

## Making sense of non-Hermitian Hamiltonians

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# Making sense of non-Hermitian Hamiltonians

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## Abstract

The Hamiltonian  $H$  specifies the energy levels and time evolution of a quantum theory. A standard axiom of quantum mechanics requires that  $H$  be Hermitian because Hermiticity guarantees that the energy spectrum is real and that time evolution is unitary (probability-preserving). This paper describes an alternative formulation of quantum mechanics in which the mathematical axiom of Hermiticity (transpose + complex conjugate) is replaced by the physically transparent condition of space–time reflection ( $\mathcal{PT}$ ) symmetry. If  $H$  has an unbroken  $\mathcal{PT}$  symmetry, then the spectrum is real. Examples of  $\mathcal{PT}$ -symmetric non-Hermitian quantum-mechanical Hamiltonians are  $H = \hat{p}^2 + i\hat{x}^3$  and  $H = \hat{p}^2 - \hat{x}^4$ . Amazingly, the energy levels of these Hamiltonians are all real and positive!

Does a  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  specify a physical quantum theory in which the norms of states are positive and time evolution is unitary? The answer is that if  $H$  has an unbroken  $\mathcal{PT}$  symmetry, then it has another symmetry represented by a linear operator  $\mathcal{C}$ . In terms of  $\mathcal{C}$ , one can construct a time-independent inner product with a positive-definite norm. Thus,  $\mathcal{PT}$ -symmetric Hamiltonians describe a new class of complex quantum theories having positive probabilities and unitary time evolution.

The Lee model provides an excellent example of a  $\mathcal{PT}$ -symmetric Hamiltonian. The renormalized Lee-model Hamiltonian has a negative-norm ‘ghost’ state because renormalization causes the Hamiltonian to become non-Hermitian. For the past 50 years there have been many attempts to find a physical interpretation for the ghost, but all such attempts failed. The correct interpretation of the ghost is simply that the non-Hermitian Lee-model Hamiltonian is  $\mathcal{PT}$ -symmetric. The  $\mathcal{C}$  operator for the Lee model is calculated exactly and in closed form and the ghost is shown to be a physical state having a positive norm. The ideas of  $\mathcal{PT}$  symmetry are illustrated by using many quantum-mechanical and quantum-field-theoretic models.

(Some figures in this article are in colour only in the electronic version)

This article was invited by Professor S Washburn.

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## 1. Introduction—new kinds of quantum theories

The theory of quantum mechanics is nearly one hundred years old and because there have been so many experimental verifications of its theoretical predictions, it has become an accepted component of modern science. In an introductory course on quantum physics, one learns the fundamental axioms that define and characterize the theory. All but one of these axioms are physical requirements. For example, the energy spectrum is required to be real because all measurements of the energy of a system yield real results. Another axiom requires that the energy spectrum be bounded below so that the system has a stable lowest-energy state. Yet another axiom requires that the time evolution of a quantum system be *unitary* (probability-conserving) because the expected result of a probability measurement of a state cannot grow or decay in time. A quantum theory of elementary particles must also satisfy the physical axioms of Lorentz covariance and causality. However, there is one axiom that stands out because it is mathematical rather than physical in character, and this is the requirement that the Hamiltonian  $H$ , which is the operator that expresses the dynamics of the quantum system, be Hermitian.

The requirement that  $H$  be Hermitian dates back to the early days of quantum mechanics. The Hermiticity of  $H$  is expressed by the equation

$$H = H^\dagger, \quad (1)$$

where the Dirac Hermitian conjugation symbol  $\dagger$  represents the combined operations of matrix transposition and complex conjugation. The mathematical symmetry condition (1) is physically obscure but very convenient because it implies that the eigenvalues of  $H$  are real and that the time-evolution operator  $e^{-iHt}$  is unitary.

Hamiltonians that are non-Hermitian have traditionally been used to describe dissipative processes, such as the phenomenon of radioactive decay. However, these non-Hermitian Hamiltonians are only approximate, phenomenological descriptions of physical processes. They cannot be regarded as fundamental because they violate the requirement of unitarity. A non-Hermitian Hamiltonian whose purpose is to describe a particle that undergoes radioactive decay predicts that the probability of finding the particle gradually decreases in time. Of course, a particle cannot just disappear because this would violate the conservation of probability; rather, the particle transforms into other particles. Thus, a non-Hermitian Hamiltonian that describes radioactive decay can at best be a simplified, phenomenological, and *non-fundamental* description of the decay process because it ignores the precise nature of the decay products. In his book on quantum field theory Barton gives the standard reasons for why a non-Hermitian Hamiltonian cannot provide a fundamental description of nature [1]: ‘A non-Hermitian Hamiltonian is unacceptable partly because it may lead to complex energy eigenvalues, but chiefly because it implies a non-unitary S matrix, which fails to conserve probability and makes a hash of the physical interpretation.’

The purpose of this paper is to describe at an elementary level the breakthroughs that have been made in the past decade which show that while the symmetry condition (1) is sufficient to guarantee that the energy spectrum is real and that time evolution is unitary, the condition of Dirac Hermiticity is *not necessary*. It is possible to describe natural processes by means of non-Hermitian Hamiltonians. We will show that the Hermiticity requirement (1) may be replaced by the analogous but physically transparent condition of space–time reflection symmetry ( $\mathcal{PT}$  symmetry)

$$H = H^{\mathcal{PT}} \quad (2)$$

without violating any of the physical axioms of quantum mechanics. If  $H$  satisfies (2), it is said to be  $\mathcal{PT}$  symmetric. This paper is an update of an earlier, shorter and more elementary review paper [2].

The notation used in this paper is as follows: the space-reflection operator, or *parity* operator, is represented by the symbol  $\mathcal{P}$ . The effect of  $\mathcal{P}$  on the quantum-mechanical coordinate operator  $\hat{x}$  and the momentum operator  $\hat{p}$  is to change their signs:

$$\mathcal{P}\hat{x}\mathcal{P} = -\hat{x} \quad \text{and} \quad \mathcal{P}\hat{p}\mathcal{P} = -\hat{p}. \tag{3}$$

Note that  $\mathcal{P}$  is a linear operator and that it leaves invariant the fundamental commutation relation (the Heisenberg algebra) of quantum mechanics,

$$\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \mathbf{1}, \tag{4}$$

where  $\mathbf{1}$  is the identity matrix. The time-reversal operator is represented by the symbol  $\mathcal{T}$ . This operator leaves  $\hat{x}$  invariant but changes the sign of  $\hat{p}$ :

$$\mathcal{T}\hat{x}\mathcal{T} = \hat{x} \quad \text{and} \quad \mathcal{T}\hat{p}\mathcal{T} = -\hat{p}. \tag{5}$$

Like the parity operator  $\mathcal{P}$ , the time-reversal operator  $\mathcal{T}$  leaves the commutation relation (4) invariant, but this requires that  $\mathcal{T}$  reverse the sign of the complex number  $i$ :

$$\mathcal{T}i\mathcal{T} = -i. \tag{6}$$

Equation (6) demonstrates that  $\mathcal{T}$  is not a linear operator;  $\mathcal{T}$  is said to be *antilinear*. Also, since  $\mathcal{P}$  and  $\mathcal{T}$  are reflection operators, their squares are the unit operator:

$$\mathcal{P}^2 = \mathcal{T}^2 = \mathbf{1}. \tag{7}$$

Finally, the  $\mathcal{P}$  and  $\mathcal{T}$  operators commute:

$$\mathcal{P}\mathcal{T} - \mathcal{T}\mathcal{P} = 0. \tag{8}$$

In terms of the  $\mathcal{P}$  and  $\mathcal{T}$  operators, we define the  $\mathcal{PT}$ -reflected Hamiltonian  $H^{\mathcal{PT}}$  in (2) as  $H^{\mathcal{PT}} \equiv (\mathcal{P}\mathcal{T})H(\mathcal{P}\mathcal{T})$ . Thus, if a Hamiltonian is  $\mathcal{PT}$  symmetric [that is, if it satisfies (2)], then the  $\mathcal{PT}$  operator commutes with  $H$ :

$$H(\mathcal{P}\mathcal{T}) - (\mathcal{P}\mathcal{T})H = 0. \tag{9}$$

A  $\mathcal{PT}$ -symmetric Hamiltonian need not be Hermitian; that is, it need not satisfy the Hermiticity symmetry condition (1). Thus, it is possible to have a fully consistent quantum theory whose dynamics is described by a non-Hermitian Hamiltonian. Some examples of such non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians are

$$H = \hat{p}^2 + i\hat{x}^3, \tag{10}$$

and

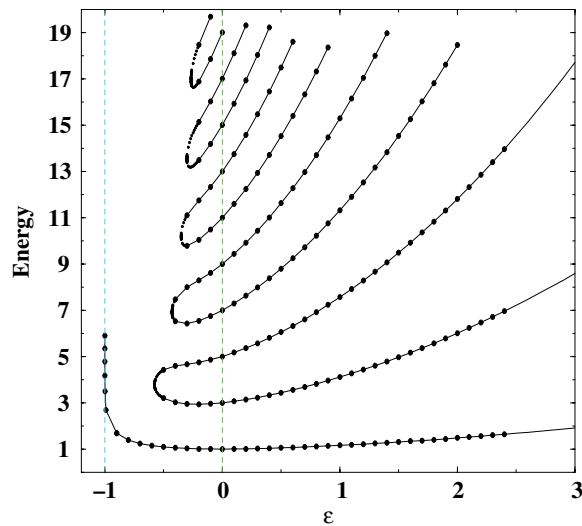
$$H = \hat{p}^2 - \hat{x}^4. \tag{11}$$

It is amazing indeed that the eigenvalues of these strange-looking Hamiltonians are all real and positive and that these two Hamiltonians specify a unitary time evolution even though they are non-Hermitian.

The Hamiltonians in (10) and (11) are special cases of the general parametric family of  $\mathcal{PT}$ -symmetric Hamiltonians

$$H = \hat{p}^2 + \hat{x}^2(i\hat{x})^\epsilon, \tag{12}$$

where the parameter  $\epsilon$  is real. These Hamiltonians are all  $\mathcal{PT}$  symmetric because they satisfy the condition in (2). It was shown in 1998 that when  $\epsilon \geq 0$  all of the eigenvalues of these Hamiltonians are entirely real and positive, but when  $\epsilon < 0$  there are complex eigenvalues [3]. We say that  $\epsilon \geq 0$  is the parametric region of *unbroken*  $\mathcal{PT}$  symmetry and that  $\epsilon < 0$  is the parametric region of *broken*  $\mathcal{PT}$  symmetry. (See figure 1.)



**Figure 1.** Energy levels of the Hamiltonian  $H = \hat{p}^2 + \hat{x}^2(i\hat{x})^\epsilon$  as a function of the real parameter  $\epsilon$ . There are three regions: when  $\epsilon \geq 0$ , the spectrum is real and positive and the energy levels rise with increasing  $\epsilon$ . The lower bound of this region,  $\epsilon = 0$ , corresponds to the harmonic oscillator, whose energy levels are  $E_n = 2n + 1$ . When  $-1 < \epsilon < 0$ , there are a finite number of real positive eigenvalues and an infinite number of complex-conjugate pairs of eigenvalues. As  $\epsilon$  decreases from 0 to  $-1$ , the number of real eigenvalues decreases; when  $\epsilon \leq -0.57793$ , the only real eigenvalue is the ground-state energy. As  $\epsilon$  approaches  $-1^+$ , the ground-state energy diverges. For  $\epsilon \leq -1$  there are no real eigenvalues. When  $\epsilon \geq 0$ , the  $\mathcal{PT}$  symmetry is unbroken, but when  $\epsilon < 0$  the  $\mathcal{PT}$  symmetry is broken.

One can think of the non-Hermitian Hamiltonians in (12) as complex extensions of the harmonic-oscillator Hamiltonian  $H = \hat{p}^2 + \hat{x}^2$ . Indeed, the quantum theories defined by  $H$  are complex extensions of the conventional quantum theory of the harmonic oscillator into the complex domain. The general constructive principle that we are using in (12) is to start with a Hamiltonian that is *both* Hermitian and  $\mathcal{PT}$  symmetric. One then introduces a real parameter  $\epsilon$  in such a way that as  $\epsilon$  increases from 0 the Hamiltonian is no longer Hermitian but its  $\mathcal{PT}$  symmetry is maintained. One need not start with the harmonic oscillator. One can, for example, begin with any of the Hermitian Hamiltonians  $H = \hat{p}^2 + \hat{x}^{2N}$ , where  $N = 1, 2, 3, \dots$ , and introduce the parameter  $\epsilon$  as follows:  $H = \hat{p}^2 + \hat{x}^{2N}(i\hat{x})^\epsilon$ . (The Hamiltonian in (12) is just the special case  $N = 1$ .) The properties of these Hamiltonians are discussed in [4].

We emphasize that these new kinds of Hamiltonians define valid and consistent quantum theories in which the mathematical condition of Dirac Hermiticity  $H = H^\dagger$  has been replaced by the physical condition of  $\mathcal{PT}$  symmetry,  $H = H^{\mathcal{PT}}$ . The condition in (2) that the Hamiltonian is  $\mathcal{PT}$  symmetric is a physical condition because  $\mathcal{P}$  and  $\mathcal{T}$  are elements of the homogeneous Lorentz group of spatial rotations and Lorentz boosts. The real Lorentz group consists of four disconnected parts [5]. (i) The first part, called the *proper orthochronous Lorentz group*, is a subgroup of the Lorentz group whose elements are continuously connected to the identity. (ii) The second part consists of all of the elements of the proper orthochronous Lorentz group multiplied by the parity operator  $\mathcal{P}$ . (iii) The third part consists of all of the elements of the proper orthochronous Lorentz group multiplied by the time-reversal operator  $\mathcal{T}$ . (iv) The fourth part consists of all of the elements of the proper orthochronous Lorentz group

multiplied by  $\mathcal{PT}$ . Note that parts (ii)–(iv) are not subgroups of the Lorentz group because they do not contain the identity element. These four parts of the Lorentz group are disconnected because there is no continuous path in group space from one part to another.

When we say that Lorentz invariance is a physical requirement of a theory, what we really mean is that the theory must be invariant under Lorentz transformations belonging to the proper, orthochronous Lorentz group. We know that the physical world is *not* invariant under the full homogeneous Lorentz group because it has been demonstrated experimentally that there exist weak processes that do not respect parity symmetry and other weak processes that do not respect time-reversal symmetry.

One can extend the real Lorentz group to the *complex* Lorentz group [5]. (To perform this extension it is necessary to make the crucial assumption that the eigenvalues of the Hamiltonian are real and bounded below.) The complex Lorentz group consists of *two* and not four disconnected parts. In the complex Lorentz group there exists a continuous path in group space from the elements of the real proper, orthochronous Lorentz group to the elements of part (iv) of the real Lorentz group. There also exists a continuous path in group space from the elements of part (ii) to the elements of part (iii) of the real Lorentz group. Thus, while we know that the world is not invariant under  $\mathcal{P}$  reflection or under  $\mathcal{T}$  reflection, we are proposing here to consider the possibility suggested by complex group analysis that a fundamental discrete symmetry of the world is  $\mathcal{PT}$  symmetry, or space–time reflection symmetry.

The most important consequence of the discovery that non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians can define acceptable theories of quantum mechanics is that we now can construct many new kinds of Hamiltonians that only a decade ago would have been rejected as being unphysical because they violate the axiom of Hermiticity. In this paper we will examine some of these new Hamiltonians and discuss the properties and possible physical implications of the theories defined by these Hamiltonians. So far, there have been no experiments that prove clearly and definitively that quantum systems defined by non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians do exist in nature. However, one should keep an open mind regarding the kinds of theories that one is willing to consider. Indeed, Gell-Mann’s ‘totalitarian principle’ states that among all possible physical theories ‘Everything which is not forbidden is compulsory.’

### 1.1. Presentation and scope of this paper

Like many research areas in science, the study of non-Hermitian Hamiltonians having real spectra began in a haphazard and diffuse fashion. There are numerous early examples of isolated and disconnected discoveries of such non-Hermitian Hamiltonians. For example, in 1980 Caliceti *et al*, who 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 selfinteraction term are real [6]. In the summer of 1993, when I was visiting CEN Saclay, I learned that Bessis and Zinn-Justin had noticed on the basis of numerical work that some of the eigenvalues of the cubic Hamiltonian in (10) seemed to be real, and they wondered if the spectrum might be entirely real [7]. (Their interest in the Hamiltonian (10) was piqued by the Lee–Yang edge singularity.) In 1982 Andrianov, who was doing perturbative studies of  $-x^4$  potentials, found evidence that such theories might have real eigenvalues [8]. In 1992 Hollowood [9] and Scholtz *et al* [10] discovered in their own areas of research surprising examples of non-Hermitian Hamiltonians having real spectra. The latter paper gave a comprehensive mathematical analysis of quasi-Hermitian operators having real eigenvalues.



The field of  $\mathcal{PT}$ -symmetric quantum mechanics was established in 1998 with the discovery by Bender and Boettcher that the numerical conjectures of Bessis and Zinn-Justin were not only valid, but were just one instance of a huge class of non-Hermitian Schrödinger eigenvalue problems whose spectra are entirely real and positive [3]. Bender and Boettcher showed that the reality of the spectra was due to a symmetry principle, namely the condition of an unbroken space–time reflection symmetry, and they argued that this symmetry principle could replace the usual requirement of Dirac Hermiticity.

This discovery by Bender and Boettcher relies on two essential mathematical ingredients. First, Bender and Boettcher used the techniques of analytic continuation of eigenvalue problems. These fundamental techniques were developed and used heavily in the early work of Bender and Wu on divergent perturbation series [11, 12] and were later used by Bender and Turbinger [13]. These techniques are crucial because they show how to analytically continue the boundary conditions of an eigenvalue problem as a function of a parameter in the Hamiltonian. Second, Bender and Boettcher used the delta-expansion techniques that had been discovered and developed by Bender *et al* [14] as a way to avoid divergent perturbation series. The delta expansion is a powerful perturbation-theory technique in which the small perturbation parameter is a measure of the nonlinearity of the problem. As a result, many crucial properties of the problem are exactly preserved as this parameter varies. In the case of  $\mathcal{PT}$ -symmetric quantum mechanics, it is the reality of the eigenvalues that is exactly maintained as the perturbation parameter  $\epsilon$  in (12) is varied.

Many researchers have contributed immensely to the development of  $\mathcal{PT}$ -symmetric quantum mechanics by discovering new examples and models, proving theorems and performing numerical and asymptotic analysis. In the past few years a large and active research community has developed and there have been half a dozen international conferences on the subject of  $\mathcal{PT}$  symmetry, pseudo-Hermiticity and non-Hermitian Hamiltonians. The proceedings of these conferences provide a complete source of references [15–20]. By now, there have been so many contributions to the field that it is impossible to describe them all in this one paper.

The purpose of this paper is to give an elementary introduction to this exciting and active field of research. In writing this paper, my hope is that the rate of new discoveries and the development of the field will continue at such a rapid pace that this review will soon become obsolete.

## 1.2. Organization of this paper

In section 2 we show that  $\mathcal{PT}$ -symmetric Hamiltonians are complex extensions of Hermitian Hamiltonians and we discuss the key property of  $\mathcal{PT}$ -symmetric Hamiltonians, namely, that their energy eigenvalues are real and bounded below. We discuss techniques for calculating eigenvalues. In section 3 we discuss classical  $\mathcal{PT}$ -symmetric Hamiltonians and show how to continue ordinary classical mechanics into the complex domain. The crucial theoretical questions of conservation of probability and unitary time evolution are addressed in section 4. In section 5 we illustrate the theory of  $\mathcal{PT}$ -symmetric quantum mechanics by using a simple  $2 \times 2$  matrix Hamiltonian. Then in section 6 we explain how to calculate the  $\mathcal{C}$  operator, which is the central pillar of  $\mathcal{PT}$  symmetry and which is needed to construct the Hilbert space for the theory. In the following two sections we discuss the many applications of  $\mathcal{PT}$ -symmetric quantum theory. We discuss quantum-mechanical applications in section 7 and quantum-field-theoretic applications in section 8. Finally, in section 9 we make some brief concluding remarks.

## 2. Determining the eigenvalues of a $\mathcal{PT}$ -symmetric Hamiltonian

In this section we show how to calculate the eigenvalues of a  $\mathcal{PT}$ -symmetric Hamiltonian. We begin by pointing out that the Hamiltonian operator defines and determines the physical properties of a quantum theory in three important ways.

- (i) *The Hamiltonian determines the energy levels of the quantum theory.* To find these energy levels one must solve the time-independent Schrödinger eigenvalue problem

$$H\psi = E\psi. \quad (13)$$

This equation usually takes the form of a differential equation that must be solved subject to boundary conditions on the eigenfunction  $\psi$ . In the case of a  $\mathcal{PT}$ -symmetric Hamiltonian it is crucial that the boundary conditions be imposed properly. We emphasize that for a quantum theory to be physically acceptable the energy eigenvalues of the Hamiltonian must be real and bounded below.

- (ii) *The Hamiltonian specifies the time evolution of the states and operators of the quantum theory.* To determine the time evolution of a state  $\psi(t)$  in the Schrödinger picture we must solve the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(t) = H\psi(t). \quad (14)$$

The solution to this first-order differential equation is straightforward because  $H$  is assumed to be independent of time:

$$\psi(t) = e^{-iHt}\psi(0). \quad (15)$$

We call  $e^{-iHt}$  the *time-evolution operator*. In conventional quantum mechanics the time-evolution operator is unitary because the Hamiltonian  $H$  is Hermitian. As a result, the norm of the state  $\psi(t)$  remains constant in time. The constancy of the norm is an essential feature of a quantum system because the norm of a state is a probability, and this probability must remain constant in time. If this probability were to grow or decay in time, we would say that the theory violates unitarity. In  $\mathcal{PT}$ -symmetric quantum mechanics  $H$  is not Dirac Hermitian, but the norms of states are still time independent.

- (iii) *The Hamiltonian incorporates the symmetries of the theory.* As an example, suppose that the Hamiltonian  $H$  commutes with the parity operator  $\mathcal{P}$ . We then say that the Hamiltonian is *parity invariant*. Since  $\mathcal{P}$  is a linear operator, we know that the eigenstates of the Hamiltonian (the solutions to (13)) will also be eigenstates of  $\mathcal{P}$ . Thus, the eigenstates of  $H$  will have a definite parity; they will be either even or odd under space reflection. (Of course, a general state, which is a linear combination of the eigenstates of  $H$ , need not have definite parity.)

### 2.1. Broken and unbroken $\mathcal{PT}$ symmetry

For the case of a  $\mathcal{PT}$ -symmetric Hamiltonian, the  $\mathcal{PT}$  operator commutes with the Hamiltonian  $H$  (see (9)). However,  $\mathcal{PT}$  symmetry is more subtle than parity symmetry because the  $\mathcal{PT}$  operator is not linear. Because  $\mathcal{PT}$  is not linear, the eigenstates of  $H$  may or may not be eigenstates of  $\mathcal{PT}$ .

Let us see what may go wrong if we assume that an eigenstate  $\psi$  of the Hamiltonian  $H$  is also an eigenstate of the  $\mathcal{PT}$  operator. Call the eigenvalue  $\lambda$  and express the eigenvalue condition as

$$\mathcal{PT}\psi = \lambda\psi. \quad (16)$$

Multiply (16) by  $\mathcal{PT}$  on the left and use the property that  $(\mathcal{PT})^2 = \mathbf{1}$  (see (7) and (8)):

$$\psi = (\mathcal{PT})\lambda(\mathcal{PT})^2\psi. \quad (17)$$

Since  $\mathcal{T}$  is antilinear [see (6)], we get

$$\psi = \lambda^*\lambda\psi = |\lambda|^2\psi. \quad (18)$$

Thus,  $|\lambda|^2 = 1$  and the eigenvalue  $\lambda$  of the  $\mathcal{PT}$  operator is a pure phase:

$$\lambda = e^{i\alpha}. \quad (19)$$

Next, multiply the eigenvalue equation (13) by  $\mathcal{PT}$  on the left and again use the property that  $(\mathcal{PT})^2 = \mathbf{1}$ :

$$(\mathcal{PT})H\psi = (\mathcal{PT})E(\mathcal{PT})^2\psi. \quad (20)$$

Using the eigenvalue equation (16) and recalling that  $\mathcal{PT}$  commutes with  $H$ , we get

$$H\lambda\psi = (\mathcal{PT})E(\mathcal{PT})\lambda\psi. \quad (21)$$

Finally, we again use the property that  $\mathcal{T}$  is antilinear to obtain

$$E\lambda\psi = E^*\lambda\psi. \quad (22)$$

Since  $\lambda$  is non-zero (see (19)), we conclude that the eigenvalue  $E$  is real:  $E = E^*$ .

