^2 + O(\epsilon^3)$$

$$h_c := p_c^2 + x_c^2 + (-3 \hbar x_c^2 p_c + 3 I \hbar^2 x_c) \epsilon + \left(-2 \hbar^2 - 6 I \hbar x_c p_c + 3 x_c^2 p_c^2 - 9 \hbar^2 p_c^2 + \frac{3 x_c^4}{2} - 6 I \hbar x_c p_c^3 \right) \epsilon^2 + O(\epsilon^3) \quad (61)$$

> eval((61), [\hbar=0])

$$p_c^2 + x_c^2 + \left(3 x_c^2 p_c^2 + \frac{3 x_c^4}{2} \right) \epsilon^2 + O(\epsilon^3) \quad (62)$$

$$H_c := p_c^2 + x_c^2 + \left(\frac{3 x_c^4}{2} + 3 x_c^2 p_c^2 \right) \epsilon^2 + O(\epsilon^3)$$

$$H_c := p_c^2 + x_c^2 + \left(3 x_c^2 p_c^2 + \frac{3 x_c^4}{2} \right) \epsilon^2 + O(\epsilon^3) \quad (63)$$

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