In general, this conclusion is false, as figure 1 clearly demonstrates. When  $\epsilon < 0$ , some of the eigenvalues have disappeared because they are complex. On the other hand, for the restricted region  $\epsilon \geq 0$  this conclusion is correct; all of the eigenvalues are indeed real. We are then led to make the following definition: if every eigenfunction of a  $\mathcal{PT}$ -symmetric Hamiltonian is also an eigenfunction of the  $\mathcal{PT}$  operator, we say that the  $\mathcal{PT}$  symmetry of  $H$  is *unbroken*. Conversely, if some of the eigenfunctions of a  $\mathcal{PT}$ -symmetric Hamiltonian are not simultaneously eigenfunctions of the  $\mathcal{PT}$  operator, we say that the  $\mathcal{PT}$  symmetry of  $H$  is *broken*.

The correct way to interpret (22) is that if a Hamiltonian has an unbroken  $\mathcal{PT}$  symmetry, then all of its eigenvalues are real. Thus, to establish that the eigenvalues of a particular  $\mathcal{PT}$ -symmetric Hamiltonian are real, it is necessary to prove that the  $\mathcal{PT}$  symmetry of  $H$  is unbroken. This is difficult to show, and it took several years after the discovery of the family of  $\mathcal{PT}$ -symmetric Hamiltonians in (12) before a complete and rigorous proof was finally constructed by Dorey *et al* in 2001 [21, 22].<sup>2</sup> Many others have contributed to the rigorous mathematical development of the theory of  $\mathcal{PT}$  symmetry. These include Shin [27], Pham [28], Delabaere [29], Trinh [30], Weigert [31, 33], Davies [34], Ralston [35] and Scholtz and Geyer [36]. Mostafazadeh generalized  $\mathcal{PT}$  symmetry to pseudo-Hermiticity (see section 4.5). See also [37].

## 2.2. Boundary conditions for the Schrödinger eigenvalue problem

Our objective in this section is to show how to calculate the eigenvalues of the Schrödinger eigenvalue problem (13). The most direct approach is to write (13) as a differential equation in coordinate space. The principal conceptual difficulty that we face in solving this differential equation is in identifying and understanding the boundary conditions on the coordinate-space eigenfunctions.

<sup>2</sup> The proof by Dorey *et al* draws from many areas of theoretical and mathematical physics and uses spectral determinants, the Bethe ansatz, the Baxter  $T$ - $Q$  relation, the monodromy group, and an array of techniques used in conformal quantum field theory. This proof is too technical to be described in this paper, but it is a significant advance because it establishes a correspondence between ordinary differential equations and integrable models. This correspondence is known as the *ODE-IM correspondence* [23–26].

To write (13) in coordinate space, we make the standard transcriptions

$$\hat{x} \rightarrow x \quad \text{and} \quad \hat{p} \rightarrow -i \frac{d}{dx}, \tag{23}$$

except that we treat the variable  $x$  as complex. The Schrödinger eigenvalue problem (13) then takes the form

$$-\psi''(x) + x^2(ix)^\epsilon \psi(x) = E\psi(x). \tag{24}$$

Although we cannot solve this equation exactly for arbitrary  $\epsilon$ , we can easily find the possible asymptotic behaviours of its solutions by using the WKB approximation. In general, for any differential equation of the form  $-y''(x) + V(x)y(x) = 0$ , where  $V(x)$  is a function that grows as  $|x| \rightarrow \infty$ , we know that the exponential component of the asymptotic behaviour of  $y(x)$  for large  $|x|$  has the form

$$y(x) \sim \exp \left[ \pm \int^x ds \sqrt{V(s)} \right]. \tag{25}$$

To identify the appropriate boundary conditions to impose on  $\psi(x)$ , we consider first the Hermitian case  $\epsilon = 0$  (the harmonic oscillator). From (25) we can see immediately that the possible asymptotic behaviours of solutions are  $\psi(x) \sim \exp(\pm \frac{1}{2}x^2)$ . The usual requirement that the eigenfunction be square-integrable implies that we must choose the negative sign in the exponent, and therefore the eigenfunctions are Gaussian-like for large  $|x|$ . This result extends into the complex- $x$  plane: If the eigenfunctions vanish exponentially on the real- $x$  axis for large  $|x|$ , they must also vanish in two wedges of opening angle  $\frac{1}{2}\pi$  in the complex plane centered about the positive-real and negative-real axes. These wedges are called *Stokes wedges* [32].

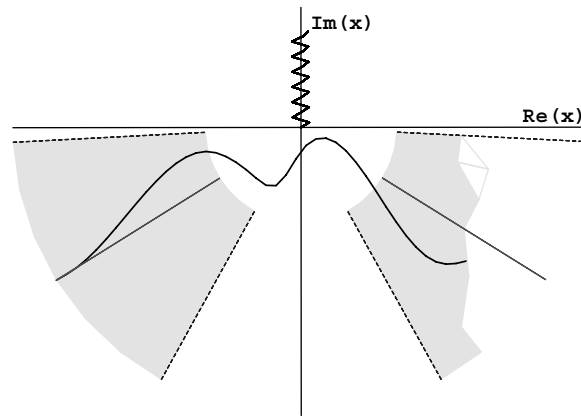
What happens as  $\epsilon$  increases from 0? As soon as  $\epsilon > 0$  ( $\epsilon$  non-integer), a logarithmic branch point appears at the origin  $x = 0$ . Without loss of generality, we may choose the branch cut to run up the imaginary axis from  $x = 0$  to  $x = i\infty$ . In this cut plane the solutions to the differential equation (24) are single-valued. From the asymptotic behaviour of  $\psi(x)$  in (25), we deduce that the Stokes wedges rotate downward into the complex- $x$  plane and that the opening angles of the wedges decrease as  $\epsilon$  increases.

There are many wedges in which  $\psi(x) \rightarrow 0$  as  $|x| \rightarrow \infty$ . Thus, there are many eigenvalue problems associated with the differential equation (24). We choose to continue the eigenvalue differential equation (24) smoothly away from the location of the harmonic-oscillator wedges at  $\epsilon = 0$ . (A detailed description of how to extend eigenvalue equations into the complex plane may be found in [13].) For  $\epsilon > 0$  the centre lines of the left and right wedges lie at the angles

$$\theta_{\text{left}} = -\pi + \frac{\epsilon}{\epsilon + 4} \frac{\pi}{2} \quad \text{and} \quad \theta_{\text{right}} = -\frac{\epsilon}{\epsilon + 4} \frac{\pi}{2}. \tag{26}$$

The opening angle of each of these wedges is  $\Delta = 2\pi/(\epsilon + 4)$ . The differential equation (24) may be integrated along any path in the complex- $x$  plane as long as the ends of the path approach complex infinity inside the left wedge and the right wedge. Note that these wedges contain the real- $x$  axis when  $-1 < \epsilon < 2$ . However, as soon as  $\epsilon$  is larger than 2, the wedges rotate below the real- $x$  axis. These wedges are shown in figure 2.

Notice that the wedges in figure 2 are mirror images of one another if they are reflected through the imaginary- $x$  axis. This left–right symmetry is the coordinate-space realization of  $\mathcal{PT}$  symmetry. If we choose any point  $x$  in the complex- $x$  plane and perform a parity reflection, then  $x \rightarrow -x$ . Time reversal replaces  $i$  by  $-i$  as we saw in (6), and so  $\mathcal{T}$  replaces  $-x$  by its



**Figure 2.** Stokes wedges in the complex- $x$  plane containing the contour on which the eigenvalue problem for the differential equation (24) for  $\epsilon = 2.2$  is posed. In these wedges  $\psi(x)$  vanishes exponentially as  $|x| \rightarrow \infty$ . The eigenfunction  $\psi(x)$  vanishes most rapidly at the centres of the wedges.

complex conjugate  $-x^*$ . Thus, in the coordinate representation  $\mathcal{PT}$  symmetry is left–right symmetry.

### 2.3. The flaw in Dyson’s argument

The quantum theories that we are considering in this paper are obtained by extending real quantum mechanics into the complex domain, as explained in section 2.2. The notion of analytically continuing a Hamiltonian into the complex plane was first discussed in 1952 by Dyson, who argued heuristically that perturbation theory for quantum electrodynamics diverges [38]. Dyson’s argument consists of rotating the electric charge  $e$  into the complex- $e$  plane:  $e \rightarrow ie$ . Applied to the standard quantum anharmonic-oscillator Hamiltonian  $H = \hat{p}^2 + g\hat{x}^4$ , Dyson’s argument goes as follows: rotate the parameter  $g$  anticlockwise in the complex- $g$  plane from positive  $g$  to  $-g$ . Now, the potential term in the Hamiltonian is *no longer bounded below*, so the resulting theory has no ground state. Hence, the ground-state energy  $E_0(g)$  has an abrupt transition at  $g = 0$ , which implies that  $E_0(g)$  must have a singularity at  $g = 0$ .

Following Dyson’s reasoning, one would think that the spectrum of the Hamiltonian (11), which is obtained by setting  $\epsilon = 2$  in (12), would not be bounded below, and one might conclude that this Hamiltonian is mathematically and physically unacceptable. However, this heuristic argument is flawed. While the ground-state energy of the quantum anharmonic oscillator does indeed have a singularity at  $g = 0$ , the spectrum of the Hamiltonian (11) that is obtained by analytically continuing a parameter in the Hamiltonian remains ambiguous until the boundary conditions satisfied by the eigenfunctions are specified. The term ‘bounded below’ is inappropriate if it relies on an ordering relation applied to a complex potential because ordering relations cannot be used for complex numbers. The concern that the spectrum of  $H$  in (11) is not bounded below is unfounded because  $\mathcal{PT}$ -symmetric boundary conditions on the Schrödinger equation (24) prohibit the occurrence of negative eigenvalues.

The eigenvalues of  $H$  in (11) depend crucially on the history of how this negative-coupling-constant Hamiltonian constant is obtained. There are two different ways to obtain  $H$  in (11): First, one can substitute  $g = |g|e^{i\theta}$  into  $H = \hat{p}^2 + g\hat{x}^4$  and rotate from  $\theta = 0$  to  $\theta = \pi$ .

Under this rotation, the ground-state energy  $E_0(g)$  becomes complex. Clearly,  $E_0(g)$  is real and positive when  $g > 0$  and complex when  $g < 0$ .<sup>3</sup> Second, one can obtain (11) as a limit of the Hamiltonian  $H$  in (12) as  $\epsilon : 0 \rightarrow 2$ . The spectrum of this complex Hamiltonian is real, positive and discrete, as is shown in figure 1.

How can the Hamiltonian (11) possess two such astonishingly different spectra? The answer lies in the boundary conditions satisfied by the eigenfunctions  $\psi(x)$ . In the first case, in which  $\theta = \arg g$  is rotated in the complex- $g$  plane from 0 to  $\pi$ ,  $\psi(x)$  vanishes in the complex- $x$  plane as  $|x| \rightarrow \infty$  inside the wedges  $-\pi/3 < \arg x < 0$  and  $-4\pi/3 < \arg x < -\pi$ . *These wedges are not  $\mathcal{PT}$ -symmetric reflections of one another.* In the second case, in which the exponent  $\epsilon$  ranges from 0 to 2,  $\psi(x)$  vanishes in the complex- $x$  plane as  $|x| \rightarrow \infty$  inside the  $\mathcal{PT}$ -symmetric pair of wedges  $-\pi/3 < \arg x < 0$  and  $-\pi < \arg x < -2\pi/3$ . We emphasize that in this second case the boundary conditions hold in wedges that are symmetric with respect to the imaginary axis; these boundary conditions enforce the  $\mathcal{PT}$  symmetry of  $H$  and are responsible for the reality of the energy spectrum.

*Illustrative example:* The harmonic oscillator Hamiltonian

$$H = \hat{p}^2 + \omega^2 \hat{x}^2 \quad (\omega > 0) \tag{27}$$

is an elementary model that illustrates the dependence of the eigenvalues on the boundary conditions imposed on the eigenfunctions. Let us assume that the eigenfunctions of  $H$  vanish on the real- $x$  axis as  $x \rightarrow \pm\infty$ . The eigenfunctions have the form of a Gaussian  $\exp(-\frac{1}{2}\omega x^2)$  multiplied by a Hermite polynomial. Thus, the Stokes wedges are centred about the positive-real- $x$  axis and have angular opening  $\frac{1}{2}\pi$ . The eigenvalues  $E_n$  are given exactly by the formula

$$E_n = (n + \frac{1}{2}) \omega \quad (n = 0, 1, 2, 3, \dots). \tag{28}$$

Now suppose that the parameter  $\omega$  is rotated by  $180^\circ$  into the complex- $\omega$  plane from the positive axis to the negative axis so that  $\omega$  is replaced by  $-\omega$ . This causes the Stokes wedges in the complex- $x$  plane to rotate by  $90^\circ$  so that the eigenfunctions now vanish exponentially on the imaginary- $x$  axis rather than on the real- $x$  axis. Also, as a consequence of this rotation, the *eigenvalues change sign*:

$$E_n = -(n + \frac{1}{2}) \omega \quad (n = 0, 1, 2, 3, \dots). \tag{29}$$

Notice that under the rotation that replaces  $\omega$  by  $-\omega$  the Hamiltonian remains invariant, and yet the signs of the eigenvalues are reversed! This shows that the eigenspectrum depends crucially on the boundary conditions that are imposed on the eigenfunctions.

Apart from the eigenvalues, there is yet another striking difference between the two theories corresponding to  $H$  in (11). The expectation value of the operator  $\hat{x}$  in the ground-state eigenfunction  $\psi_0(x)$  is given by

$$\frac{\langle 0|x|0\rangle}{\langle 0|0\rangle} \equiv \frac{\int_C dx x \psi_0^2(x)}{\int_C dx \psi_0^2(x)}, \tag{30}$$

where  $C$  is a complex contour that lies in the asymptotic wedges described above. The value of  $\langle 0|x|0\rangle/\langle 0|0\rangle$  for  $H$  in (11) depends on the limiting process by which we obtain  $H$ . If we

<sup>3</sup> Rotating from  $\theta = 0$  to  $\theta = -\pi$ , we obtain the same Hamiltonian as in (11), but the spectrum is the complex conjugate of the spectrum obtained when we rotate from  $\theta = 0$  to  $\theta = \pi$ .

substitute  $g = g_0 e^{i\theta}$  into the Hamiltonian  $H = \hat{p}^2 + g\hat{x}^4$  and rotate  $g$  from  $\theta = 0$  to  $\theta = \pi$ , we find by an elementary symmetry argument that this expectation value vanishes for all  $g$  on the semicircle in the complex- $g$  plane. The expectation value vanishes because this rotation in the complex- $g$  plane preserves parity symmetry ( $x \rightarrow -x$ ). However, if we define  $H$  in (11) by using the Hamiltonian in (12) and by allowing  $\epsilon$  to range from 0 to 2, we find that this expectation value is non-zero. In fact, this expectation value is non-vanishing for all  $\epsilon > 0$ . On this alternate path  $\mathcal{PT}$  symmetry (reflection about the imaginary axis,  $x \rightarrow -x^*$ ) is preserved, but parity symmetry is permanently broken. (We suggest in section 8.4 that, as a consequence of broken parity symmetry, one might be able to describe the dynamics of the Higgs sector by using a  $\mathcal{PT}$ -symmetric  $-g\varphi^4$  quantum field theory.)

2.4. Using WKB phase-integral techniques to calculate eigenvalues

Now that we have identified the boundary conditions to be imposed on the eigenfunctions of the  $\mathcal{PT}$ -symmetric Hamiltonian (12), we can use a variety of techniques to calculate the eigenvalues of this Hamiltonian. Not surprisingly, it is impossible to solve the differential-equation eigenvalue problem (24) analytically and in closed form except in two special cases, namely, for  $\epsilon = 0$  (the harmonic oscillator) and for  $\epsilon \rightarrow \infty$  (the  $\mathcal{PT}$ -symmetric version of the square-well potential, whose solution is given in [39]). Thus, it is necessary to use approximate analytic or numerical methods.

The simplest analytic approach uses WKB theory, which gives an excellent approximation to the eigenvalues when  $\epsilon > 0$ . The WKB calculation is interesting because it must be performed in the complex plane rather than on the real- $x$  axis. The turning points  $x_{\pm}$  are those roots of  $E = x^2(ix)^{\epsilon}$  that *analytically continue* off the real axis as  $\epsilon$  increases from 0. These turning points,

$$x_- = E^{\frac{1}{\epsilon+2}} e^{i\pi(\frac{3}{2} - \frac{1}{\epsilon+2})}, \quad x_+ = E^{\frac{1}{\epsilon+2}} e^{-i\pi(\frac{1}{2} - \frac{1}{\epsilon+2})}, \tag{31}$$

lie in the lower-half (upper-half)  $x$  plane in figure 2 when  $\epsilon > 0$  ( $\epsilon < 0$ ).

The leading-order WKB phase-integral quantization condition is given by

$$(n + 1/2)\pi = \int_{x_-}^{x_+} dx \sqrt{E - x^2(ix)^{\epsilon}}. \tag{32}$$

When  $\epsilon > 0$  this path lies entirely in the lower-half  $x$  plane, and when  $\epsilon = 0$  (the case of the harmonic oscillator) the path lies on the real axis. However, when  $\epsilon < 0$  the path lies in the upper-half  $x$  plane and crosses the cut on the positive imaginary- $x$  axis. In this case there is no *continuous path joining the turning points*. Hence, WKB fails when  $\epsilon < 0$ .

When  $\epsilon \geq 0$ , we deform the phase-integral contour so that it follows the rays from  $x_-$  to 0 and from 0 to  $x_+$ :

$$(n + \frac{1}{2})\pi = 2 \sin\left(\frac{\pi}{\epsilon + 2}\right) E^{\frac{1}{\epsilon+2} + \frac{1}{2}} \int_0^1 ds \sqrt{1 - s^{\epsilon+2}}. \tag{33}$$

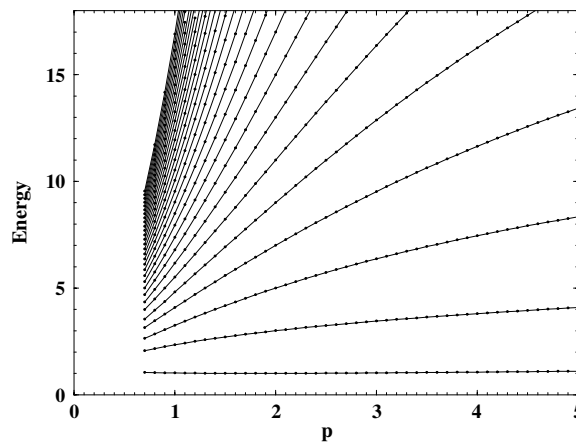
We then solve for  $E_n$ :

$$E_n \sim \left[ \frac{\Gamma\left(\frac{3}{2} + \frac{1}{\epsilon + 2}\right) \sqrt{\pi} \left(n + \frac{1}{2}\right)}{\sin\left(\frac{\pi}{\epsilon + 2}\right) \Gamma\left(1 + \frac{1}{\epsilon + 2}\right)} \right]^{\frac{2\epsilon+4}{\epsilon+4}} \quad (n \rightarrow \infty). \tag{34}$$

This formula gives a very accurate approximation to the eigenvalues plotted in figure 1 and it shows, at least in the WKB approximation, that the energy eigenvalues of  $H$  in (12) are real and positive (see table 1). We can, in addition, perform a higher-order WKB calculation

**Table 1.** Comparison of the exact eigenvalues (obtained with Runge–Kutta) and the WKB result in (34).

$\epsilon$	$n$	$E_{\text{exact}}$	$E_{\text{WKB}}$	$\epsilon$	$n$	$E_{\text{exact}}$	$E_{\text{WKB}}$
1	0	1.156 267 072	1.0943	2	0	1.477 149 753	1.3765
	1	4.109 228 752	4.0895		1	6.003 386 082	5.9558
	2	7.562 273 854	7.5489		2	11.802 433 593	11.7690
	3	11.314 421 818	11.3043		3	18.458 818 694	18.4321
	4	15.291 553 748	15.2832		4	25.791 792 423	25.7692
	5	19.451 529 125	19.4444		5	33.694 279 298	33.6746
	6	23.766 740 439	23.7606		6	42.093 814 569	42.0761
	7	28.217 524 934	28.2120		7	50.937 278 826	50.9214
	8	32.789 082 922	32.7841		8	60.185 767 651	60.1696
9	37.469 824 697	37.4653	9	69.795 703 031	69.7884		



**Figure 3.** Energy levels of the Hamiltonian  $H = p^2 + |x|^P$  as a function of the real parameter  $P$ . This figure is similar to figure 1, but the eigenvalues do not pinch off and go into the complex plane because the Hamiltonian is Hermitian. (The spectrum becomes dense at  $P = 0$ .)

by replacing the phase integral by a *closed contour* that encircles the path joining the turning points (see [4, 32]).

It is interesting that the spectrum of the real  $|x|^{\epsilon+2}$  potential strongly resembles that of the  $x^2(ix)^\epsilon$  potential. The leading-order WKB quantization condition (accurate for  $\epsilon > -2$ ) is like that in (34) except that the factor of  $\sin(\frac{\pi}{\epsilon+2})$  is absent. However, as  $\epsilon \rightarrow \infty$ , the spectrum of  $|x|^{\epsilon+2}$  approaches that of the square-well potential [ $E_n = (n + 1)^2\pi^2/4$ ], while the energies of the complex  $x^2(ix)^\epsilon$  potential diverge, as figure 1 indicates. The energies of the  $|x|^P$  potential are shown in figure 3. Additional work on the WKB approximation applied to  $\mathcal{PT}$ -symmetric potentials can be found in [40, 41].

### 2.5. Numerical calculation of eigenvalues

There are several highly accurate numerical techniques for computing the energy spectrum that is displayed in figure 1. The simplest and most direct method is to integrate the Schrödinger differential equation (24) using a Runge–Kutta approach. To do so, we convert this complex differential equation to a system of coupled, real, second-order equations. The convergence is most rapid when we integrate along paths located at the centers of the Stokes wedges and



follow these paths out to  $\infty$ . We then patch the two solutions in each Stokes wedge together at the origin. This procedure, which is described in detail in [3], gives highly accurate numerical results.

An alternative is to perform a variational calculation in which we determine the energy levels by finding the stationary points of the functional

$$\langle H \rangle(a, b, c) \equiv \frac{\int_C dx \psi(x) H \psi(x)}{\int_C dx \psi^2(x)}, \quad (35)$$

where

$$\psi(x) = (ix)^c \exp[a(ix)^b] \quad (36)$$

is a three-parameter class of  $\mathcal{PT}$ -invariant trial wave functions [42]. The integration contour  $C$  used to define  $\langle H \rangle(a, b, c)$  must lie inside the wedges in the complex- $x$  plane in which the wave function falls off exponentially at infinity (see figure 2). Rather than having a local minimum, the functional has a saddle point in  $(a, b, c)$ -space. At this saddle point the numerical prediction for the ground-state energy is extremely accurate for a wide range of  $\epsilon$ . This method also determines approximate eigenfunctions and eigenvalues of the excited states of these non-Hermitian Hamiltonians. Handy used the numerical technique of solving the coupled moment problem [43]. This technique, which produces accurate results for the eigenvalues, is the exact quantum-mechanical analog of solving the Schwinger-Dyson equations in quantum field theory.

## 2.6. The remarkable case of a $\mathcal{PT}$ -symmetric $-x^4$ potential

The  $\mathcal{PT}$ -symmetric  $-x^4$  Hamiltonian in (11), which is obtained by setting  $\epsilon = 2$  in (12), is particularly interesting because it is possible to obtain the energy spectrum by using real analysis alone; that is, one can focus on real  $x$  only and avoid having to perform analysis in the complex- $x$  plane. One way to proceed is to deform the integration contour shown in figure 2 to the upper edges of the wedges so that it lies entirely on the real- $x$  axis. If this is done carefully, the exact eigenvalues for this potential can be obtained by solving the Schrödinger equation (24) subject to the boundary conditions that the potential be *reflectionless* [44]. That is, an incoming incident wave from the left gives rise to an outgoing transmitted wave on the right, but no reflected wave on the left. (This observation may have consequences in cosmological models, as explained in section 8.7.)

Another way to proceed is to show that the eigenvalues of the non-Hermitian  $-x^4$  Hamiltonian are identical with the eigenvalues of a conventional Hermitian Hamiltonian having a positive  $x^4$  potential. A number of authors have observed and discussed this equivalence [8, 45–47]. Here, we use elementary differential-equation methods [48] to prove that the spectrum of the non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian

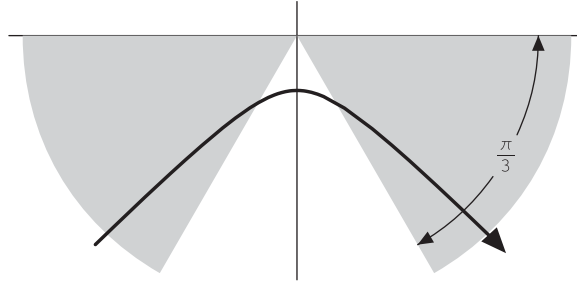
$$H = \frac{1}{2m} \hat{p}^2 - g \hat{x}^4 \quad (g > 0) \quad (37)$$

is identical to the spectrum of the Hermitian Hamiltonian

$$\tilde{H} = \frac{1}{2m} \hat{p}^2 + 4g \hat{x}^4 - \hbar \sqrt{\frac{2g}{m}} \hat{x} \quad (g > 0). \quad (38)$$

(We have included the dimensional constants  $m$ ,  $g$ , and  $\hbar$  because they help to elucidate the physical significance of the spectral equivalence of these two very different Hamiltonians.) To show that  $H$  in (37) and  $\tilde{H}$  in (38) are equivalent, we examine the corresponding Schrödinger eigenvalue equations

$$-\frac{\hbar^2}{2m} \psi''(x) - gx^4 \psi(x) = E \psi(x) \quad (39)$$



**Figure 4.** Stokes wedges in the lower-half complex- $x$  plane for the Schrödinger equation (39) arising from the Hamiltonian  $H$  in (37). The eigenfunctions of  $H$  decay exponentially as  $|x| \rightarrow \infty$  inside these wedges. Also shown is the contour in (41).

and

$$-\frac{\hbar^2}{2m}\Phi''(x) + \left(-\hbar\sqrt{\frac{2g}{m}}x + 4gx^4\right)\Phi(x) = E\Phi(x). \tag{40}$$

We begin by moving the complex integration contour for the Schrödinger equation (39) to the real axis. To do so, we parameterize the integration contour using

$$x = -2iL\sqrt{1 + iy/L}, \tag{41}$$

where

$$L = \lambda [\hbar^2/(mg)]^{1/6} \tag{42}$$

and  $y$  is a real parameter that ranges from  $-\infty$  to  $\infty$ . A graph of the contour in (41) is shown in figure 4. The transformed differential equation then reads

$$-\frac{\hbar^2}{2m}\left(1 + \frac{iy}{L}\right)\phi''(y) - \frac{i\hbar^2}{4Lm}\phi'(y) - 16gL^4\left(1 + \frac{iy}{L}\right)^2\phi(y) = E\phi(y). \tag{43}$$

Next, we perform a Fourier transform defined by

$$\tilde{f}(p) \equiv \int_{-\infty}^{\infty} dy e^{-iyp/\hbar} f(y). \tag{44}$$

By this definition the Fourier transforms of a derivative and a product are given by

$$f'(y) \rightarrow ip\tilde{f}(p)/\hbar \quad \text{and} \quad yf(y) \rightarrow i\hbar\tilde{f}'(p). \tag{45}$$

Thus, the transformed version of (43) reads

$$\frac{1}{2m}\left(1 - \frac{\hbar}{L}\frac{d}{dp}\right)p^2\tilde{\phi}(p) + \frac{\hbar}{4Lm}p\tilde{\phi}(p) - 16gL^4\left(1 - \frac{\hbar}{L}\frac{d}{dp}\right)^2\tilde{\phi}(p) = E\tilde{\phi}(p). \tag{46}$$

We expand and simplify the differential equation in (46) and get

$$-16gL^2\hbar^2\tilde{\phi}''(p) + \left(-\frac{\hbar p^2}{2mL} + 32gL^3\hbar\right)\tilde{\phi}'(p) + \left(\frac{p^2}{2m} - \frac{3p\hbar}{4mL} - 16gL^4\right)\tilde{\phi}(p) = E\tilde{\phi}(p). \tag{47}$$

Next, we eliminate the one-derivative term in the differential equation (47) to convert it to the form of a Schrödinger equation. To do so, we substitute

$$\tilde{\phi}(p) = e^{F(p)}\Phi(p), \tag{48}$$

where

$$F(p) = \frac{L}{\hbar} p - \frac{1}{192gmL^3\hbar} p^3. \quad (49)$$

The resulting equation is

$$-16gL^2\hbar^2\Phi''(p) + \left( \frac{p^4}{256gm^2L^4} - \frac{\hbar p}{4mL} \right) \Phi(p) = E\Phi(p). \quad (50)$$

Last, we rescale (50) by substituting

$$p = xL\sqrt{32mg} \quad (51)$$

and we obtain the Schrödinger differential equation (40). This completes the proof and verifies that the eigenvalues of the two Hamiltonians (37) and (38) have identical eigenvalues. This demonstration of equivalence is exact; no approximations were made in this argument<sup>4</sup>.

### 2.7. Parity anomaly

The proof in section 2.6 that the Hamiltonians in (37) and (38) are equivalent helps to clarify some of the physical content of the non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian (37). The interpretation of the result in (40) is that the linear term in the potential of the equivalent quartic Hermitian Hamiltonian in (38) is a parity *anomaly*. In general, an *anomaly* is a purely quantum (non-classical) effect that vanishes in the classical limit  $\hbar \rightarrow 0$ . There is no classical analog of an anomaly because Planck's constant  $\hbar$  does not appear in classical mechanics.

We refer to the linear term in (38) as a *parity anomaly* for the following reason: even though the  $\mathcal{PT}$ -symmetric Hamiltonian (37) is symmetric under the parity reflections defined in (3),  $H$  does not respect parity symmetry. The violation of parity symmetry is subtle because it is contained in the boundary conditions that the eigenfunctions of the associated Schrödinger equation must satisfy. Since these boundary conditions are given at  $|x| = \infty$ , the violation of parity symmetry is not detectable in any finite domain in the complex- $x$  plane. Classical motion is a local phenomenon. Therefore, a classical particle that is moving under the influence of this Hamiltonian (see section 3) will act as if it is subject to parity-symmetric forces; the classical particle cannot feel the influences of quantum boundary conditions imposed at  $|x| = \infty$ . In contrast, a quantum wave function is inherently non-local because it must obey boundary conditions that are imposed at  $|x| = \infty$ . Thus, only a quantum particle 'knows' about the violation of parity symmetry. To establish the equivalence between the Hamiltonians in (37) and (38) it was necessary to perform a Fourier transform (see (46)). This transformation maps the point at  $x = \infty$  to the point at  $p = 0$ , and this explains the presence of the linear parity-violating term in the potential of  $\tilde{H}$  in (38). The violation of parity is now a visible local effect in the Hamiltonian  $\tilde{H}$ . However, this violation of parity is proportional to  $\hbar$  and evaporates in the classical limit  $\hbar \rightarrow 0$ .

The Hamiltonian (38) is Hermitian in the usual Dirac sense and its energy spectrum is bounded below. This Hamiltonian is also  $\mathcal{PT}$ -symmetric because at every stage in the sequence of differential-equation transformations in section 2.6,  $\mathcal{PT}$  symmetry is preserved. However, the variable  $x$  that gives rise to the parity anomaly in (40) is *not* a coordinate variable. Its behaviour is that of a momentum variable because  $x$  changes sign under time reversal.

The violation of parity symmetry at the quantum level has important physical implications. It is the lack of parity symmetry which implies that the one-point Green's function in the

<sup>4</sup> A simple and exact transformation like the one presented in this section for mapping a  $\mathcal{PT}$ -symmetric non-Hermitian Hamiltonian to a Hermitian Hamiltonian has been found only for the isolated case  $\epsilon = 2$  in (12). (A more complicated spectral equivalence exists for the special case  $\epsilon = 4$  (see [21, 22]).)

corresponding quantum field theory does not vanish. A possible consequence of this is that the elusive Higgs particle, which is a fundamental ingredient in the standard model of particle physics, is a quantum anomaly. In the following section, we show that the parity anomaly has a major impact on the spectrum of bound states in a quantum theory.

2.8. *Physical consequence of the parity anomaly: appearance of bound states in a  $\mathcal{PT}$ -symmetric quartic potential*

A direct physical consequence of the parity anomaly is the appearance of bound states. To elucidate the connection between the parity anomaly and bound states, we generalize the Hamiltonian (37) to include a harmonic ( $\hat{x}^2$ ) term in the potential:

$$H = \frac{1}{2m} \hat{p}^2 + \frac{\mu^2}{2} \hat{x}^2 - g \hat{x}^4. \tag{52}$$

The same differential-equation analysis used in section 2.6 straightforwardly yields the equivalent Hermitian Hamiltonian [45, 46]

$$\tilde{H} = \frac{\hat{p}^2}{2m} - \hbar \sqrt{\frac{2g}{m}} \hat{x} + 4g \left( \hat{x}^2 - \frac{\mu^2}{8g} \right)^2. \tag{53}$$

Note that for these more general Hamiltonians the linear anomaly term remains unchanged from that in (38).

It was shown in an earlier paper [49] that the Hamiltonian (52) exhibits bound states. In particle physics a *bound state* is a state having a negative binding energy. Bound states in the context of quantum mechanics are defined as follows: let the energy levels of the Hamiltonian be  $E_n$  ( $n = 0, 1, 2, \dots$ ). The *renormalized mass* is the mass gap; that is,  $M = E_1 - E_0$ . Higher excitations must be measured relative to the vacuum energy:  $E_n - E_0$  ( $n = 2, 3, 4, \dots$ ). We say that the  $n$ th higher excitation is a bound state if the binding energy

$$B_n \equiv E_n - E_0 - nM \tag{54}$$

is negative. If  $B_n$  is positive, then we regard the state as *unbound* because this state can decay into  $n$  1-particle states of mass  $M$  in the presence of an external field.

In [49] it was shown numerically that for small positive values of  $g$  the first few states of  $H$  in (52) are bound. As  $g$  increases, the number of bound states decreases until, when  $g/\mu^3$  is larger than the critical value 0.0465, there are no bound states at all<sup>5</sup>.

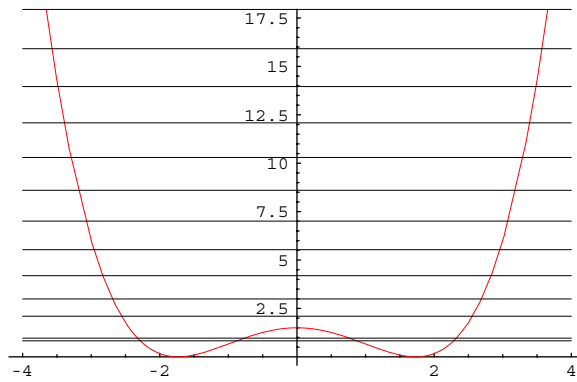
Because  $H$  in (52) has the same spectrum as the Hermitian Hamiltonian in (53), it is easy to explain the appearance of bound states and to show that the bound states are a direct consequence of the linear anomaly term. To probe the influence of the anomaly, we generalize (53) by inserting a dimensionless parameter  $\epsilon$  that measures the strength of the anomaly term:

$$\tilde{H} = \frac{1}{2} \hat{p}^2 - \epsilon \sqrt{2g} \hat{x} + 4g \left( \hat{x}^2 - \frac{1}{8g} \right)^2, \tag{55}$$

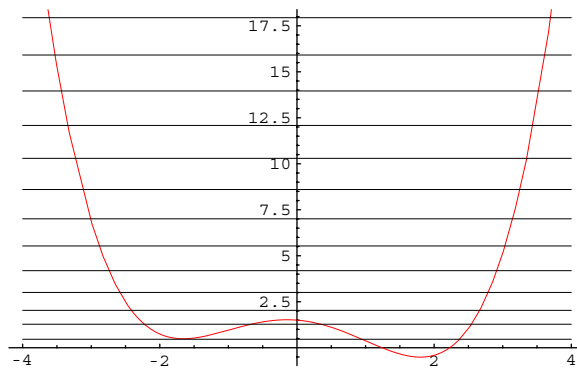
where for simplicity we have set  $m = \mu = \hbar = 1$ .

If we set  $\epsilon = 0$ , there is no anomaly term and the potential is a *symmetric* double well. The mass gap for a double well is exponentially small because it is a result of the tunnelling between the wells and thus the renormalized mass  $M$  is very small. Therefore,  $B_n$  in (54) is positive and there are no bound states. In figure 5 we display the double-well potential and the first several states of the system for the case  $g = 0.046$  and  $\epsilon = 0$ . There is a very small splitting between the lowest two states.

<sup>5</sup> In [49] a heuristic argument was given to explain why there is such a critical value. This argument is heuristic because the non-Hermitian Hamiltonian is evaluated for  $x$  in the complex plane. As explained in section 2.3, when  $x$  is complex, one cannot use order relationships such as  $>$  or  $<$ , which only apply to real numbers.



**Figure 5.** Potential of the Hermitian Hamiltonian (55) plotted as a function of the real variable  $x$  for the case  $\epsilon = 0$  and  $g = 0.046$ . The energy levels are indicated by horizontal lines. Because  $\epsilon = 0$ , there is no anomaly and the double-well potential is symmetric. Therefore, the mass gap is very small and thus there are no bound states.

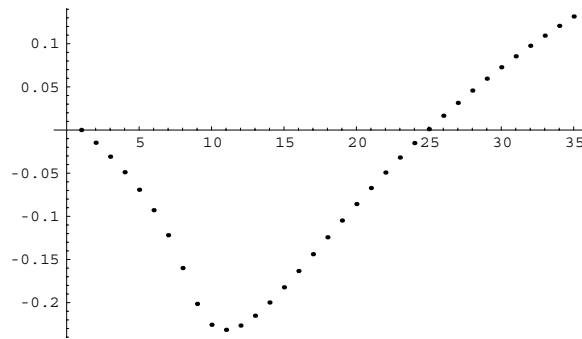


**Figure 6.** Asymmetric potential well plotted as a function of the real variable  $x$  for the Hermitian Hamiltonian (55) with  $\epsilon = 1$  and  $g = 0.046$ . The energy levels are indicated by horizontal lines. There is one bound state. The occurrence of bound states is due to the anomaly.

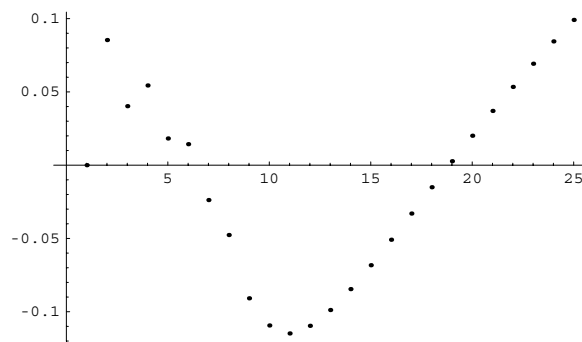
If  $\epsilon = 1$ , the double-well potential is asymmetric and the two lowest states are not approximately degenerate. Therefore, bound states can occur near the bottom of the potential well. Higher-energy states eventually become unbound because, as we know from WKB theory, in a quartic well the  $n$ th energy level grows like  $n^{4/3}$  for large  $n$ . As  $g$  becomes large, the number of bound states becomes smaller because the depth of the double well decreases. For large enough  $g$  there are no bound states. In figure 6 we display the potential for  $\epsilon = 1$  and for  $g = 0.046$ ; for this  $g$  there is one bound state.

Another way to display the bound states is to plot the value of the binding energy  $B_n$  as a function of  $n$ . For example, in figure 7 we display the bound states for  $\epsilon = 1$  and  $g = 0.008333$ . Note that for these values there are 23 bound states. Observe also that the binding energy  $B_n$  is a smooth function of  $n$ .

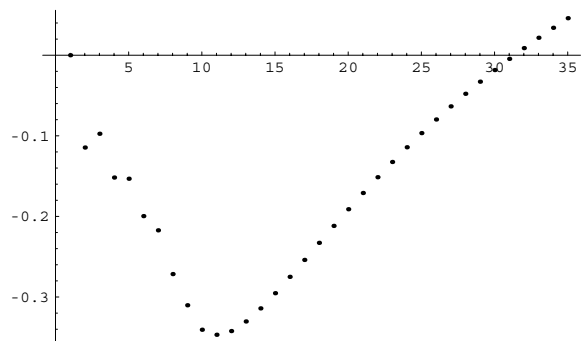
It is worth noting that the bound-state spectrum depends so sensitively on the strength of the anomaly term in the Hamiltonian (55). If  $\epsilon$  is slightly less than 1, the first few states become unbound, as shown in figure 8. In this figure  $g = 0.008333$  and  $\epsilon = 0.9$ . If  $\epsilon$  is slightly greater than 1, the binding energy  $B_n$  is not a smooth function of  $n$  for small  $n$ .



**Figure 7.** Binding energies  $B_n = E_n - E_0 - nM$  plotted as a function of  $n$  for  $g = 0.008333$  and  $\epsilon = 1$ . A negative value of  $B_n$  indicates a bound state. Observe that there are 23 bound states for these parameter values. Note that  $B_n$  is a smooth function of  $n$ .



**Figure 8.** Binding energies  $B_n$  plotted as a function of  $n$  for  $g = 0.008333$  and  $\epsilon = 0.9$ . The first five states have now become unbound and  $B_n$  is not a smooth function of  $n$  for  $n \leq 6$ . The next 12 states are bound, and in this region  $B_n$  is a smooth function of  $n$ . Comparison of this figure with figure 7 shows that the bound-state spectrum is exquisitely sensitive to the strength of the linear anomaly term.



**Figure 9.** Binding energies  $B_n$  plotted as a function of  $n$  for  $g = 0.008333$  and  $\epsilon = 1.1$ . Note that there are 30 bound states and that  $B_n$  is not a smooth function of  $n$  when  $n$  is small.

In figure 9 we plot  $B_n$  as a function of  $n$  for  $g = 0.008333$  and  $\epsilon = 1.1$ . Note that for these values of the parameters there are 30 bound states. Figures 7–9 are strikingly different, which demonstrates the extreme sensitivity of the bound-state spectrum to the anomaly term.

### 3. $\mathcal{PT}$ -symmetric classical mechanics—the strange dynamics of a classical particle subject to complex forces

In this section we describe the properties of the  $\mathcal{PT}$ -symmetric classical-mechanical theory that underlies the quantum-mechanical theory described by the Hamiltonian (12). We describe the motion of a particle that feels complex forces and responds by moving about in the complex plane. Several papers have been published in this area [4, 50–55] and we summarize here some of the surprising discoveries.

One objective here is to explain heuristically how an upside-down potential like that in (11) can have *positive*-energy quantum-mechanical eigenstates. One might think (incorrectly!) that since a classical particle would slide down the positive-real axis to infinity, the corresponding quantum states would be unstable and the spectrum of the quantum system would be unbounded below. In fact, when  $\epsilon \geq 0$  (the region of unbroken  $\mathcal{PT}$  symmetry), all but a set of measure zero of the possible classical paths are confined and periodic, and thus the classical particle does not slide off to infinity. When  $\epsilon < 0$  (the region of broken  $\mathcal{PT}$  symmetry), the classical trajectories do indeed run off to infinity, and we can begin to understand why the energy levels of the corresponding quantum system are complex.

The equation of motion of a classical particle described by  $H$  in (12) follows from Hamilton's equations:

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = 2p, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial x} = i(2 + \epsilon)(ix)^{1+\epsilon}. \quad (56)$$

Combining these two equations gives

$$\frac{d^2x}{dt^2} = 2i(2 + \epsilon)(ix)^{1+\epsilon}, \quad (57)$$

which is the *complex* version of Newton's second law,  $F = ma$ .

We can integrate (57) to give

$$\frac{1}{2} \frac{dx}{dt} = \pm \sqrt{E + (ix)^{2+\epsilon}}, \quad (58)$$

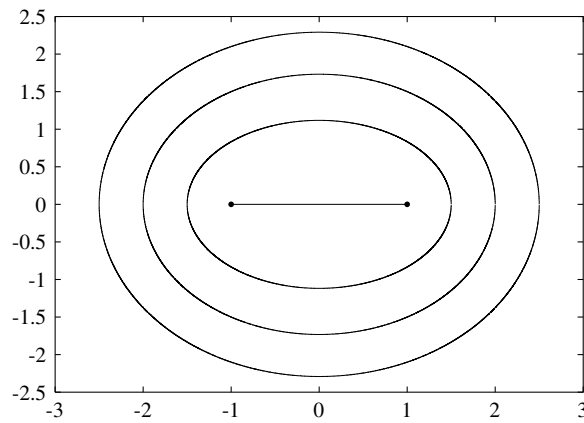
where  $E$  is the energy of the classical particle (the time-independent value of  $H$ ). We treat time  $t$  as a real variable that parametrizes the complex path  $x(t)$  of this particle. Equation (58) is a complex generalization of the concept that the velocity is the time derivative of the position ( $v = \frac{dx}{dt}$ ). Here,  $t$  is real, but  $v$  and  $x$  are complex.

We now describe and classify the solutions to equation (58). Because the corresponding quantum theory possesses  $\mathcal{PT}$  invariance, we restrict our attention to real values of  $E$ . Given this restriction, we can rescale  $x$  and  $t$  by real numbers so that without loss of generality equation (58) reduces to

$$\frac{dx}{dt} = \pm \sqrt{1 + (ix)^{2+\epsilon}}. \quad (59)$$

#### 3.1. The case $\epsilon = 0$

The classical solutions to equation (59) have elaborate topologies, so we begin by considering some special values of  $\epsilon$ . For the simplest case,  $\epsilon = 0$ , there are two turning points and these lie on the real axis at  $\pm 1$ . To solve equation (59) we must specify the initial condition  $x(0)$ . An obvious choice for  $x(0)$  is a turning point. If the path begins at  $\pm 1$ , there is a unique trajectory



**Figure 10.** Classical trajectories in the complex- $x$  plane for the harmonic-oscillator Hamiltonian  $H = p^2 + x^2$ . These trajectories are the complex paths of a particle whose energy is  $E = 1$ . The trajectories are nested ellipses with foci located at the turning points at  $x = \pm 1$ . The real line segment (degenerate ellipse) connecting the turning points is the conventional real periodic classical solution to the harmonic oscillator. All paths are closed orbits having the same period  $2\pi$ .

in the complex- $x$  plane that solves (59). This trajectory lies on the real axis and oscillates between the turning points. This is the usual sinusoidal harmonic motion.

Choosing the energy determines the locations of the turning points, and choosing the initial position of the particle determines the initial velocity (up to a plus or minus sign) as well. So if the path of the particle begins anywhere on the real axis between the turning points, the initial velocity is fixed up to a sign and the trajectory of the particle still oscillates between the turning points.

In conventional classical mechanics the only possible initial positions for the particle are on the real- $x$  axis between the turning points because the velocity is real; all other points on the real axis belong to the so-called classically forbidden region. However, because we are analytically continuing classical mechanics into the complex plane, we can choose any point  $x(0)$  in the complex plane as an initial position. For all complex initial positions outside the conventional classically allowed region the classical trajectory is an ellipse whose foci are the turning points. The ellipses are nested because no trajectories may cross. These ellipses are shown in figure 10.

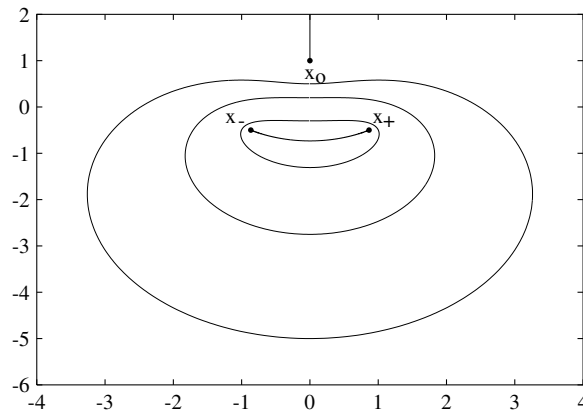
The exact harmonic-oscillator ( $\epsilon = 0$ ) solution to (59) is

$$x(t) = \cos[\arccos x(0) \pm t], \quad (60)$$

where the sign of  $t$  determines the direction (clockwise or anticlockwise) in which the particle traces out the ellipse. For *any* ellipse the period is  $2\pi$ . The period is the same for all trajectories because we can join the square-root branch points by a single finite branch cut lying along the real axis from  $x = -1$  to  $x = 1$ . The complex path integral that determines the period can then be shrunk (by Cauchy's theorem) to the usual real integral joining the turning points.

Note that all of the elliptical orbits in figure 10 are symmetric with respect to parity  $\mathcal{P}$  (reflections through the origin) and time reversal  $\mathcal{T}$  (reflections about the real axis) as well as to  $\mathcal{PT}$  (reflections about the imaginary axis). Furthermore,  $\mathcal{P}$  and  $\mathcal{T}$  individually preserve the directions in which the ellipses are traversed.





**Figure 11.** Classical trajectories in the complex- $x$  plane for a particle of energy  $E = 1$  described by the Hamiltonian  $H = p^2 + ix^3$ . An oscillatory trajectory connects the turning points  $x_{\pm}$ . This trajectory is enclosed by a set of closed, nested paths that fill the finite complex- $x$  plane except for points on the imaginary axis at or above the turning point  $x_0 = i$ . Trajectories that originate on the imaginary axis above  $x = i$  either move off to  $i\infty$  or else approach  $x_0$ , stop, turn around and then move up the imaginary axis to  $i\infty$ .

### 3.2. The case $\epsilon = 1$

When  $\epsilon = 1$ , there are three turning points. These turning points solve the equation  $ix^3 = 1$ . Two lie below the real axis and are symmetric with respect to the imaginary axis:

$$x_- = e^{-5i\pi/6} \quad \text{and} \quad x_+ = e^{-i\pi/6}. \quad (61)$$

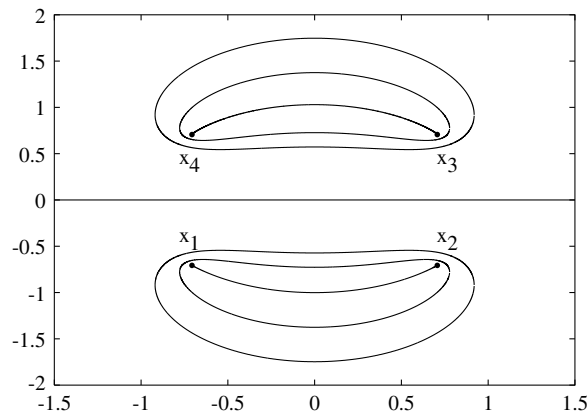
Under  $\mathcal{PT}$  reflection  $x_-$  and  $x_+$  are interchanged. The third turning point lies on the imaginary axis at  $x_0 = i$ .

Like the case  $\epsilon = 0$ , the trajectory of a particle that begins at the turning point  $x_-$  follows a path in the complex- $x$  plane to the turning point at  $x_+$ . Then, the particle retraces its path back to the turning point at  $x_-$ , and it continues to oscillate between these two turning points. This path is shown in figure 11. The period of this motion is  $2\sqrt{3}\pi\Gamma(\frac{4}{3})/\Gamma(\frac{5}{6})$ . A particle beginning at the third turning point  $x_0$  exhibits a completely distinct motion: it travels up the imaginary axis and reaches  $i\infty$  in a finite time  $\sqrt{\pi}\Gamma(\frac{4}{3})/\Gamma(\frac{5}{6})$ . This motion is not periodic.

Paths originating from all other points in the finite complex- $x$  plane follow closed periodic orbits. No two orbits may intersect; rather they are all nested, like the ellipses for the case  $\epsilon = 0$ . All of these orbits encircle the turning points  $x_{\pm}$  and, by virtue of Cauchy's theorem, have the same period  $2\sqrt{3}\pi\Gamma(\frac{4}{3})/\Gamma(\frac{5}{6})$  as the oscillatory path connecting  $x_{\pm}$ . Because these orbits must avoid crossing the trajectory that runs up the positive imaginary axis from the turning point at  $x_0 = i$ , they are pinched in the region just below  $x_0$ , as shown in figure 11.

### 3.3. The case $\epsilon = 2$

When  $\epsilon = 2$ , there are four turning points, two below the real axis and symmetric with respect to the imaginary axis,  $x_1 = e^{-3i\pi/4}$  and  $x_2 = e^{-i\pi/4}$ , and two more located above the real axis and symmetric with respect to the imaginary axis,  $x_3 = e^{i\pi/4}$  and  $x_4 = e^{3i\pi/4}$ . These turning points are solutions to the equation  $-x^4 = 1$ . Classical trajectories that oscillate between the pair  $x_1$  and  $x_2$  and the pair  $x_3$  and  $x_4$  are shown in figure 12. The period of these oscillations is  $2\sqrt{2}\pi\Gamma(\frac{5}{4})/\Gamma(\frac{3}{4})$ . Trajectories that begin elsewhere in the complex- $x$  plane are also shown



**Figure 12.** Classical trajectories in the complex- $x$  plane for a particle described by the Hamiltonian  $H = p^2 - x^4$  and having energy  $E = 1$ . There are two oscillatory trajectories connecting the pairs of turning points  $x_1$  and  $x_2$  in the lower-half  $x$ -plane and  $x_3$  and  $x_4$  in the upper-half  $x$ -plane. (A trajectory joining any other pair of turning points is forbidden because it would violate the  $\mathcal{PT}$  (left–right) symmetry.) The oscillatory trajectories are surrounded by closed orbits of the same period. In contrast to these periodic orbits, there is a special class of trajectories having unbounded path length and running along the real- $x$  axis.

in figure 10. By virtue of Cauchy’s theorem all these nested non-intersecting trajectories have the same period. All classical motion is periodic except for the special trajectories that begin on the real axis. A particle that begins on the real- $x$  axis runs off to  $\pm\infty$ ; its trajectory is non-periodic.

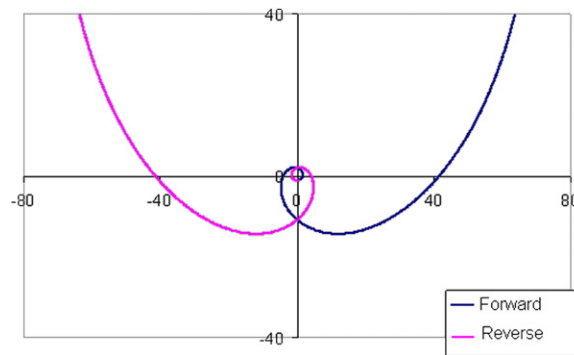
### 3.4. Broken and unbroken classical $\mathcal{PT}$ symmetry

We can now understand heuristically why the energies of the corresponding  $\mathcal{PT}$ -symmetric quantum systems are real. In each of figures 10, 11 and 12 we can see that all of the orbits are localized and periodic. We may regard the pictured classical motions as representing particles confined to and orbiting around *complex atoms*! We can then use Bohr–Sommerfeld quantization to determine the discrete energies of the system:

$$\oint_C dx p = \oint_C dx \sqrt{E - x^2(ix)^\epsilon} = (n + \frac{1}{2}) \pi, \tag{62}$$

where  $C$  represents the orbit of a classical particle in the complex- $x$  plane. By Cauchy’s theorem, any closed orbit leads to the same result for the energy  $E_n$ , and because of  $\mathcal{PT}$  symmetry the integral above gives a *real* value for the energy.

The key difference between classical paths for  $\epsilon > 0$  and for  $\epsilon < 0$  is that in the former case the paths (except for isolated examples) are closed orbits and in the latter case the paths are open orbits. In figure 13 we consider the case  $\epsilon = -0.2$  and display two paths that begin on the negative imaginary axis. Because  $\epsilon$  is non-integer, there is a branch cut and the classical particle travels on a Riemann surface rather than on a single sheet of the complex plane. In this figure one path evolves forwards in time and the other path evolves backwards in time. Each path spirals outward and eventually moves off to infinity. Note that the pair of paths forms a  $\mathcal{PT}$ -symmetric structure. We remark that the paths do not cross because they are on different sheets of the Riemann surface. The function  $(ix)^{-0.2}$  requires a branch cut, and we take this branch cut to lie along the positive imaginary axis. The forward-evolving path leaves



**Figure 13.** Classical trajectories in the complex- $x$  plane for the Hamiltonian in (21) with  $\epsilon = -0.2$ . These trajectories begin on the negative imaginary axis very close to the origin. One trajectory evolves forwards in time and the other goes backwards in time. The trajectories are open orbits and show the particle spiraling off to infinity. The trajectories begin on the principal sheet of the Riemann surface; as they cross the branch cut on the positive imaginary axis, they visit the higher and lower sheets of the surface. The trajectories do not cross because they lie on different Riemann sheets.

the principal sheet (sheet 0) of the Riemann surface and crosses the branch cut in the positive sense and continues on sheet 1. The reverse path crosses the branch cut in the negative sense and continues on sheet  $-1$ . Figure 13 shows the projection of the classical orbit onto the principal sheet.

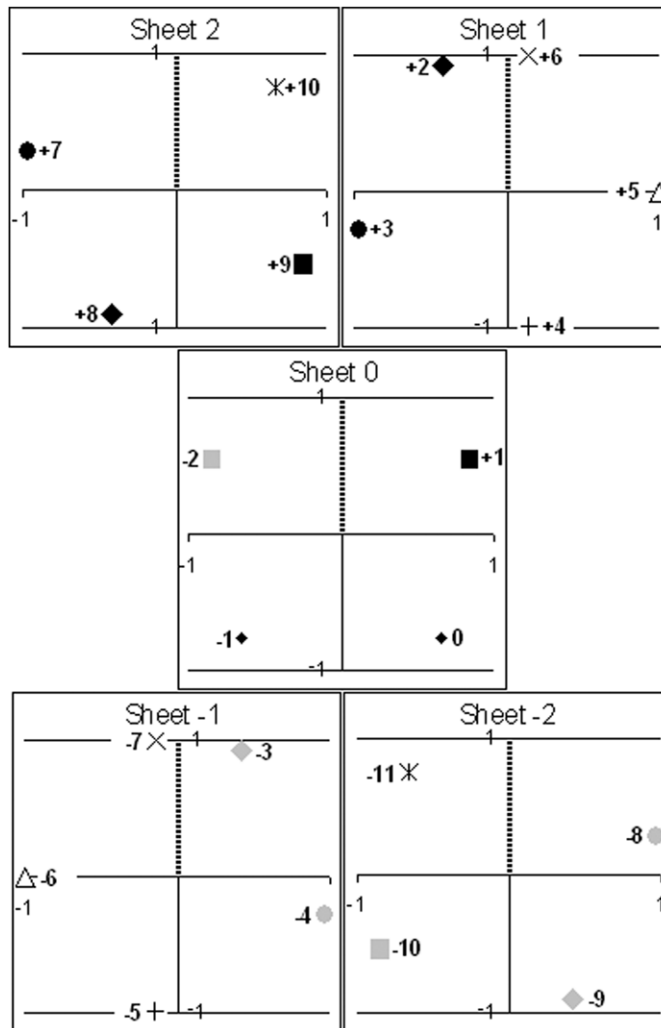
Figure 13 shows why the energies of the quantum system in the broken  $\mathcal{PT}$ -symmetric region  $\epsilon < 0$  are not real. The answer is simply that the trajectories are not closed orbits; the trajectories are *open* orbits, and all classical particles drift off to  $x = \infty$ . As explained after (32), if we attempt to quantize the system for the case  $\epsilon < 0$  using the Bohr–Sommerfeld integral in (62), the integral does not exist because the integration contour is not closed.

### 3.5. Noninteger values of $\epsilon$

As  $\epsilon$  increases from 0, the turning points at  $x = 1$  (and at  $x = -1$ ), as shown in figure 10 rotate downwards and clockwise (anticlockwise) into the complex- $x$  plane. These turning points are solutions to the equation  $1 + (ix)^{2+\epsilon} = 0$ . When  $\epsilon$  is non-integer, this equation has many solutions that all lie on the unit circle and have the form

$$x = \exp\left(i\pi \frac{4N - \epsilon}{4 + 2\epsilon}\right) \quad (N \text{ integer}). \quad (63)$$

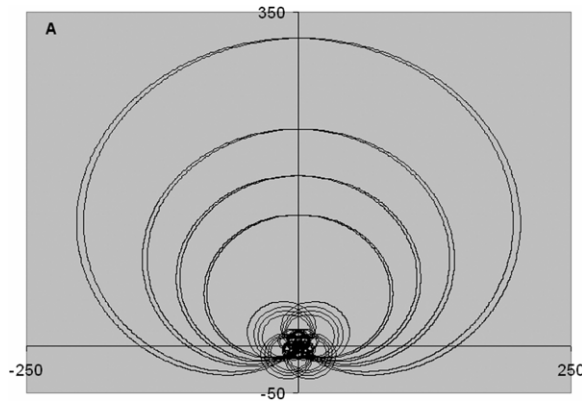
These turning points occur in  $\mathcal{PT}$ -symmetric pairs (pairs that are symmetric when reflected through the imaginary axis) corresponding to the  $N$  values  $(N = -1, N = 0)$ ,  $(N = -2, N = 1)$ ,  $(N = -3, N = 2)$ ,  $(N = -4, N = 3)$  and so on. We label these pairs by the integer  $K$  ( $K = 0, 1, 2, 3, \dots$ ) so that the  $K$ th pair corresponds to  $(N = -K - 1, N = K)$ . The pair of turning points on the real- $x$  axis for  $\epsilon = 0$  deforms continuously into the  $K = 0$  pair of turning points when  $\epsilon > 0$ . When  $\epsilon$  is rational, there are a finite number of turning points in the complex- $x$  Riemann surface. For example, when  $\epsilon = \frac{12}{5}$ , there are five sheets in the Riemann surface and 11 pairs of turning points. The  $K = 0$  pair of turning points is labelled  $N = -1$  and  $N = 0$ , the  $K = 1$  pair is labelled  $N = -2$  and  $N = 1$ , and so on. The last ( $K = 10$ ) pair of turning points is labelled  $N = -11$  and  $N = 10$ . These turning points are shown in figure 14.



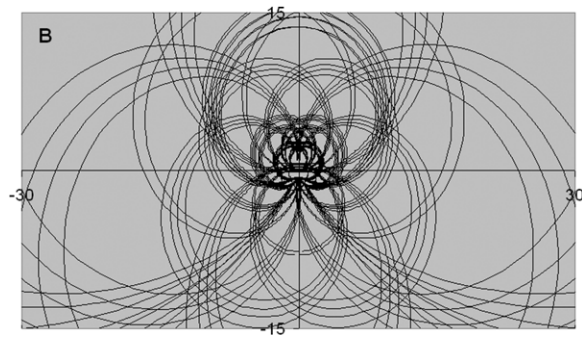
**Figure 14.** Locations of the turning points for  $\epsilon = \frac{12}{5}$ . There are 11  $\mathcal{PT}$ -symmetric pairs of turning points, with each pair being mirror images under reflection through the imaginary- $x$  axis on the principal sheet. All 22 turning points lie on the unit circle on a five-sheeted Riemann surface, where the sheets are joined by cuts on the positive imaginary axis.

As  $\epsilon$  increases from 0, the elliptical complex trajectories in figure 10 for the harmonic oscillator begin to distort but the trajectories remain closed and periodic except for special singular trajectories that run off to complex infinity, as we see in figure 11. These singular trajectories only occur when  $\epsilon$  is an integer. Nearly all of the orbits that one finds are  $\mathcal{PT}$  symmetric (left–right symmetric), and until very recently it was thought that all closed periodic orbits are  $\mathcal{PT}$  symmetric. This is, in fact, not so [53]. Closed non- $\mathcal{PT}$ -symmetric orbits exist, and these orbits are crucial for understanding the behaviour of the periods of the complex orbits as  $\epsilon$  varies.

In figure 15 we display a  $\mathcal{PT}$ -symmetric orbit of immense topological intricacy that visits many sheets of the Riemann surface. This figure shows a classical trajectory corresponding to



**Figure 15.** A classical trajectory in the complex- $x$  plane for the complex Hamiltonian  $H = p^2 x^2 (ix)^{\pi-2}$ . This complicated trajectory begins at  $x(0) = -7.1i$  and visits 11 sheets of the Riemann surface. Its period is approximately  $T = 255.3$ . This figure displays the projection of the trajectory onto the principal sheet of the Riemann surface. This trajectory does not cross itself.



**Figure 16.** An enlargement of the classical trajectory  $x(t)$  in figure 15 showing the detail near the origin in the complex- $x$  plane. We emphasize that this classical path never crosses itself; the apparent self-intersections are paths that lie on different sheets of the Riemann surface.

$\epsilon = \pi - 2$ . The trajectory starts at  $x(0) = -7.1i$  and visits 11 sheets of the Riemann surface. Its period is  $T = 255.3$ . The structure of this orbit near the origin is so complicated that we provide a magnified version in figure 16.

The period of any classical orbit depends on the specific pairs of turning points that are enclosed by the orbit and on the number of times that the orbit encircles each pair. As shown in [51], any given orbit can be deformed to a simpler orbit of exactly the same period. This simpler orbit connects two turning points and oscillates between them rather than encircling them. For the elementary case of orbits that enclose only the  $K = 0$  pair of turning points, the formula for the period of the closed orbit is

$$T_0(\epsilon) = 2\sqrt{\pi} \frac{\Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right)}{\Gamma\left(\frac{4+\epsilon}{4+2\epsilon}\right)} \cos\left(\frac{\epsilon\pi}{4+2\epsilon}\right) \quad (\epsilon \geq 0). \quad (64)$$

The derivation of (64) goes as follows: the period  $T_0$  is given by a closed contour integral along the trajectory in the complex- $x$  plane. This trajectory encloses the square-root branch cut that

joins the  $K = 0$  pair of turning points. This contour can be deformed into a pair of rays that run from one turning point to the origin and then from the origin to the other turning point. The integral along each ray is easily evaluated as a beta function, which is then written in terms of gamma functions.

When the classical orbit encloses more than just the  $K = 0$  pair of turning points, the formula for the period of the orbit becomes more complicated [51]. In general, there are contributions to the period integral from many enclosed pairs of turning points. We label each such pair by the integer  $j$ . The formula for the period of the topological class of classical orbits whose central orbit terminates on the  $K$ th pair of turning points is

$$T_K(\epsilon) = 2\sqrt{\pi} \frac{\Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right)}{\Gamma\left(\frac{4+\epsilon}{4+2\epsilon}\right)} \sum_{j=0}^{\infty} a_j(K, \epsilon) \left| \cos\left(\frac{(2j+1)\epsilon\pi}{4+2\epsilon}\right) \right|. \quad (65)$$

In this formula the cosines originate from the angular positions of the turning points in (63). The coefficients  $a_j(K, \epsilon)$  are all non-negative integers. The  $j$ th coefficient is non-zero only if the classical path encloses the  $j$ th pair of turning points. Each coefficient is an *even* integer except for the  $j = K$  coefficient, which is an odd integer. The coefficients  $a_j(K, \epsilon)$  satisfy

$$\sum_{j=0}^{\infty} a_j(K, \epsilon) = k, \quad (66)$$

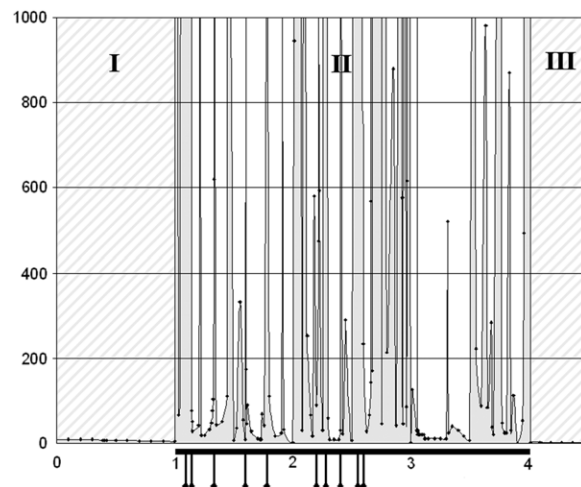
where  $k$  is the number of times that the central classical path crosses the imaginary axis. Equation (66) truncates the summation in (65) to a finite number of terms.

The period  $T_0$  in (64) of orbits connecting the  $K = 0$  turning points is a smoothly decreasing function of  $\epsilon$ . However, for classical orbits connecting the  $K$ th ( $K > 0$ ) pair of turning points, the classical orbits exhibit fine structure that is exquisitely sensitive to the value of  $\epsilon$ . Small variations in  $\epsilon$  can cause huge changes in the topology and in the periods of the closed orbits. Depending on  $\epsilon$ , there are orbits having short periods as well as orbits having long and possibly arbitrarily long periods.

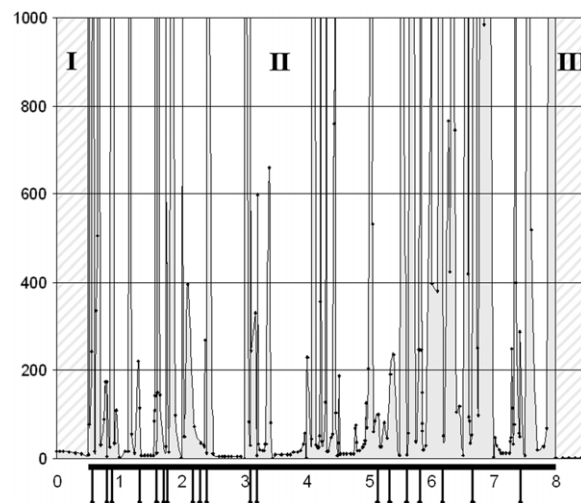
### 3.6. Classical orbits having spontaneously broken $\mathcal{PT}$ symmetry

There is a general pattern that holds for all  $K$ . For classical orbits that oscillate between the  $K$ th pair of turning points, there are three regions of  $\epsilon$ . The domain of region I is  $0 \leq \epsilon \leq \frac{1}{K}$ , the domain of region II is  $\frac{1}{K} < \epsilon < 4K$  and the domain of region III is  $4K < \epsilon$ . In regions I and III the period is a small and smoothly decreasing function of  $\epsilon$ . However, in region II the period is a rapidly varying and noisy function of  $\epsilon$ . We illustrate this behaviour for the case  $K = 1$  and  $K = 2$  in figures 17 and 18.

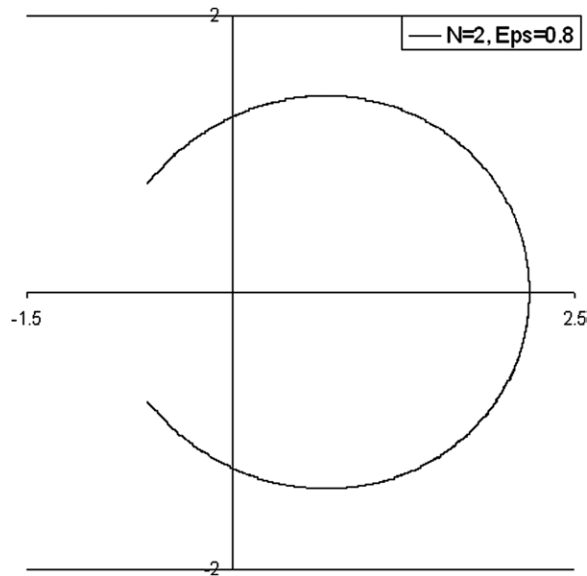
The abrupt changes in the topology and the periods of the orbits for  $\epsilon$  in region II are associated with the appearance of orbits having *spontaneously broken*  $\mathcal{PT}$  symmetry. In region II there are short patches where the period is relatively small and is a slowly varying function of  $\epsilon$ . These patches are bounded by special values of  $\epsilon$  for which the period of the orbit suddenly becomes extremely long. Numerical studies of the orbits connecting the  $K$ th pair of turning points indicate that these special values of  $\epsilon$  are always *rational* [55]. Furthermore, at these special rational values of  $\epsilon$ , the closed orbits are *not*  $\mathcal{PT}$ -symmetric (left–right symmetric). Such orbits exhibit *spontaneously broken*  $\mathcal{PT}$  symmetry. Some special values of  $\epsilon$  at which spontaneously broken  $\mathcal{PT}$ -symmetric orbits occur are indicated in figures 17 and 18 by short vertical lines below the horizontal axis. These special values of  $\epsilon$  have the form  $\frac{p}{q}$ , where  $p$  is a multiple of 4 and  $q$  is odd.



**Figure 17.** Period of a classical trajectory beginning at the  $N = 1$  turning point in the complex- $x$  plane. The period is plotted as a function of  $\epsilon$ . The period decreases smoothly for  $0 \leq \epsilon < 1$  (region I). However, when  $1 \leq \epsilon \leq 4$  (region II), the period becomes a rapidly varying and noisy function of  $\epsilon$ . For  $\epsilon > 4$  (region III) the period is once again a smoothly decaying function of  $\epsilon$ . Region II contains short subintervals where the period is a small and smoothly varying function of  $\epsilon$ . At the edges of these subintervals the period suddenly becomes extremely long. Detailed numerical analysis shows that the edges of the subintervals lie at special rational values of  $\epsilon$ . Some of these special rational values of  $\epsilon$  are indicated by vertical line segments that cross the horizontal axis. At these rational values the orbit does not reach the  $N = -2$  turning point and the  $\mathcal{PT}$  symmetry of the classical orbit is spontaneously broken.



**Figure 18.** Period of a classical trajectory joining (except when  $\mathcal{PT}$  symmetry is broken) the  $K = 2$  pair of turning points. The period is plotted as a function of  $\epsilon$ . As in the  $K = 1$  case shown in figure 17, there are three regions. When  $0 \leq \epsilon \leq \frac{1}{2}$  (region I), the period is a smooth decreasing function of  $\epsilon$ ; when  $\frac{1}{2} < \epsilon \leq 8$  (region II), the period is a rapidly varying and choppy function of  $\epsilon$ ; when  $8 < \epsilon$  (region III), the period is again a smooth and decreasing function of  $\epsilon$ .



**Figure 19.** A horseshoe-shaped non- $\mathcal{PT}$ -symmetric orbit. This orbit is not symmetric with respect to the imaginary axis, but it is symmetric with respect to the real axis. The orbit terminates at a complex-conjugate pair of turning points. For this orbit  $\epsilon = \frac{4}{5}$ .

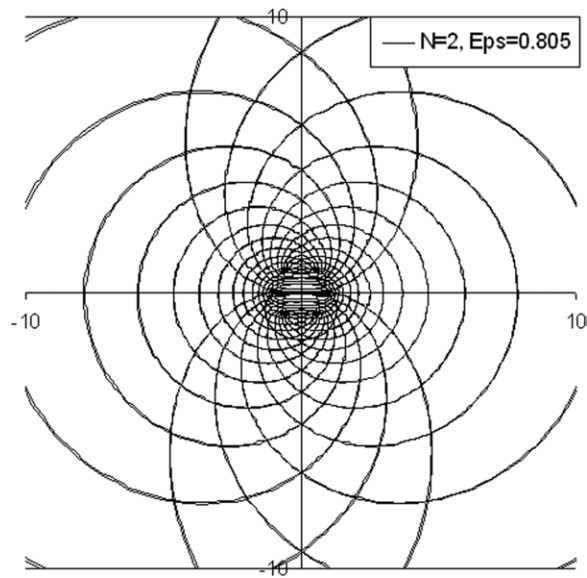
A broken- $\mathcal{PT}$ -symmetric orbit is a failed  $\mathcal{PT}$ -symmetric orbit. Figure 19 displays a spontaneously broken- $\mathcal{PT}$ -symmetric orbit for  $\epsilon = \frac{4}{5}$ . The orbit starts at the  $N = 2$  turning point, but it never reaches the  $\mathcal{PT}$ -symmetric turning point  $N = -3$ . Rather, the orbit terminates when it runs into and is reflected back from the complex conjugate  $N = 4$  turning point (see (63)). The period of the orbit is short ( $T = 4.63$ ). While this orbit is not  $\mathcal{PT}$  (left–right) symmetric, it does possess complex-conjugate (up–down) symmetry. In general, for a non- $\mathcal{PT}$ -symmetric orbit to exist, it must join or encircle a pair of complex-conjugate turning points.

If we change  $\epsilon$  slightly,  $\mathcal{PT}$  symmetry is restored and one can only find orbits that are  $\mathcal{PT}$  symmetric. For example, if we take  $\epsilon = 0.805$ , we obtain the complicated orbit in figure 20. The period of this orbit is large ( $T = 173.36$ ).

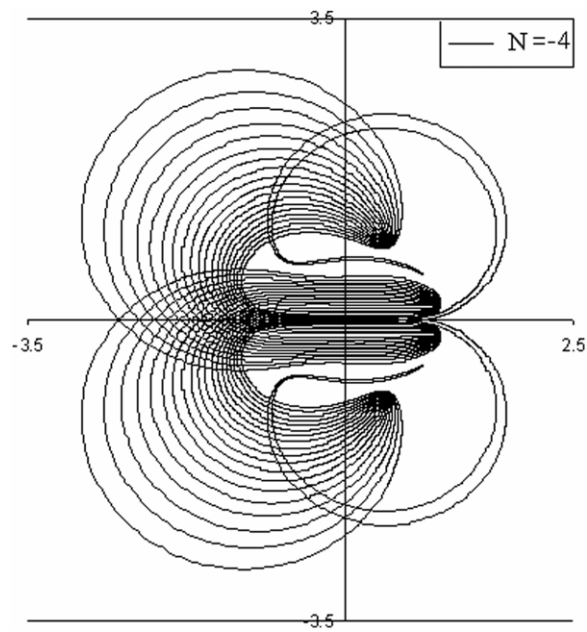
Broken- $\mathcal{PT}$ -symmetric orbits need not be simple looking, like the orbit shown in figure 19. Indeed, they can have an elaborate topology. As an example we plot in figure 21 the complicated orbit that arises when  $\epsilon = \frac{16}{9}$ . This orbit is a failed  $K = 3$   $\mathcal{PT}$ -symmetric orbit that originates at the  $N = -4$  turning point, but never reaches the  $\mathcal{PT}$ -symmetric  $N = 3$  turning point. Instead, it is reflected back by the complex-conjugate  $N = -14$  turning point.

This study of classical orbits provides a heuristic explanation of the quantum transition from a broken to an unbroken  $\mathcal{PT}$  symmetry as  $\epsilon$  increases past 0. The quantum transition corresponds to a change from open to closed classical orbits. Furthermore, we can now see why the quantum theory in the unbroken region is unitary. At the classical level, particles are bound in a complex atom and cannot escape to infinity; at the quantum level the probability is conserved and does not leak away as time evolves. Quantum mechanics is obtained by summing over all possible classical trajectories, and in the case of  $\mathcal{PT}$ -symmetric classical mechanics we have seen some bizarre classical trajectories. To understand how summing over such trajectories produces  $\mathcal{PT}$ -symmetric quantum mechanics will require much more research.





**Figure 20.**  $\mathcal{PT}$ -symmetric orbit for  $\epsilon = 0.805$ . This orbit connects the  $K = 2$  pair of turning points.



**Figure 21.** Non- $\mathcal{PT}$ -symmetric orbit for  $\epsilon = \frac{16}{9}$ . This topologically complicated orbit originates at the  $N = -4$  turning point but does not reach the  $\mathcal{PT}$ -symmetric  $N = 3$  turning point. Instead, it is reflected back at the complex-conjugate  $N = -14$  turning point. The period of this orbit is  $T = 186.14$ .

#### 4. $\mathcal{PT}$ -symmetric quantum mechanics

Establishing that the eigenvalues of many  $\mathcal{PT}$ -symmetric Hamiltonians are real and positive raises an obvious question: does a non-Hermitian Hamiltonian such as  $H$  in (12) define a physical theory of quantum mechanics or is the reality and positivity of the spectrum merely an intriguing mathematical curiosity exhibited by some special classes of complex eigenvalue problems? Recall that a *physical* quantum theory must (i) have an energy spectrum that is bounded below; (ii) possess a Hilbert space of state vectors that is endowed with an inner product having a positive norm and (iii) have unitary time evolution. The simplest condition on the Hamiltonian  $H$  that guarantees that the quantum theory satisfies these three requirements is that  $H$  be real and symmetric. However, this condition is overly restrictive. One can allow  $H$  to be complex as long as it is Dirac Hermitian:  $H^\dagger = H$ . In this section we explain why we can replace the condition of Hermiticity by the condition that  $H$  have an unbroken  $\mathcal{PT}$  symmetry and still satisfy the above requirements for a physical quantum theory<sup>6</sup>.

##### 4.1. Recipe for a quantum-mechanical theory defined by a Hermitian Hamiltonian

For purposes of comparison, we summarize in this section the standard textbook procedure that one follows in analysing a theory defined by a conventional Hermitian quantum-mechanical Hamiltonian. In the following section we repeat these procedures for a non-Hermitian Hamiltonian.

- (a) *Eigenfunctions and eigenvalues of  $H$ .* Given the Hamiltonian  $H$  one can write down the time-independent Schrödinger equation associated with  $H$  and calculate the eigenvalues  $E_n$  and eigenfunctions  $\psi_n(x)$ . Usually, this calculation is difficult to perform analytically, so it must be done numerically.
- (b) *Orthogonality of eigenfunctions.* Because  $H$  is Hermitian, the eigenfunctions of  $H$  will be orthogonal with respect to the standard Hermitian inner product:

$$(\psi, \phi) \equiv \int dx [\psi(x)]^* \phi(x). \tag{67}$$

*Orthogonality* means that the inner product of two eigenfunctions  $\psi_m(x)$  and  $\psi_n(x)$  associated with different eigenvalues  $E_m \neq E_n$  vanishes:

$$(\psi_m, \phi_n) = 0. \tag{68}$$

(We do not discuss here the technical problems associated with degenerate spectra.)

- (c) *Orthonormality of eigenfunctions.* Since the Hamiltonian is Hermitian, the norm of any vector is guaranteed to be positive. This means that we can normalize the eigenfunctions of  $H$  so that the norm of every eigenfunction is unity:

$$(\psi_n, \psi_n) = 1. \tag{69}$$

- (d) *Completeness of eigenfunctions.* It is a deep theorem of the theory of linear operators on Hilbert spaces that the eigenfunctions of a Hermitian Hamiltonian are *complete*. This means that any (finite-norm) vector  $\chi$  in the Hilbert space can be expressed as a linear combination of the eigenfunctions of  $H$ :

$$\chi = \sum_{n=0}^{\infty} a_n \psi_n. \tag{70}$$

<sup>6</sup> All the  $\mathcal{PT}$ -symmetric Hamiltonians considered in this paper are symmetric under matrix transposition. This matrix symmetry condition is not necessary, but it has the simplifying advantage that we do not need to have a biorthogonal set of basis states. We can consider  $\mathcal{PT}$ -symmetric Hamiltonians that are not symmetric under matrix transposition, but only at the cost of introducing a biorthogonal basis [33, 56].

The formal statement of completeness in coordinate space is the reconstruction of the unit operator (the delta function) as a sum over the eigenfunctions:

$$\sum_{n=0}^{\infty} [\psi_n(x)]^* \psi_n(y) = \delta(x - y). \quad (71)$$

- (e) *Reconstruction of the Hamiltonian  $H$  and Green's function  $G$ , and calculation of the spectral Zeta function.* The Hamiltonian matrix in coordinate space has the form

$$\sum_{n=0}^{\infty} [\psi_n(x)]^* \psi_n(y) E_n = H(x, y) \quad (72)$$

and Green's function is given by

$$\sum_{n=0}^{\infty} [\psi_n(x)]^* \psi_n(y) \frac{1}{E_n} = G(x, y). \quad (73)$$

Green's function is the matrix inverse of the Hamiltonian in the sense that

$$\int dy H(x, y) G(y, z) = \delta(x - z). \quad (74)$$

The formula for Green's function in (73) allows us to calculate the sum of the reciprocals of the energy eigenvalues. We simply set  $x = y$  in (73), integrate with respect to  $x$ , and use the normalization condition in (69) to obtain the result that

$$\int dx G(x, x) = \sum_{n=0}^{\infty} \frac{1}{E_n}. \quad (75)$$

The summation on the right side of (75) is called the *spectral zeta function*. This sum is convergent if the energy levels  $E_n$  rise faster than linearly with  $n$ . Thus, the spectral zeta function for the harmonic oscillator is divergent, but it exists for the  $|x|^{\epsilon+2}$  and  $x^2(ix)^\epsilon$  potentials if  $\epsilon > 0$ .

- (f) *Time evolution and unitarity.* For a Hermitian Hamiltonian the time-evolution operator  $e^{-iHt}$  (see (15)) is unitary, and it automatically preserves the inner product:

$$(\chi(t), \chi(t)) = (\chi(0)e^{iHt}, e^{-iHt}\chi(t)) = (\chi(0), \chi(0)). \quad (76)$$

- (g) *Observables.* An observable is represented by a linear Hermitian operator. The outcome of a measurement is one of the *real* eigenvalues of this operator.

- (h) *Miscellany.* One can study a number of additional topics, such as the classical and semiclassical limits of the quantum theory, probability density and currents, perturbative and non-perturbative calculations and so on. We do not address these issues in depth in this paper.

#### 4.2. Recipe for $\mathcal{PT}$ -symmetric quantum mechanics

Let us follow the recipe outlined in section 4.1 for the case of a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian having an unbroken  $\mathcal{PT}$  symmetry. For definiteness, we will imagine that the non-Hermitian Hamiltonian has the form in (12). The novelty here is that we do not know *a priori* the definition of the inner product, as we do in the case of ordinary Hermitian quantum mechanics. We will have to discover the correct inner product in the course of our analysis. The inner product is determined by the Hamiltonian itself, so  $\mathcal{PT}$ -symmetric quantum mechanics is a kind of 'bootstrap' theory. The Hamiltonian operator chooses its own Hilbert space (and

associated inner product) in which it prefers to live!

- (a) *Eigenfunctions and eigenvalues of  $H$ .* In section 2 we discussed various techniques for determining the coordinate-space eigenfunctions and eigenvalues of a non-Hermitian Hamiltonian. We assume here that we have found the eigenvalues  $E_n$  by using either analytical or numerical methods and that these eigenvalues are all real. (This is equivalent to assuming that the  $\mathcal{PT}$  symmetry of  $H$  is unbroken; that is, all eigenfunctions  $\psi_n(x)$  of  $H$  are also eigenfunctions of  $\mathcal{PT}$ .) The zeros of  $\mathcal{PT}$ -symmetric eigenfunctions have interesting complex interlacing properties [57–59].
- (b) *Orthogonality of eigenfunctions.* To test the orthogonality of the eigenfunctions, we must specify an inner product. (A pair of vectors can be orthogonal with respect to one inner product and not orthogonal with respect to another inner product.) Since we do not yet know what inner product to use, one might try to guess an inner product. Arguing by analogy, one might think that since the inner product in (67) is appropriate for Hermitian Hamiltonians ( $H = H^\dagger$ ), a good choice for an inner product associated with a  $\mathcal{PT}$ -symmetric Hamiltonian ( $H = H^{\mathcal{PT}}$ ) might be

$$\langle \psi, \phi \rangle \equiv \int_C dx [\psi(x)]^{\mathcal{PT}} \phi(x) = \int_C dx [\psi(-x)]^* \phi(x), \tag{77}$$

where  $C$  is a contour in the Stokes wedges shown in figure 2. With this inner-product definition one can show by a trivial integration-by-parts argument using the time-independent Schrödinger equation (24) that pairs of eigenfunctions of  $H$  associated with different eigenvalues are orthogonal. However, this guess for an inner product is not acceptable for formulating a valid quantum theory because the norm of a state is not necessarily positive.

- (c) *The  $\mathcal{CPT}$  inner product.* To construct an inner product with a positive norm for a complex non-Hermitian Hamiltonian having an *unbroken*  $\mathcal{PT}$  symmetry, we will construct a new linear operator  $\mathcal{C}$  that commutes with both  $H$  and  $\mathcal{PT}$ . Because  $\mathcal{C}$  commutes with the Hamiltonian, it represents a *symmetry* of  $H$ . We use the symbol  $\mathcal{C}$  to represent this symmetry because, as we will see, the properties of  $\mathcal{C}$  are similar to those of the charge conjugation operator in particle physics. The inner product with respect to  $\mathcal{CPT}$  conjugation is defined as

$$\langle \psi | \chi \rangle^{\mathcal{CPT}} = \int dx \psi^{\mathcal{CPT}}(x) \chi(x), \tag{78}$$

where  $\psi^{\mathcal{CPT}}(x) = \int dy \mathcal{C}(x, y) \psi^*(-y)$ . We will show that this inner product satisfies the requirements for the quantum theory defined by  $H$  to have a Hilbert space with a positive norm and to be a unitary theory of quantum mechanics. We will represent the  $\mathcal{C}$  operator as a sum over the eigenfunctions of  $H$ , but before doing so we must first show how to normalize these eigenfunctions.

- (d)  *$\mathcal{PT}$ -symmetric normalization of the eigenfunctions and the strange statement of completeness.* We showed in (19) that the eigenfunctions  $\psi_n(x)$  of  $H$  are also eigenfunctions of the  $\mathcal{PT}$  operator with eigenvalue  $\lambda = e^{i\alpha}$ , where  $\lambda$  and  $\alpha$  depend on  $n$ . Thus, we can construct  $\mathcal{PT}$ -normalized eigenfunctions  $\phi_n(x)$  defined by

$$\phi_n(x) \equiv e^{-i\alpha/2} \psi_n(x). \tag{79}$$

By this construction,  $\phi_n(x)$  is still an eigenfunction of  $H$  and it is also an eigenfunction of  $\mathcal{PT}$  with eigenvalue 1. One can also show both numerically and analytically that the algebraic sign of the  $\mathcal{PT}$  norm in (77) of  $\phi_n(x)$  is  $(-1)^n$  for all  $n$  and for all values of  $\epsilon > 0$  [60]. Thus, we *define* the eigenfunctions so that their  $\mathcal{PT}$  norms are exactly  $(-1)^n$ :

$$\int_C dx [\phi_n(x)]^{\mathcal{PT}} \phi_n(x) = \int_C dx [\phi_n(-x)]^* \phi_n(x) = (-1)^n, \tag{80}$$

where the contour  $C$  lies in the Stokes wedges shown in figure 2. In terms of these  $\mathcal{PT}$ -normalized eigenfunctions there is a simple but unusual statement of completeness:

$$\sum_{n=0}^{\infty} (-1)^n \phi_n(x) \phi_n(y) = \delta(x - y). \tag{81}$$

This unusual statement of completeness has been verified both numerically and analytically to great precision for all  $\epsilon > 0$  [61, 62] and a mathematical proof has been given [33]. It is easy to verify using (80) that the left side of (81) satisfies the integration rule for delta functions:  $\int dy \delta(x - y) \delta(y - z) = \delta(x - z)$ .

*Example:  $\mathcal{PT}$ -symmetric normalization of harmonic-oscillator eigenfunctions.*

For the harmonic-oscillator Hamiltonian  $H = \hat{p}^2 + \hat{x}^2$ , the eigenfunctions are Gaussians multiplied by Hermite polynomials:  $\psi_0(x) = \exp(-\frac{1}{2}x^2)$ ,  $\psi_1(x) = x \exp(-\frac{1}{2}x^2)$ ,  $\psi_2(x) = (2x^2 - 1) \exp(-\frac{1}{2}x^2)$ ,  $\psi_3(x) = (2x^3 - 3x) \exp(-\frac{1}{2}x^2)$ , and so on. To normalize these eigenfunctions so that they are also eigenfunctions of the  $\mathcal{PT}$  operator with eigenvalue 1, we choose

$$\begin{aligned} \phi_0(x) &= a_0 \exp(-\frac{1}{2}x^2), \\ \phi_1(x) &= a_1 i x \exp(-\frac{1}{2}x^2), \\ \psi_2(x) &= a_2 (2x^2 - 1) \exp(-\frac{1}{2}x^2), \\ \psi_3(x) &= a_3 i (2x^3 - 3x) \exp(-\frac{1}{2}x^2), \end{aligned} \tag{82}$$

and so on, where the real numbers  $a_n$  are chosen so that the integral in (80) evaluates to  $(-1)^n$  for all  $n$ . It is easy to verify that if the eigenfunctions  $\phi_n(x)$  are substituted into (81) and the summation is performed, then the result is the Dirac delta function on the right side of (81).

- (e) *Coordinate-space representation of  $H$  and  $G$  and the spectral Zeta function.* From the statement of completeness in (81) we can construct coordinate-space representations of the linear operators. For example, since the coordinate-space representation of the parity operator is  $\mathcal{P}(x, y) = \delta(x + y)$ , we have

$$\mathcal{P}(x, y) = \sum_{n=0}^{\infty} (-1)^n \phi_n(x) \phi_n(-y). \tag{83}$$

We can also construct the coordinate-space representations of the Hamiltonian and Green's function,

$$\begin{aligned} H(x, y) &= \sum_{n=0}^{\infty} (-1)^n E_n \phi_n(x) \phi_n(y), \\ G(x, y) &= \sum_{n=0}^{\infty} (-1)^n \frac{1}{E_n} \phi_n(x) \phi_n(y), \end{aligned} \tag{84}$$

and using (80) it is straightforward to show that  $G$  is the functional inverse of  $H$ :  $\int dy H(x, y) G(y, z) = \delta(x - z)$ . For the class of  $\mathcal{PT}$ -symmetric Hamiltonians in (12) this equation takes the form of a differential equation satisfied by  $G(x, y)$ :

$$\left( -\frac{d^2}{dx^2} + x^2 (ix)^\epsilon \right) G(x, y) = \delta(x - y). \tag{85}$$

Equation (85) can be solved in terms of associated Bessel functions in each of two regions,  $x > y$  and  $x < y$ . The solutions can then be patched together at  $x = y$  to obtain a closed-form expression for  $G(x, y)$  [61, 62]. One then uses (75) to find an exact formula for the spectral zeta function for all values of  $\epsilon$ :

$$\sum_n \frac{1}{E_n} = \left[ 1 + \frac{\cos\left(\frac{3\epsilon\pi}{2\epsilon+8}\right) \sin\left(\frac{\pi}{4+\epsilon}\right)}{\cos\left(\frac{\epsilon\pi}{4+2\epsilon}\right) \sin\left(\frac{3\pi}{4+\epsilon}\right)} \right] \frac{\Gamma\left(\frac{1}{4+\epsilon}\right) \Gamma\left(\frac{2}{4+\epsilon}\right) \Gamma\left(\frac{\epsilon}{4+\epsilon}\right)}{(4+\epsilon)^{\frac{4+2\epsilon}{4+\epsilon}} \Gamma\left(\frac{1+\epsilon}{4+\epsilon}\right) \Gamma\left(\frac{2+\epsilon}{4+\epsilon}\right)}. \quad (86)$$

- (f) *Construction of the  $\mathcal{C}$  operator.* The situation here in which half of the energy eigenstates have positive norm and half have negative norm (see (80)) is analogous to the problem that Dirac encountered in formulating the spinor wave equation in relativistic quantum theory [63]. Following Dirac, we attack the problem of an indefinite norm by finding an interpretation of the negative-norm states. For any Hamiltonian  $H$  having an unbroken  $\mathcal{PT}$  symmetry there exists an additional symmetry of  $H$  connected with the fact that there are equal numbers of positive- and negative-norm states. The linear operator  $\mathcal{C}$  that embodies this symmetry can be represented in coordinate space as a sum over the  $\mathcal{PT}$ -normalized eigenfunctions of the  $\mathcal{PT}$ -symmetric Hamiltonian in (12):

$$\mathcal{C}(x, y) = \sum_{n=0}^{\infty} \phi_n(x)\phi_n(y). \quad (87)$$

Notice that this equation is identical to the statement of completeness in (81) except that the factor of  $(-1)^n$  is absent. We can use (80) and (81) to verify that the square of  $\mathcal{C}$  is unity ( $\mathcal{C}^2 = \mathbf{1}$ ):

$$\int dy \mathcal{C}(x, y)\mathcal{C}(y, z) = \delta(x - z). \quad (88)$$

Thus, the eigenvalues of  $\mathcal{C}$  are  $\pm 1$ . Also,  $\mathcal{C}$  commutes with  $H$ . Therefore, since  $\mathcal{C}$  is linear, the eigenstates of  $H$  have definite values of  $\mathcal{C}$ . Specifically,

$$\begin{aligned} \mathcal{C}\phi_n(x) &= \int dy \mathcal{C}(x, y)\phi_n(y) \\ &= \sum_{m=0}^{\infty} \phi_m(x) \int dy \phi_m(y)\phi_n(y) = (-1)^n \phi_n(x). \end{aligned} \quad (89)$$

This new operator  $\mathcal{C}$  resembles the charge-conjugation operator in quantum field theory. However, the precise meaning of  $\mathcal{C}$  is that it represents the measurement of the sign of the  $\mathcal{PT}$  norm in (80) of an eigenstate.

The operators  $\mathcal{P}$  and  $\mathcal{C}$  are distinct square roots of the unity operator  $\delta(x - y)$ . That is,  $\mathcal{P}^2 = \mathcal{C}^2 = \mathbf{1}$ , but  $\mathcal{P} \neq \mathcal{C}$  because  $\mathcal{P}$  is real, while  $\mathcal{C}$  is complex. The parity operator in coordinate space is explicitly real ( $\mathcal{P}(x, y) = \delta(x + y)$ ), while the operator  $\mathcal{C}(x, y)$  is complex because it is a sum of products of complex functions. The two operators  $\mathcal{P}$  and  $\mathcal{C}$  do not commute. However,  $\mathcal{C}$  does commute with  $\mathcal{PT}$ .

- (g) *Positive norm and unitarity in  $\mathcal{PT}$ -symmetric quantum mechanics.* Having constructed the operator  $\mathcal{C}$ , we can now use the new  $\mathcal{CPT}$  inner product defined in (78). Like the  $\mathcal{PT}$  inner product, this new inner product is phase independent. Also, because the time-evolution operator (as in ordinary quantum mechanics) is  $e^{-iHt}$  and because  $H$  commutes with  $\mathcal{PT}$  and with  $\mathcal{CPT}$ , both the  $\mathcal{PT}$  inner product and the  $\mathcal{CPT}$  inner product remain time independent as the states evolve. However, unlike the  $\mathcal{PT}$  inner product, the  $\mathcal{CPT}$

inner product is *positive definite* because  $\mathcal{C}$  contributes a factor of  $-1$  when it acts on states with negative  $\mathcal{PT}$  norm. In terms of the  $\mathcal{CPT}$  conjugate, the completeness condition reads

$$\sum_{n=0}^{\infty} \phi_n(x) [\mathcal{CPT} \phi_n(y)] = \delta(x - y). \quad (90)$$

#### 4.3. Comparison of Hermitian and $\mathcal{PT}$ -symmetric quantum theories

We have shown in sections 4.1 and 4.2 how to construct quantum theories based on Hermitian and on non-Hermitian Hamiltonians. In the formulation of a conventional quantum theory defined by a Hermitian Hamiltonian, the Hilbert space of physical states is specified even before the Hamiltonian is known. The inner product (67) in this vector space is defined with respect to Dirac Hermitian conjugation (complex conjugate and transpose). The Hamiltonian is then chosen and the eigenvectors and eigenvalues of the Hamiltonian are determined. In contrast, the inner product for a quantum theory defined by a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian depends on the Hamiltonian itself and thus is determined *dynamically*. One must solve for the eigenstates of  $H$  before knowing the Hilbert space and the associated inner product of the theory because the  $\mathcal{C}$  operator is defined and constructed in terms of the eigenstates of the Hamiltonian. The Hilbert space, which consists of all complex linear combinations of the eigenstates of  $H$ , and the  $\mathcal{CPT}$  inner product are determined by these eigenstates.

The operator  $\mathcal{C}$  does not exist as a distinct entity in ordinary Hermitian quantum mechanics. Indeed, if we allow the parameter  $\epsilon$  in (12) to tend to 0, the operator  $\mathcal{C}$  in this limit becomes identical to  $\mathcal{P}$  and the  $\mathcal{CPT}$  operator becomes  $\mathcal{T}$ , which performs complex conjugation. Hence, the inner product defined with respect to  $\mathcal{CPT}$  conjugation reduces to the inner product of conventional quantum mechanics and (81) reduces to the usual statement of completeness  $\sum_n \phi_n(x) \phi_n^*(y) = \delta(x - y)$ .

The  $\mathcal{CPT}$  inner product is independent of the choice of integration contour  $C$  as long as  $C$  lies inside the asymptotic wedges associated with the boundary conditions for the eigenvalue problem. In ordinary quantum mechanics, where the positive-definite inner product has the form  $\int dx f^*(x)g(x)$ , the integral must be taken along the real axis and the path of integration cannot be deformed into the complex plane because the integrand is not analytic. The  $\mathcal{PT}$  inner product shares with the  $\mathcal{CPT}$  inner-product the advantage of analyticity and path independence, but it suffers from non-positivity. It is surprising that we can construct a positive-definite metric by using  $\mathcal{CPT}$  conjugation without disturbing the path independence of the inner-product integral.

Time evolution is expressed by the operator  $e^{-iHt}$  whether the theory is determined by a  $\mathcal{PT}$ -symmetric Hamiltonian or just an ordinary Hermitian Hamiltonian. To establish unitarity we must show that as a state vector evolves, its norm does not change in time. If  $\psi_0(x)$  is any given initial vector belonging to the Hilbert space spanned by the energy eigenstates, then it evolves into the state  $\psi_t(x)$  at time  $t$  according to  $\psi_t(x) = e^{-iHt} \psi_0(x)$ . With respect to the  $\mathcal{CPT}$  inner product the norm of  $\psi_t(x)$  does not change in time because  $H$  commutes with  $\mathcal{CPT}$ .

#### 4.4. Observables

How do we represent an observable in  $\mathcal{PT}$ -symmetric quantum mechanics? Recall that in ordinary quantum mechanics the condition for a linear operator  $A$  to be an observable is that  $A = A^\dagger$ . This condition guarantees that the expectation value of  $A$  in a state is real. Operators in the Heisenberg picture evolve in time according to  $A(t) = e^{iHt} A(0) e^{-iHt}$ , so this Hermiticity condition is maintained in time. In  $\mathcal{PT}$ -symmetric quantum mechanics the equivalent condition

is that at time  $t = 0$  the operator  $A$  must obey the condition  $A^T = \mathcal{CPT}A\mathcal{CPT}$ , where  $A^T$  is the *transpose* of  $A$  [60]. If this condition holds at  $t = 0$ , then it will continue to hold for all time because we have assumed that  $H$  is symmetric ( $H = H^T$ ). This condition also guarantees that the expectation value of  $A$  in any state is real<sup>7</sup>.

The operator  $\mathcal{C}$  itself satisfies this requirement, so it is an observable. The Hamiltonian is also an observable. However, the  $\hat{x}$  and  $\hat{p}$  operators are not observables. Indeed, the expectation value of  $\hat{x}$  in the ground state is a negative imaginary number. Thus, there is no position operator in  $\mathcal{PT}$ -symmetric quantum mechanics. In this sense  $\mathcal{PT}$ -symmetric quantum mechanics is similar to fermionic quantum field theories. In such theories the fermion field corresponds to the  $\hat{x}$  operator. The fermion field is complex and does not have a classical limit. One cannot measure the position of an electron; one can only measure the position of the *charge* or the *energy* of the electron!

One can see why the expectation of the  $x$  operator in  $\mathcal{PT}$ -symmetric quantum mechanics is a negative imaginary number by examining a classical trajectory like that shown in figure 15. Note that this classical trajectory has left–right ( $\mathcal{PT}$ ) symmetry, but not up–down symmetry. Also, the classical paths favour (spend more time in) the lower-half complex- $x$  plane. Thus, the average classical position is a negative imaginary number. Just as the classical particle moves about in the complex plane, the quantum probability current flows about in the complex plane. It may be that the correct interpretation is to view  $\mathcal{PT}$ -symmetric quantum mechanics as describing the interaction of extended, rather than point-like objects.

#### 4.5. Pseudo-Hermiticity, quasi-Hermiticity and $\mathcal{PT}$ symmetry

The thesis of this paper—replacing the mathematical condition of Hermiticity by the more physical condition of  $\mathcal{PT}$  symmetry—can be placed in a more general mathematical context known as *pseudo-Hermiticity*. A linear operator  $A$  is pseudo-Hermitian if there is a Hermitian operator  $\eta$  such that

$$A^\dagger = \eta A \eta. \quad (91)$$

The operator  $\eta$  is often called an *intertwining* operator. The condition in (91) reduces to ordinary Hermiticity when the intertwining operator  $\eta$  is the identity  $\mathbf{1}$  and reduces to  $\mathcal{PT}$  symmetry when  $\eta = \mathcal{P}$ . The concept of pseudo-Hermiticity was introduced in the 1940s by Dirac and Pauli and later discussed by Lee, Wick and Sudarshan, who were trying to resolve the problems that arise in quantizing electrodynamics and other quantum field theories in which negative-norm states appear as a consequence of renormalization [67–71]. These problems are illustrated very clearly by the Lee model, which is discussed in section 8.3.

The related notion of quasi-Hermiticity was discussed in detail in 1992 by Scholtz *et al* [10]. This deep paper is relevant to  $\mathcal{PT}$  symmetry because it was the first to show how to construct a similarity transformation that maps Hermitian operators onto the corresponding quasi-Hermitian operators and also the first to consider the corresponding transformations of infinite-dimensional Hilbert-space inner products.

Mostafazadeh first pointed out that because the parity operator  $\mathcal{P}$  is Hermitian, it may be used as an intertwining operator. The class of Hamiltonians  $H$  in (12) is pseudo-Hermitian because the parity operator  $\mathcal{P}$  changes the sign of  $\hat{x}$  while Dirac Hermitian conjugation changes the sign of  $i$  [65, 72–74]:

$$H^\dagger = \mathcal{P} H \mathcal{P}. \quad (92)$$

<sup>7</sup> The requirement given here for  $A$  to be an observable involves matrix transposition. This condition is more restrictive than is necessary and it has been generalized by Mostafazadeh. See [64–66]. Note that if the matrix transpose symmetry condition on the Hamiltonian is removed we must introduce a biorthogonal basis. See [33,56].



For other references on the generalization of  $\mathcal{PT}$  symmetry to pseudo-Hermiticity see [75].

### 5. Illustrative $2 \times 2$ matrix example of a $\mathcal{PT}$ -symmetric Hamiltonian

It is always useful to study exactly solvable models when one is trying to understand a formal procedure like that discussed in section 4. One exactly solvable model, which has been used in many papers on  $\mathcal{PT}$  symmetry, is due to Swanson [76]. This model is exactly solvable because it is quadratic in  $\hat{x}$  and  $\hat{p}$ . In this section we use an even simpler model to illustrate the construction of a quantum theory described by a  $\mathcal{PT}$ -symmetric Hamiltonian. We consider the elementary  $2 \times 2$  Hamiltonian matrix

$$H = \begin{pmatrix} r e^{i\theta} & s \\ s & r e^{-i\theta} \end{pmatrix}, \quad (93)$$

where the three parameters  $r$ ,  $s$  and  $\theta$  are real [77]. The Hamiltonian in (93) is not Hermitian, but it is easy to see that it is  $\mathcal{PT}$  symmetric, where we define the parity operator as

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (94)$$

and we define the operator  $\mathcal{T}$  to perform complex conjugation.

As a first step in analysing the Hamiltonian (93), we calculate its two eigenvalues:

$$E_{\pm} = r \cos \theta \pm (s^2 - r^2 \sin^2 \theta)^{1/2}. \quad (95)$$

There are clearly two parametric regions to consider, one for which the square root in (95) is real and the other for which it is imaginary. When  $s^2 < r^2 \sin^2 \theta$ , the energy eigenvalues form a complex-conjugate pair. This is the region of broken  $\mathcal{PT}$  symmetry. On the other hand, when  $s^2 \geq r^2 \sin^2 \theta$ , the eigenvalues  $\varepsilon_{\pm} = r \cos \theta \pm (s^2 - r^2 \sin^2 \theta)^{1/2}$  are real. This is the region of unbroken  $\mathcal{PT}$  symmetry. In the unbroken region the simultaneous eigenstates of the operators  $H$  and  $\mathcal{PT}$  are

$$|E_{+}\rangle = \frac{1}{\sqrt{2 \cos \alpha}} \begin{pmatrix} e^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix} \quad \text{and} \quad |E_{-}\rangle = \frac{i}{\sqrt{2 \cos \alpha}} \begin{pmatrix} e^{-i\alpha/2} \\ -e^{i\alpha/2} \end{pmatrix}, \quad (96)$$

where

$$\sin \alpha = \frac{r}{s} \sin \theta. \quad (97)$$

The  $\mathcal{PT}$  inner product gives

$$(E_{\pm}, E_{\pm}) = \pm 1 \quad \text{and} \quad (E_{\pm}, E_{\mp}) = 0, \quad (98)$$

where  $(u, v) = (\mathcal{PT}u) \cdot v$ . With respect to the  $\mathcal{PT}$  inner product, the vector space spanned by the energy eigenstates has a metric of signature  $(+, -)$ . If the condition  $s^2 > r^2 \sin^2 \theta$  for an unbroken  $\mathcal{PT}$  symmetry is violated, the states (96) are no longer eigenstates of  $\mathcal{PT}$  because  $\alpha$  becomes imaginary. When  $\mathcal{PT}$  symmetry is broken, the  $\mathcal{PT}$  norm of the energy eigenstate vanishes.

Next, we construct the operator  $\mathcal{C}$  using (87):

$$\mathcal{C} = \frac{1}{\cos \alpha} \begin{pmatrix} i \sin \alpha & 1 \\ 1 & -i \sin \alpha \end{pmatrix}. \quad (99)$$

Note that  $\mathcal{C}$  is distinct from  $H$  and  $\mathcal{P}$  and it has the key property that

$$\mathcal{C}|E_{\pm}\rangle = \pm|E_{\pm}\rangle. \quad (100)$$

The operator  $\mathcal{C}$  commutes with  $H$  and satisfies  $\mathcal{C}^2 = 1$ . The eigenvalues of  $\mathcal{C}$  are precisely the signs of the  $\mathcal{PT}$  norms of the corresponding eigenstates. Using the operator  $\mathcal{C}$  we construct the new inner-product structure  $\langle u|v\rangle = (\mathcal{CPT}u) \cdot v$ . This inner product is positive definite because  $\langle E_{\pm}|E_{\pm}\rangle = 1$ . Thus, the two-dimensional Hilbert space spanned by  $|E_{\pm}\rangle$ , with inner product  $\langle \cdot|\cdot\rangle$ , has signature  $(+, +)$ .

Finally, we prove that the  $\mathcal{CPT}$  norm of any vector is positive. For the arbitrary vector  $\psi = \begin{pmatrix} a \\ b \end{pmatrix}$ , where  $a$  and  $b$  are any complex numbers, we see that

$$\begin{aligned} T\psi &= \begin{pmatrix} a^* \\ b^* \end{pmatrix}, & \mathcal{PT}\psi &= \begin{pmatrix} b^* \\ a^* \end{pmatrix}, \\ \mathcal{CPT}\psi &= \frac{1}{\cos\alpha} \begin{pmatrix} a^* + ib^* \sin\alpha \\ b^* - ia^* \sin\alpha \end{pmatrix}. \end{aligned} \tag{101}$$

Thus,  $\langle\psi|\psi\rangle = (\mathcal{CPT}\psi) \cdot \psi = \frac{1}{\cos\alpha}[a^*a + b^*b + i(b^*b - a^*a) \sin\alpha]$ . Now let  $a = x + iy$  and  $b = u + iv$ , where  $x, y, u$  and  $v$  are real. Then

$$\langle\psi|\psi\rangle = \frac{1}{\cos\alpha} (x^2 + v^2 + 2xv \sin\alpha + y^2 + u^2 - 2yu \sin\alpha), \tag{102}$$

which is explicitly positive and vanishes only if  $x = y = u = v = 0$ .

Since  $\langle u|$  denotes the  $\mathcal{CPT}$ -conjugate of  $|u\rangle$ , the completeness condition reads

$$|E_+\rangle\langle E_+| + |E_-\rangle\langle E_-| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{103}$$

Furthermore, using the  $\mathcal{CPT}$  conjugate  $\langle E_{\pm}|$ , we can represent  $\mathcal{C}$  as

$$\mathcal{C} = |E_+\rangle\langle E_+| - |E_-\rangle\langle E_-|. \tag{104}$$

In the limit  $\theta \rightarrow 0$ , the Hamiltonian (93) for this two-state system becomes Hermitian and  $\mathcal{C}$  reduces to the parity operator  $\mathcal{P}$ . Thus,  $\mathcal{CPT}$  invariance reduces to the standard condition of Hermiticity for a symmetric matrix; namely,  $H = H^*$ .

### 6. Calculation of the $\mathcal{C}$ operator in quantum mechanics

The distinguishing feature of  $\mathcal{PT}$ -symmetric quantum mechanics is the  $\mathcal{C}$  operator. In ordinary Hermitian quantum mechanics there is no such operator. Only a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian possesses a  $\mathcal{C}$  operator distinct from the parity operator  $\mathcal{P}$ . Indeed, if we were to sum the series in (87) for a  $\mathcal{PT}$ -symmetric Hermitian Hamiltonian, the result would be  $\mathcal{P}$ , which in coordinate space is  $\delta(x + y)$ . (See (83).)

While the  $\mathcal{C}$  operator is represented formally in (87) as an infinite series, it is not easy to evaluate the sum of this series. Calculating  $\mathcal{C}$  by direct brute-force evaluation of the sum in (87) is not easy in quantum mechanics because it is necessary to find all the eigenfunctions  $\phi_n(x)$  of  $H$ . Furthermore, such a procedure cannot be used in quantum field theory because in field theory there is no simple analog of the Schrödinger eigenvalue differential equation and its associated coordinate-space eigenfunctions.

The first attempt to calculate  $\mathcal{C}$  relied on a perturbative approach [78]. In this paper the  $\mathcal{PT}$ -symmetric Hamiltonian

$$H = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + i\epsilon\hat{x}^3 \tag{105}$$

is considered, where  $\epsilon$  is treated as a small real parameter. When  $\epsilon = 0$ , the Hamiltonian reduces to the Hamiltonian for the quantum harmonic oscillator, all of whose eigenfunctions

can be calculated exactly. Thus, it is possible to express the eigenfunctions of  $H$  in (105) in the form of perturbation series in powers of  $\epsilon$ . For each of the eigenfunctions the first few terms in the perturbation series were calculated. These perturbation series were then substituted into (87) and the summation over the  $n$ th eigenfunction was performed. The result is a perturbation-series expansion of the  $\mathcal{C}$  operator. This calculation is long and tedious and the final result is quite complicated. However, the calculation turned out to be of great value because while the final answer is complicated, it was discovered that the answer in coordinate space simplified dramatically if the  $\mathcal{C}$  operator is written as the exponential of a derivative operator  $Q$  multiplying the parity operator  $\mathcal{P}$ :

$$\mathcal{C}(x, y) = \exp \left[ Q \left( x, -i \frac{d}{dx} \right) \right] \delta(x + y). \tag{106}$$

The simplification that occurs when  $\mathcal{C}$  is written in the form  $\mathcal{C} = e^{Q\mathcal{P}}$  is that while the expression for  $\mathcal{C}$  is a series in all positive integer powers of  $\epsilon$ ,  $Q$  is a series in *odd* powers of  $\epsilon$  only. Since  $Q$  is a series in odd powers of  $\epsilon$ , in the limit  $\epsilon \rightarrow 0$  the function  $Q$  vanishes. Thus, in this limit the  $\mathcal{C}$  operator tends to the parity operator  $\mathcal{P}$ .

The expression in (106) need not be limited to coordinate space. A more general way to represent the  $\mathcal{C}$  operator is to express it generically in terms of the fundamental dynamical operators  $\hat{x}$  and  $\hat{p}$ :

$$\mathcal{C} = e^{Q(\hat{x}, \hat{p})} \mathcal{P}. \tag{107}$$

Written in this form,  $Q$  is a *real* function of its two variables. By seeking the  $\mathcal{C}$  operator in the form (107) we will be able to devise powerful analytic tools for calculating it.

We illustrate the representation  $\mathcal{C} = e^{Q\mathcal{P}}$  by using two elementary Hamiltonians. First, consider the shifted harmonic oscillator  $H = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + i\epsilon\hat{x}$ . This Hamiltonian has an unbroken  $\mathcal{PT}$  symmetry for all real  $\epsilon$ . Its eigenvalues  $E_n = n + \frac{1}{2} + \frac{1}{2}\epsilon^2$  are all real. The exact formula for  $\mathcal{C}$  for this theory is given exactly by  $\mathcal{C} = e^{Q\mathcal{P}}$ , where

$$Q = -\epsilon\hat{p}. \tag{108}$$

Note that in the limit  $\epsilon \rightarrow 0$ , where the Hamiltonian becomes Hermitian,  $\mathcal{C}$  becomes identical with  $\mathcal{P}$ .

As a second example, consider the non-Hermitian  $2 \times 2$  matrix Hamiltonian (93). The associated  $\mathcal{C}$  operator in (99) can be rewritten in the form  $\mathcal{C} = e^{Q\mathcal{P}}$ , where

$$Q = \frac{1}{2}\sigma_2 \ln \left( \frac{1 - \sin \alpha}{1 + \sin \alpha} \right) \tag{109}$$

and

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{110}$$

is the Pauli sigma matrix. Again, observe that in the limit  $\theta \rightarrow 0$ , where the Hamiltonian becomes Hermitian, the  $\mathcal{C}$  operator becomes identical with  $\mathcal{P}$ .

### 6.1. Algebraic equations satisfied by the $\mathcal{C}$ operator

Fortunately, there is a relatively easy algebraic way to calculate the  $\mathcal{C}$  operator, and the procedure circumvents the difficult problem of evaluating the sum in (87). As a result, the technique readily generalizes from quantum mechanics to quantum field theory. In this section we show how to use this technique to calculate  $\mathcal{C}$  for the  $\mathcal{PT}$ -symmetric Hamiltonian in (105). We explain how to calculate  $\mathcal{C}$  perturbatively to high order in powers of  $\epsilon$  for this cubic

Hamiltonian. Calculating  $\mathcal{C}$  for other kinds of interactions is more difficult and may require the use of semiclassical approximations [79].

To calculate  $\mathcal{C}$  we make use of its three crucial algebraic properties. First,  $\mathcal{C}$  commutes with the space–time reflection operator  $\mathcal{PT}$ ,

$$[\mathcal{C}, \mathcal{PT}] = 0, \tag{111}$$

although  $\mathcal{C}$  does not, in general, commute with  $\mathcal{P}$  or  $\mathcal{T}$  separately. Second, the square of  $\mathcal{C}$  is the identity,

$$\mathcal{C}^2 = \mathbf{1}, \tag{112}$$

which allows us to interpret  $\mathcal{C}$  as a reflection operator. Third,  $\mathcal{C}$  commutes with  $H$ ,

$$[\mathcal{C}, H] = 0, \tag{113}$$

and thus is time independent. To summarize,  $\mathcal{C}$  is a time-independent  $\mathcal{PT}$ -symmetric reflection operator.

The procedure for calculating  $\mathcal{C}$  is simply to substitute the generic operator representation in (107) into the three algebraic equations (111)–(113) in turn and to solve the resulting equations for the function  $Q$ . First, we substitute (107) into the condition (111) to obtain

$$e^{Q(\hat{x}, \hat{p})} = \mathcal{PT}e^{Q(\hat{x}, \hat{p})}\mathcal{PT} = e^{Q(-\hat{x}, \hat{p})}, \tag{114}$$

from which we conclude that  $Q(\hat{x}, \hat{p})$  is an *even* function of  $\hat{x}$ .

Second, we substitute (107) into the condition (112) and find that

$$e^{Q(\hat{x}, \hat{p})}\mathcal{P}e^{Q(\hat{x}, \hat{p})}\mathcal{P} = e^{Q(\hat{x}, \hat{p})}e^{Q(-\hat{x}, -\hat{p})} = 1, \tag{115}$$

which implies that  $Q(\hat{x}, \hat{p}) = -Q(-\hat{x}, -\hat{p})$ . Since we already know that  $Q(\hat{x}, \hat{p})$  is an even function of  $\hat{x}$ , we conclude that it is also an *odd* function of  $\hat{p}$ .

The remaining condition (113) to be imposed is that the operator  $\mathcal{C}$  commutes with  $H$ . While the first two conditions are, in effect, *kinematic* conditions on  $Q$  that are generally true for any Hamiltonian, condition (113) is equivalent to imposing the specific dynamics of the particular Hamiltonian that defines the quantum theory. Substituting  $\mathcal{C} = e^{Q(\hat{x}, \hat{p})}\mathcal{P}$  into (113), we get

$$e^{Q(\hat{x}, \hat{p})}[\mathcal{P}, H] + [e^{Q(\hat{x}, \hat{p})}, H]\mathcal{P} = 0. \tag{116}$$

This equation is difficult to solve in general, and to do so we must use perturbative methods, as we explain in the following section.

### 6.2. Perturbative calculation of $\mathcal{C}$

To solve (116) for the Hamiltonian in (105), we express this Hamiltonian in the form  $H = H_0 + \epsilon H_1$ . Here,  $H_0$  is the harmonic-oscillator Hamiltonian  $H_0 = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2$ , which commutes with the parity operator  $\mathcal{P}$ , and  $H_1 = i\hat{x}^3$ , which *anticommutes* with  $\mathcal{P}$ . Thus, the condition (116) becomes

$$2\epsilon e^{Q(\hat{x}, \hat{p})} H_1 = [e^{Q(\hat{x}, \hat{p})}, H]. \tag{117}$$

We expand the operator  $Q(\hat{x}, \hat{p})$  as a perturbation series in odd powers of  $\epsilon$ :

$$Q(\hat{x}, \hat{p}) = \epsilon Q_1(\hat{x}, \hat{p}) + \epsilon^3 Q_3(\hat{x}, \hat{p}) + \epsilon^5 Q_5(\hat{x}, \hat{p}) + \dots \tag{118}$$

Substituting the expansion in (118) into the exponential  $e^{Q(\hat{x}, \hat{p})}$ , we get after some algebra a sequence of equations that can be solved systematically for the operator-valued functions

$Q_n(\hat{x}, \hat{p})$  ( $n = 1, 3, 5, \dots$ ) subject to the symmetry constraints that ensure the conditions (111) and (112). The first three of these equations are

$$\begin{aligned} [H_0, Q_1] &= -2H_1, \\ [H_0, Q_3] &= -\frac{1}{6}[Q_1, [Q_1, H_1]], \\ [H_0, Q_5] &= \frac{1}{360}[Q_1, [Q_1, [Q_1, [Q_1, H_1]]]] - \frac{1}{6}[Q_1, [Q_3, H_1]] + \frac{1}{6}[Q_3, [Q_1, H_1]]. \end{aligned} \quad (119)$$

Let us solve these equations for the Hamiltonian in (105), for which  $H_0 = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2$  and  $H_1 = i\hat{x}^3$ . The procedure is to substitute the most general polynomial form for  $Q_n$  using arbitrary coefficients and then to solve for these coefficients. For example, to solve  $[H_0, Q_1] = -2i\hat{x}^3$ , the first of the equations in (119), we take as an ansatz for  $Q_1$  the most general Hermitian cubic polynomial that is even in  $\hat{x}$  and odd in  $p$ :

$$Q_1(\hat{x}, \hat{p}) = M\hat{p}^3 + N\hat{x}\hat{p}\hat{x}, \quad (120)$$

where  $M$  and  $N$  are numerical coefficients to be determined. The operator equation for  $Q_1$  is satisfied if  $M = -\frac{4}{3}$  and  $N = -2$ .

It is algebraically tedious but completely straightforward to continue this process. In order to present the solutions for  $Q_n(\hat{x}, \hat{p})$  ( $n > 1$ ), it is convenient to introduce the following notation: let  $S_{m,n}$  represent the *totally symmetrized* sum over all terms containing  $m$  factors of  $\hat{p}$  and  $n$  factors of  $\hat{x}$ . For example,

$$S_{0,0} = 1, \quad S_{0,3} = \hat{x}^3, \quad S_{1,1} = \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}), \quad S_{1,2} = \frac{1}{3}(\hat{x}^2\hat{p} + \hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2), \quad (121)$$

and so on. (The properties of the operators  $S_{m,n}$  are summarized in [80].)

In terms of the symmetrized operators  $S_{m,n}$  the first three functions  $Q_{2n+1}$  are

$$\begin{aligned} Q_1 &= -\frac{4}{3}\hat{p}^3 - 2S_{1,2}, \\ Q_3 &= \frac{128}{15}\hat{p}^5 + \frac{40}{3}S_{3,2} + 8S_{1,4} - 12\hat{p}, \\ Q_5 &= -\frac{320}{3}\hat{p}^7 - \frac{544}{3}S_{5,2} - \frac{512}{3}S_{3,4} - 64S_{1,6} + \frac{24736}{45}\hat{p}^3 + \frac{6368}{15}S_{1,2}. \end{aligned} \quad (122)$$

Together, (107) (118) and (122) represent an explicit perturbative expansion of  $\mathcal{C}$  in terms of the operators  $\hat{x}$  and  $\hat{p}$ , correct to order  $\epsilon^6$ .

To summarize, using the ansatz (107) we can calculate  $\mathcal{C}$  to high order in perturbation theory. We are able to perform this calculation because this ansatz obviates the necessity of calculating the  $\mathcal{PT}$ -normalized wave functions  $\phi_n(x)$ . We show how use these same techniques for quantum field theory in section 8.

### 6.3. Perturbative calculation of $\mathcal{C}$ for other quantum-mechanical Hamiltonians

The  $\mathcal{C}$  operator has been calculated perturbatively for a variety of quantum-mechanical models. For example, let us consider first the case of the Hamiltonian

$$H = \frac{1}{2}(\hat{p}^2 + \hat{q}^2) + \frac{1}{2}(\hat{x}^2 + \hat{y}^2) + i\epsilon\hat{x}^2\hat{y}, \quad (123)$$

which has two degrees of freedom. The energy levels of this complex Hénon–Heiles theory were studied in [81]. The  $\mathcal{C}$  operator for this Hamiltonian was calculated in [82–84]. The perturbative result for the  $Q = Q_1\epsilon + Q_3\epsilon^3 + \dots$  operator is

$$\begin{aligned} Q_1(\hat{x}, \hat{y}, \hat{p}, \hat{q}) &= -\frac{4}{3}\hat{p}^2\hat{q} - \frac{1}{3}S_{1,1}y - \frac{2}{3}\hat{x}^2\hat{q}, \\ Q_3(\hat{x}, \hat{y}, \hat{p}, \hat{q}) &= \frac{512}{405}\hat{p}^2\hat{q}^3 + \frac{512}{405}\hat{p}^4\hat{q} + \frac{1088}{405}S_{1,1}T_{2,1} - \frac{256}{405}\hat{p}^2T_{1,2} + \frac{512}{405}S_{3,1}\hat{y} + \frac{288}{405}S_{2,2}\hat{q} \\ &\quad - \frac{32}{405}\hat{x}^2\hat{q}^3 + \frac{736}{405}\hat{x}^2T_{1,2} - \frac{256}{405}S_{1,1}\hat{y}^3 + \frac{608}{405}S_{1,3}\hat{y} - \frac{128}{405}\hat{x}^4\hat{q} - \frac{8}{9}q, \end{aligned} \quad (124)$$

where  $T_{m,n}$  represents a totally symmetric product of  $m$  factors of  $\hat{q}$  and  $n$  factors of  $\hat{y}$ .

For the Hamiltonian

$$H = \frac{1}{2}(\hat{p}^2 + \hat{q}^2 + \hat{r}^2) + \frac{1}{2}(\hat{x}^2 + \hat{y}^2 + \hat{z}^2) + i\epsilon\hat{x}\hat{y}\hat{z}, \quad (125)$$

which has three degrees of freedom, we have [82–84]

$$\begin{aligned} Q_1(\hat{x}, \hat{y}, \hat{z}, \hat{p}, \hat{q}, \hat{r}) &= -\frac{2}{3}(\hat{y}\hat{z}\hat{p} + \hat{x}\hat{z}\hat{q} + \hat{x}\hat{y}\hat{r}) - \frac{4}{3}\hat{p}\hat{q}\hat{r}, \\ Q_3(\hat{x}, \hat{y}, \hat{z}, \hat{p}, \hat{q}, \hat{r}) &= \frac{128}{405}(\hat{p}^3\hat{q}\hat{r} + \hat{q}^3\hat{p}\hat{r} + \hat{r}^3\hat{q}\hat{p}) + \frac{136}{405}[\hat{p}\hat{x}\hat{p}(\hat{y}\hat{r} + \hat{z}\hat{q}) + \hat{q}\hat{y}\hat{q}(\hat{x}\hat{r} + \hat{z}\hat{p}) \\ &\quad + \hat{r}\hat{z}\hat{r}(\hat{x}\hat{q} + \hat{y}\hat{p})] - \frac{64}{405}(\hat{x}\hat{p}\hat{x}\hat{q}\hat{r} + \hat{y}\hat{q}\hat{y}\hat{p}\hat{r} + \hat{z}\hat{r}\hat{z}\hat{p}\hat{q}) + \frac{184}{405}(\hat{x}\hat{p}\hat{x}\hat{y}\hat{z} + \hat{y}\hat{q}\hat{y}\hat{x}\hat{z} \\ &\quad + \hat{z}\hat{r}\hat{z}\hat{x}\hat{y}) - \frac{32}{405}[\hat{x}^3(\hat{y}\hat{r} + \hat{z}\hat{q}) + \hat{y}^3(\hat{x}\hat{r} + \hat{z}\hat{p}) + \hat{z}^3(\hat{x}\hat{q} + \hat{y}\hat{p})] \\ &\quad - \frac{8}{405}(\hat{p}^3\hat{y}\hat{z} + \hat{q}^3\hat{x}\hat{z} + \hat{r}^3\hat{x}\hat{y}). \end{aligned} \quad (126)$$

An extremely interesting and deceptively simple quantum-mechanical model is the  $\mathcal{PT}$ -symmetric square well, whose Hamiltonian on the domain  $0 < x < \pi$  is given by

$$H = \hat{p}^2 + V(\hat{x}), \quad (127)$$

where in the coordinate representation  $V(x) = \infty$  for  $x < 0$  and  $x > \pi$  and

$$V(x) = \begin{cases} i\epsilon & \text{for } \frac{\pi}{2} < x < \pi, \\ -i\epsilon & \text{for } 0 < x < \frac{\pi}{2}. \end{cases} \quad (128)$$

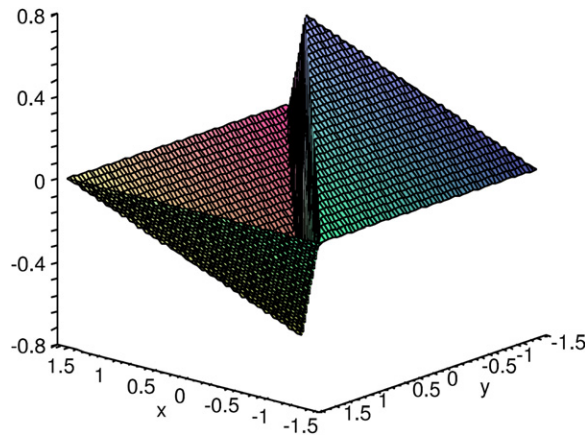
The  $\mathcal{PT}$ -symmetric square-well Hamiltonian was invented by Znojil [85] and it has been heavily studied by many researchers [64, 86–88]. This Hamiltonian reduces to the conventional Hermitian square well in the limit as  $\epsilon \rightarrow 0$ . For  $H$  in (127) the parity operator  $\mathcal{P}$  performs a reflection about  $x = \frac{\pi}{2}$ :  $\mathcal{P} : x \rightarrow \pi - x$ .

In all the examples discussed so far the coordinate-space representation of the  $\mathcal{C}$  operator is a combination of integer powers of  $x$  and integer numbers of derivatives multiplying the parity operator  $\mathcal{P}$ . Hence, the  $Q$  operator is a polynomial in the operators  $\hat{x}$  and  $\hat{p} = -i\frac{d}{dx}$ . The novelty of the  $\mathcal{PT}$ -symmetric square-well Hamiltonian (127) and (128) is that  $\mathcal{C}$  contains *integrals* of  $\mathcal{P}$ . Thus, the  $Q$  operator, while it is a simple function, is *not* a polynomial in  $\hat{x}$  and  $\hat{p}$  and therefore it cannot be found easily by the algebraic perturbative methods introduced in section 6.1.

Instead, in [89] the  $\mathcal{C}$  operator for the square-well Hamiltonian was calculated by using the brute-force approach of calculating the  $\mathcal{PT}$ -normalized eigenfunctions  $\phi_n(x)$  of  $H$  and summing over these eigenfunctions. The eigenfunctions  $\phi_n(x)$  were obtained as perturbation series to second order in powers of  $\epsilon$ . The eigenfunctions were then normalized according to (80), substituted into the formula (87), and the sum was evaluated directly to obtain the  $\mathcal{C}$  operator accurate to order  $\epsilon^2$ . The advantage of the domain  $0 < x < \pi$  is that this sum reduces to a set of Fourier sine and cosine series that can be evaluated in closed form. After evaluating the sum, the result was translated to the symmetric region  $-\frac{\pi}{2} < x < \frac{\pi}{2}$ . On this domain the parity operator in coordinate space is  $\mathcal{P}(x, y) = \delta(x + y)$ .

The last step in the calculation is to show that the  $\mathcal{C}$  operator to order  $\epsilon^2$  has the form  $e^{Q\mathcal{P}}$  and then to evaluate the function  $Q$  to order  $\epsilon^2$ . The final result for  $Q(x, y)$  on the domain  $-\frac{\pi}{2} < x < \frac{\pi}{2}$  has the relatively simple structure

$$Q(x, y) = \frac{1}{4}i\epsilon[x - y + \epsilon(x - y)(|x + y| - \pi)] + \mathcal{O}(\epsilon^3), \quad (129)$$



**Figure 22.** Three-dimensional plot of the imaginary part of  $C^{(1)}(x, y)$ , the first-order perturbative contribution in (131) to the  $\mathcal{C}$  operator in coordinate space. The plot is on the symmetric square domain  $-\frac{\pi}{2} < (x, y) < \frac{\pi}{2}$ . Note that  $C^{(1)}(x, y)$  vanishes on the boundary of this square domain because the eigenfunctions  $\phi_n(x)$  are required to vanish at  $x = 0$  and  $x = \pi$ .

where  $\varepsilon(x)$  is the standard step function

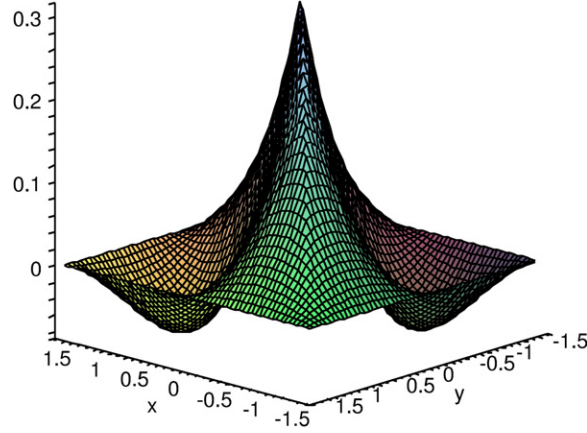
$$\varepsilon(x) = \begin{cases} 1 & (x > 0), \\ 0 & (x = 0), \\ -1 & (x < 0). \end{cases} \tag{130}$$

When we say that the formula for  $Q(x, y)$  has a relatively simple structure, we mean that this structure is simple in comparison with the formula for the  $\mathcal{C}$  operator expressed as an expansion  $C(x, y) = C^{(0)} + \varepsilon C^{(1)} + \varepsilon^2 C^{(2)} + \mathcal{O}(\varepsilon^3)$ . The formulas for the first three coefficients in this series for  $\mathcal{C}$  are

$$\begin{aligned} C^{(0)}(x, y) &= \delta(x + y), \\ C^{(1)}(x, y) &= \frac{1}{4}i[x + y + \varepsilon(x + y) (|x - y| - \pi)], \\ C^{(2)}(x, y) &= \frac{1}{96}\pi^3 - \frac{1}{24}(x^3 + y^3) \varepsilon(x + y) - \frac{1}{24}(y^3 - x^3) \varepsilon(y - x) \\ &\quad + \frac{1}{8}xy\pi - \frac{1}{16}\pi^2(x + y) \varepsilon(x + y) + \frac{1}{8}\pi(x|x| + y|y|) \varepsilon(x + y) \\ &\quad - \frac{1}{4}xy\{ |x|[\theta(x - y)\theta(-x - y) + \theta(y - x)\theta(x + y)] \\ &\quad + |y|[\theta(y - x)\theta(-x - y) + \theta(x - y)\theta(x + y)] \}. \end{aligned} \tag{131}$$

We plot the imaginary part of  $C^{(1)}(x, y)$  in figure 22, and we plot  $C^{(2)}(x, y)$  in figure 23. These three-dimensional plots show  $C^{(1)}(x, y)$  and  $C^{(2)}(x, y)$  on the symmetric domain  $-\frac{\pi}{2} < (x, y) < \frac{\pi}{2}$ .

The most noteworthy property of the  $\mathcal{C}$  operator for the square-well model is that the associated operator  $Q$  is a non-polynomial function, and this kind of structure had not been seen in previous studies of  $\mathcal{C}$ . It was originally believed that for such a simple  $\mathcal{PT}$ -symmetric Hamiltonian it would be possible to calculate the  $\mathcal{C}$  operator in closed form. It is a surprise that for this elementary model the  $\mathcal{C}$  operator is so non-trivial.



**Figure 23.** Three-dimensional plot of  $\mathcal{C}^{(2)}(x, y)$  in (131) on the symmetric square domain  $-\frac{\pi}{2} < (x, y) < \frac{\pi}{2}$ . The function  $\mathcal{C}^{(2)}(x, y)$  vanishes on the boundary of this square domain because the eigenfunctions  $\phi_n(x)$  from which it was constructed vanish at the boundaries of the square well.

#### 6.4. Mapping from a $\mathcal{PT}$ -symmetric Hamiltonian to a Hermitian Hamiltonian

Mostafazadeh observed that the square root of the positive operator  $e^Q$  can be used to construct a similarity transformation that maps a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  to an equivalent Hermitian Hamiltonian  $h$  [72, 90]:

$$h = e^{-Q/2} H e^{Q/2}. \quad (132)$$

He noted that  $h$  is equivalent to  $H$  because it has the same eigenvalues as  $H$ .

To understand why (132) is valid, recall from (107) that the  $\mathcal{C}$  operator has the general form  $\mathcal{C} = e^Q \mathcal{P}$ , where  $Q = Q(\hat{x}, \hat{p})$  is a Hermitian function of the fundamental dynamical operator variables of the quantum theory. Multiplying  $\mathcal{C}$  on the right by  $\mathcal{P}$  gives an expression for  $e^Q$ :

$$e^Q = \mathcal{C} \mathcal{P}, \quad (133)$$

which indicates that  $\mathcal{C} \mathcal{P}$  is a positive and invertible operator.

To verify that  $h$  in (132) is Hermitian, take the Hermitian conjugate of (132)

$$h^\dagger = e^{Q/2} H^\dagger e^{-Q/2}, \quad (134)$$

which can be rewritten as

$$h^\dagger = e^{-Q/2} e^Q H^\dagger e^{-Q} e^{Q/2}. \quad (135)$$

Use (133) to replace  $e^Q$  by  $\mathcal{C} \mathcal{P}$  and  $e^{-Q}$  by  $\mathcal{P} \mathcal{C}$

$$h^\dagger = e^{-Q/2} \mathcal{C} \mathcal{P} H^\dagger \mathcal{P} \mathcal{C} e^{Q/2} \quad (136)$$

and recall from (92) that  $H^\dagger$  can be replaced by  $\mathcal{P} H \mathcal{P}$ . This gives

$$h^\dagger = e^{-Q/2} \mathcal{C} \mathcal{P} \mathcal{P} H \mathcal{P} \mathcal{P} \mathcal{C} e^{Q/2} = e^{-Q/2} \mathcal{C} H \mathcal{C} e^{Q/2}. \quad (137)$$

Finally, one uses the fact that  $\mathcal{C}$  commutes with  $H$  (see (113)) and that the square of  $\mathcal{C}$  is unity (see (112)) to reduce the right side of (136) to the right side of (132). This verifies that  $h$  is Hermitian in the Dirac sense.

We conclude from this calculation that for every non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  whose  $\mathcal{PT}$  symmetry is unbroken, it is, in principle, possible to construct



via (132) a Hermitian Hamiltonian  $h$  that has exactly the same eigenvalues as  $H$ . Note that it is crucial that  $H$  has an unbroken  $\mathcal{PT}$  symmetry because this allows us to construct  $\mathcal{C}$ , which in turn allows us to construct the similarity operator  $e^{Q/2}$ .

This construction poses the following question: are  $\mathcal{PT}$ -symmetric Hamiltonians physically new and distinct from ordinary Hermitian Hamiltonians, or do they describe exactly the same physical processes that ordinary Hermitian Hamiltonians describe?

There are two answers to this question, the first being technical and practical and the second being an answer in principle. First, while it is theoretically possible to construct the Hermitian Hamiltonian  $h$  whose spectrum is identical to that of  $H$ , it cannot in general be done except at the perturbative level because the transformation is so horribly complicated. (See, for example, the discussion of the square well in section 6.3.) Furthermore, while the  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  is simple in structure and easy to use in calculations because the interaction term is local, it is shown in [91] that  $h$  is *non-local* (its interaction term has arbitrarily high powers of the variables  $\hat{x}$  and  $\hat{p}$ ). Thus, it is not just difficult to calculate using  $h$ ; it is almost impossible because the usual regulation schemes are hopelessly inadequate.

There is only one known non-trivial example for which there is actually a closed-form expression for both  $H$  and  $h$ , and this is the case of the quartic Hamiltonian discussed in sections 2.6–2.8. Even in this case, it is not possible to construct the  $\mathcal{C}$  operator in closed form because this operator is non-local (it contains a Fourier transform) and it performs a transformation in the complex plane. This is the only known example for which it is practical to calculate with both  $H$  and  $h$ . Hence, while the mapping from  $H$  to  $h$  is of great theoretical interest, it does not have much practical value.

The second answer is of greater importance because it leads immediately to physical considerations. The transformation from  $H$  to  $h$  in (132) is a *similarity* and not a unitary transformation. Thus, while the eigenvalues of  $H$  and  $h$  are the same, relationships between vectors are changed; pairs of vectors that are orthogonal are mapped into pairs of vectors that are not orthogonal. Thus, experiments that measure vectorial relationships can distinguish between  $H$  and  $h$ . One plausible experiment, which involves the speed of unitary time evolution, is described in detail in section 7.3.

## 7. Applications of $\mathcal{PT}$ -symmetric Hamiltonians in quantum mechanics

It is not yet known whether non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians describe phenomena that can be observed experimentally. However, non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians have *already* appeared in the literature very often and their remarkable properties have been noticed and used by many authors. For example, in 1959 Wu showed that the ground state of a Bose system of hard spheres is described by a non-Hermitian Hamiltonian [92]. Wu found that the ground-state energy of this system is real and he conjectured that all the energy levels were real. Hollowood showed that the non-Hermitian Hamiltonian of a complex Toda lattice has real energy levels [9]. Cubic non-Hermitian Hamiltonians of the form  $H = \hat{p}^2 + i\hat{x}^3$  (and also cubic quantum field theories) arise in studies of the Lee-Yang edge singularity [93–96] and in various Reggeon field-theory models [97, 98]. In all these cases a non-Hermitian Hamiltonian having a real spectrum appeared mysterious at the time, but now the explanation is simple: In every case the non-Hermitian Hamiltonian is  $\mathcal{PT}$  symmetric. In each case the Hamiltonian is constructed so that the position operator  $\hat{x}$  or the field operator  $\phi$  is always multiplied by  $i$ . Hamiltonians having  $\mathcal{PT}$  symmetry have also been used to describe magnetohydrodynamic systems [99, 100] and to study non-dissipative time-dependent systems interacting with electromagnetic fields [101].

In this section we describe briefly four areas of quantum mechanics in which non-Hermitian  $\mathcal{PT}$ -Hamiltonians play a crucial and significant role.

7.1. New  $\mathcal{PT}$ -symmetric quasi-exactly solvable Hamiltonians

A quantum-mechanical Hamiltonian is said to be *quasi-exactly solvable* (QES) if a finite portion of its energy spectrum and associated eigenfunctions can be found exactly and in closed form [102]. QES potentials depend on an integer parameter  $J$ ; for positive values of  $J$  one can find exactly the first  $J$  eigenvalues and eigenfunctions, typically of a given parity. QES systems are classified using an algebraic approach in which the Hamiltonian is expressed in terms of the generators of a Lie algebra [104]. This approach generalizes the dynamical-symmetry analysis of *exactly solvable* quantum-mechanical systems whose *entire* spectrum may be found in closed form by algebraic means.

Prior to the discovery of non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians the lowest-degree one-dimensional QES polynomial potential that was known was a sextic potential having one continuous parameter as well as a discrete parameter  $J$ . A simple case of such a potential is [103]

$$V(x) = x^6 - (4J - 1)x^2. \tag{138}$$

For this potential, the Schrödinger equation  $-\psi''(x) + [V(x) - E]\psi(x) = 0$  has  $J$  even-parity solutions of the form

$$\psi(x) = e^{-x^4/4} \sum_{k=0}^{J-1} c_k x^{2k}. \tag{139}$$

The coefficients  $c_k$  for  $0 \leq k \leq J - 1$  satisfy the recursion relation

$$4(J - k)c_{k-1} + Ec_k + 2(k + 1)(2k + 1)c_{k+1} = 0, \tag{140}$$

where  $c_{-1} = c_J = 0$ . The linear equations (140) have a non-trivial solution for  $c_0, c_1, \dots, c_{J-1}$  if the determinant of the coefficients vanishes. For each integer  $J$  this determinant is a polynomial of degree  $J$  in the variable  $E$ . The roots of this polynomial are all real and they are the  $J$  quasi-exact energy eigenvalues of the potential (138).

The discovery of  $\mathcal{PT}$  symmetry allows us to introduce an entirely new class of QES *quartic* polynomial potentials having *two* continuous parameters in addition to the discrete parameter  $J$ . The Hamiltonian has the form [105]

$$H = \hat{p}^2 - \hat{x}^4 + 2ia\hat{x}^3 + (a^2 - 2b)\hat{x}^2 + 2i(ab - J)\hat{x}, \tag{141}$$

where  $a$  and  $b$  are real and  $J$  is a positive integer. The spectra of this family of Hamiltonians are real, discrete and bounded below. Like the eigenvalues of the potential (138), the lowest  $J$  eigenvalues of  $H$  are the roots of a polynomial of degree  $J$ .

The eigenfunction  $\psi(x)$  satisfies  $\mathcal{PT}$ -symmetric boundary conditions; it vanishes in the Stokes wedges shown in figure 4. The eigenfunction satisfies

$$-\psi''(x) + [-x^4 + 2iax^3 + (a^2 - 2b)x^2 + 2i(ab - J)x] \psi(x) = E\psi(x). \tag{142}$$

We obtain the QES portion of the spectrum of  $H$  in (141) by making the ansatz  $\psi(x) = \exp(-\frac{1}{3}ix^3 - \frac{1}{2}ax^2 - ibx) P_{J-1}(x)$ , where

$$P_{J-1}(x) = x^{J-1} + \sum_{k=0}^{J-2} c_k x^k \tag{143}$$

is a polynomial in  $x$  of degree  $J - 1$ . Substituting  $\psi(x)$  into the differential equation (142), dividing off the exponential and collecting powers of  $x$ , we obtain a polynomial in  $x$  of

degree  $J - 1$ . Setting the coefficients of  $x^k$  ( $1 \leq k \leq J - 1$ ) to 0 gives a system of  $J - 1$  simultaneous linear equations for the coefficients  $c_k$  ( $0 \leq k \leq J - 2$ ). We solve these equations and substitute the values of  $c_k$  into the coefficient of  $x^0$ . This gives a polynomial  $Q_J(E)$  of degree  $J$  in the eigenvalue  $E$ . The coefficients of this polynomial are functions of the parameters  $a$  and  $b$ . The first two of these polynomials are

$$\begin{aligned} Q_1 &= E - b^2 - a, \\ Q_2 &= E^2 - (2b^2 + 4a)E + b^4 + 4ab^2 - 4b + 3a^2. \end{aligned} \quad (144)$$

The roots of  $Q_J(E)$  are the QES portion of the spectrum of  $H$ .

The polynomials  $Q_J(E)$  simplify dramatically when we substitute

$$E = F + b^2 + Ja \quad \text{and} \quad K = 4b + a^2. \quad (145)$$

The new polynomials then have the form

$$\begin{aligned} Q_1 &= F, \\ Q_2 &= F^2 - K, \\ Q_3 &= F^3 - 4KF - 16, \\ Q_4 &= F^4 - 10KF^2 - 96F + 9K^2, \\ Q_5 &= F^5 - 20KF^3 - 336F^2 + 64K^2F + 768K. \end{aligned} \quad (146)$$

The roots of these polynomials are all real as long as  $K \geq K_{\text{critical}}$ , where  $K_{\text{critical}}$  is a function of  $J$ .

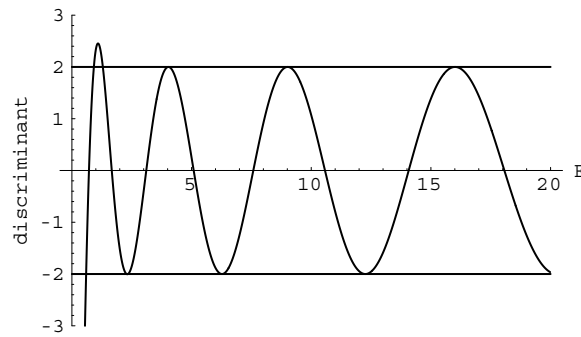
Had  $\mathcal{PT}$ -symmetric quantum mechanics not been discovered, this beautiful family of quartic QES Hamiltonians would never have been considered because the quartic term has a negative sign. Lacking the discovery that  $\mathcal{PT}$ -symmetric Hamiltonians have positive spectra, the Hamiltonians in (141) would have been rejected because it would have been assumed that the spectra of such Hamiltonians would be unbounded below. Quasi-exactly solvable sextic  $\mathcal{PT}$ -symmetric Hamiltonians are studied in [106].

## 7.2. Complex crystals

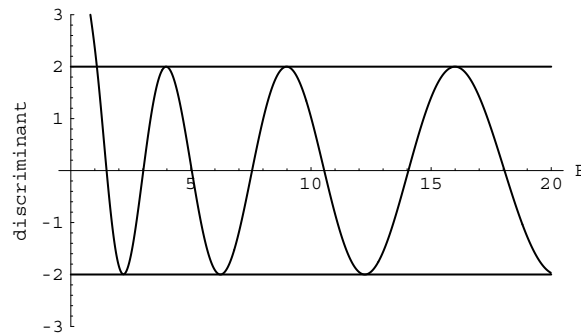
An experimental signal of a complex Hamiltonian might be found in the context of condensed matter physics. Consider the complex crystal lattice whose potential is  $V(x) = i \sin x$ . The optical properties of complex crystal lattices were first studied by Berry and O'Dell, who referred to them as complex diffraction gratings [107].

While the Hamiltonian  $H = \hat{p}^2 + i \sin \hat{x}$  is not Hermitian, it is  $\mathcal{PT}$  symmetric and all of its energy bands are *real*. At the edge of the bands the wave function of a particle in such a lattice is bosonic ( $2\pi$ -periodic), and unlike the case of ordinary crystal lattices, the wave function is never fermionic ( $4\pi$ -periodic). The discriminant for a Hermitian  $\sin(x)$  potential is plotted in figure 24 and the discriminant for a non-Hermitian  $i \sin(x)$  potential is plotted in figure 25. The difference between these two figures is subtle. In figure 25 the discriminant does not go below  $-2$ , and thus there are half as many gaps [108]. Direct observation of such a band structure would give unambiguous evidence of a  $\mathcal{PT}$ -symmetric Hamiltonian<sup>8</sup>. Complex periodic potentials having more elaborate band structures have also been found [109–112].

<sup>8</sup> We hope that some of the delicate experiments performed by A Zeilinger on models of this type (private communication, M V Berry) will eventually be able to verify by direct observation the theoretical band-edge predictions that are illustrated in figures 24 and 25.



**Figure 24.** Discriminant  $\Delta(E)$  plotted as a function of  $E$  for the real periodic potential  $V(x) = \sin(x)$ . Although it cannot be seen in the figure, all local maxima lie *above* the line  $\Delta = 2$  and all local minima lie *below* the line  $\Delta = -2$ . The regions of energy  $E$  for which  $|\Delta| \leq 2$  correspond to allowed energy bands and the regions where  $|\Delta| > 2$  correspond to gaps. There are infinitely many gaps and these gaps become exponentially narrow as  $E$  increases. It is clear in this figure that the first maximum lies above 2. The first minimum occurs at  $E = 2.3138$ , where the discriminant has the value  $-2.003\ 8787$ . The second maximum occurs at  $E = 4.0336$ , where the discriminant is  $2.000\ 007$ . Similar behaviour is found for other potentials in the class  $V(x) = \sin^{2N+1}(x)$ .



**Figure 25.** Discriminant  $\Delta(E)$  plotted as a function of  $E$  for the complex periodic potential  $V(x) = i \sin(x)$ . For  $E > 2$  it is not possible to see any difference between this figure and figure 24. However, although it cannot be seen, all local maxima in this figure lie *above* the line  $\Delta = -2$ . This behaviour is distinctly different from the behaviour in figure 24 exhibited by the real periodic potential  $V(x) = \sin x$ . In stark contrast with real periodic potentials, for the potentials of the form  $V(x) = i \sin^{2N+1}(x)$ , while the maxima of the discriminant lie above +2, the minima of the discriminant lie above  $-2$ . Thus, for these potentials there are no antiperiodic wave functions. Lengthy and delicate numerical analysis verifies that for the potential  $V(x) = i \sin(x)$  the first three maxima of the discriminant  $\Delta(E)$  are located at  $E = 3.966\ 4284$ ,  $E = 8.985\ 7320$  and  $E = 15.992\ 066\ 213\ 46$ . The value of the discriminant  $\Delta(E)$  at these energies is  $2.000\ 007$ ,  $2.000\ 000\ 000\ 000\ 000\ 69$  and  $2.000\ 000\ 000\ 000\ 000\ 000\ 04$ . The first two minima of the discriminant are located at  $E = 2.1916$  and  $E = 6.229\ 223$  and at these energies  $\Delta(E)$  has the values  $-1.995\ 3386$  and  $-1.999\ 999\ 995\ 27$ . Similar behaviour is found for the other complex periodic potentials in the class.

### 7.3. Quantum brachistochrone

We pointed out in section 6.4 that there is a similarity transformation that maps a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian  $H$  to a Hermitian Hamiltonian  $h$  [see (132)]. The two Hamiltonians,  $H$  and  $h$ , have the same eigenvalues, but this does not mean they describe

the same physics. To illustrate the differences between  $H$  and  $h$ , we show how to solve the quantum brachistochrone problem for  $\mathcal{PT}$ -symmetric and for Hermitian quantum mechanics, and we show that the solution to this problem in these two formulations of quantum mechanics is not the same.

The fancy word *brachistochrone* means ‘shortest time.’ Thus, the *quantum brachistochrone* problem is defined as follows: suppose we are given initial and final quantum states  $|\psi_I\rangle$  and  $|\psi_F\rangle$  in a Hilbert space. There exist infinitely many Hamiltonians  $H$  under which  $|\psi_I\rangle$  evolves into  $|\psi_F\rangle$  in some time  $t$ :

$$|\psi_F\rangle = e^{-iHt/\hbar}|\psi_I\rangle. \quad (147)$$

The problem is to find the Hamiltonian  $H$  that minimizes the evolution time  $t$  subject to the constraint that  $\omega$ , the difference between the largest and smallest eigenvalues of  $H$ , is held fixed. The shortest evolution time is denoted by  $\tau$ .

In Hermitian quantum mechanics there is an unavoidable lower bound  $\tau$  on the time required to transform one state into another. Thus, the minimum time required to flip unitarily a spin-up state into a spin-down state of an electron is an important physical quantity because it gives an upper bound on the speed of a quantum computer.

In this paper we have shown that Hermitian quantum mechanics can be extended into the complex domain while retaining the reality of the energy eigenvalues, the unitarity of time evolution and the probabilistic interpretation. It has recently been discovered that within this complex framework a spin-up state can be transformed *arbitrarily quickly* to a spin-down state by a simple non-Hermitian Hamiltonian [113].

Let us first show how to find the value of  $\tau$  for the case of a Hermitian Hamiltonian: this problem is easy because finding the optimal evolution time  $\tau$  requires only the solution to the simpler problem of finding the optimal evolution time for the  $2 \times 2$  matrix Hamiltonians acting on the two-dimensional subspace spanned by  $|\psi_I\rangle$  and  $|\psi_F\rangle$  [115]. To solve the Hermitian version of the two-dimensional quantum brachistochrone problem, we choose the basis so that the initial and final states are given by

$$|\psi_I\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\psi_F\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \quad (148)$$

where  $|a|^2 + |b|^2 = 1$ . The most general  $2 \times 2$  Hermitian Hamiltonian is

$$H = \begin{pmatrix} s & re^{-i\theta} \\ re^{i\theta} & u \end{pmatrix}, \quad (149)$$

where the parameters  $r, s, u$  and  $\theta$  are real. The eigenvalue constraint is

$$\omega^2 = (s - u)^2 + 4r^2. \quad (150)$$

The Hamiltonian  $H$  in (149) can be expressed in terms of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (151)$$

as  $H = \frac{1}{2}(s + u)\mathbf{1} + \frac{1}{2}\omega\boldsymbol{\sigma} \cdot \mathbf{n}$ , where  $\mathbf{n} = \frac{2}{\omega}(r \cos \theta, r \sin \theta, \frac{s-u}{2})$  is a unit vector. The matrix identity

$$\exp(i\phi \boldsymbol{\sigma} \cdot \mathbf{n}) = \cos \phi \mathbf{1} + i \sin \phi \boldsymbol{\sigma} \cdot \mathbf{n} \quad (152)$$

then simplifies the relation  $|\psi_F\rangle = e^{-iH\tau/\hbar}|\psi_I\rangle$  to

$$\begin{pmatrix} a \\ b \end{pmatrix} = e^{-i(s+u)\tau/(2\hbar)} \begin{pmatrix} \cos\left(\frac{\omega\tau}{2\hbar}\right) - i\frac{s-u}{\omega} \sin\left(\frac{\omega\tau}{2\hbar}\right) \\ -i\frac{2r}{\omega} e^{i\theta} \sin\left(\frac{\omega\tau}{2\hbar}\right) \end{pmatrix}. \quad (153)$$

From the second component of (153) we obtain  $|b| = \frac{2r}{\omega} \sin\left(\frac{\omega t}{2\hbar}\right)$ , which gives the time required to transform the initial state:  $t = \frac{2\hbar}{\omega} \arcsin\left(\frac{\omega|b|}{2r}\right)$ . To optimize this relation over all  $r > 0$ , we note that (150) implies that the maximum value of  $r$  is  $\frac{1}{2}\omega$  and that at this maximum  $s = u$ . The optimal time is thus

$$\tau = \frac{2\hbar}{\omega} \arcsin |b|. \tag{154}$$

Note that if  $a = 0$  and  $b = 1$  we have  $\tau = 2\pi\hbar/\omega$  for the smallest time required to transform  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  to the orthogonal state  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

For general  $a$  and  $b$ , at the optimal time  $\tau$  we have  $a = e^{i\tau s/\hbar} \sqrt{1 - |b|^2}$  and  $b = ie^{i\tau s/\hbar} |b| e^{i\theta}$ , which satisfies the condition  $|a|^2 + |b|^2 = 1$  that the norm of the state does not change under unitary time evolution. The parameters  $s$  and  $\theta$  are determined by the phases of  $a$  and  $b$ . We set  $a = |a|e^{i\arg(a)}$  and  $b = |b|e^{i\arg(b)}$  and find that the optimal Hamiltonian is

$$H = \begin{pmatrix} \frac{\omega \arg(a)}{2 \arcsin |b|} & \frac{\omega}{4} e^{-i[\arg(b) - \arg(a) - \frac{\pi}{2}]} \\ \frac{\omega}{4} e^{i[\arg(b) - \arg(a) - \frac{\pi}{2}]} & \frac{\omega \arg(a)}{2 \arcsin |b|} \end{pmatrix}. \tag{155}$$

The overall phase of  $|\psi_F\rangle$  is not physically relevant, so the quantity  $\arg(a)$  may be chosen arbitrarily; we may thus assume that it is 0. We are free to choose  $\arg(a)$  because there is no absolute energy in quantum mechanics; one can add a constant to the eigenvalues of the Hamiltonian without altering the physics. Equivalently, this means that the value of  $\tau$  cannot depend on the trace  $s + u$  of  $H$ .

How do we interpret the result for  $\tau$  in (154)? While this equation resembles the time-energy uncertainty principle, it is really the much simpler statement that *rate × time = distance*. The constraint (150) on  $H$  is a bound on the standard deviation  $\Delta H$  of the Hamiltonian, where  $\Delta H$  in a normalized state  $|\psi\rangle$  is given by  $(\Delta H)^2 = \langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2$ . The maximum value of  $\Delta H$  is  $\omega/2$ . From the Anandan–Aharonov relation [116], the speed of evolution of a quantum state is given by  $\Delta H$ . The distance between the initial state  $|\psi_I\rangle$  and the final state  $|\psi_F\rangle$  is  $\delta = 2 \arccos(|\langle \psi_F | \psi_I \rangle|)$ . Thus, the shortest time  $\tau$  for  $|\psi_I\rangle$  to evolve to  $|\psi_F\rangle = e^{-iH\tau/\hbar} |\psi_I\rangle$  is bounded below because the speed is bounded above while the distance is held fixed. The Hamiltonian  $H$  that realizes the shortest time evolution can be understood as follows: the standard deviation  $\Delta H$  of the Hamiltonian in (149) is  $r$ . Since  $\Delta H$  is bounded by  $\omega/2$ , to maximize the speed of evolution (and minimize the time of evolution) we choose  $r = \omega/2$ .

We now perform the same optimization for the complex  $2 \times 2$  non-Hermitian  $\mathcal{PT}$  Hamiltonian in (93). Following the same procedure used for Hermitian Hamiltonians, we rewrite  $H$  in (93) in the form  $H = (r \cos \theta)\mathbf{1} + \frac{1}{2}\omega\boldsymbol{\sigma} \cdot \mathbf{n}$ , where  $\mathbf{n} = \frac{2}{\omega}(s, 0, ir \sin \theta)$  is a unit vector and the squared difference between the energy eigenvalues (see (95)) is

$$\omega^2 = 4s^2 - 4r^2 \sin^2 \theta. \tag{156}$$

The condition of unbroken  $\mathcal{PT}$  symmetry ensures the positivity of  $\omega^2$ . This equation emphasizes the key difference between Hermitian and  $\mathcal{PT}$ -symmetric Hamiltonians: the corresponding equation (150) for the Hermitian Hamiltonian has a *sum* of squares, while this equation for  $\omega^2$  has a *difference* of squares. Thus, Hermitian Hamiltonians exhibit elliptic behaviour, which leads to a non-zero lower bound for the optimal time  $\tau$ . The hyperbolic nature of (156) allows  $\tau$  to approach zero because, as we will see, the matrix elements of the  $\mathcal{PT}$ -symmetric Hamiltonian can be made large without violating the energy constraint  $E_+ - E_- = \omega$ .

The  $\mathcal{PT}$ -symmetric analog of the evolution equation (153) is

$$e^{-iHt/\hbar} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{e^{-itr \cos \theta/\hbar}}{\cos \alpha} \begin{pmatrix} \cos \left( \frac{\omega t}{2\hbar} - \alpha \right) \\ -i \sin \left( \frac{\omega t}{2\hbar} \right) \end{pmatrix}. \quad (157)$$

We apply this result to the same pair of vectors examined in the Hermitian case:  $|\psi_I\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $|\psi_F\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . (Note that these vectors are not orthogonal with respect to the  $\mathcal{CP}\mathcal{T}$  inner product.) Equation (157) shows that the evolution time to reach  $|\psi_F\rangle$  from  $|\psi_I\rangle$  is  $t = (2\alpha - \pi)\hbar/\omega$ . Optimizing this result over allowable values for  $\alpha$ , we find that as  $\alpha$  approaches  $\frac{1}{2}\pi$  the optimal time  $\tau$  tends to zero. This result is quite general and even holds for broad classes of non-Hermitian Hamiltonians [114].

Note that in the limit  $\alpha \rightarrow \frac{1}{2}\pi$  we get  $\cos \alpha \rightarrow 0$ . However, in terms of  $\alpha$ , the energy constraint (156) becomes  $\omega^2 = 4s^2 \cos^2 \alpha$ . Since  $\omega$  is fixed, in order to have  $\alpha$  approach  $\frac{1}{2}\pi$  we must require that  $s \gg 1$ . It then follows from the relation  $\sin \alpha = (r/s) \sin \theta$  that  $|r| \sim |s|$ , so we must also require that  $r \gg 1$ . Evidently, in order to make  $\tau \ll 1$ , the matrix elements of the  $\mathcal{PT}$ -symmetric Hamiltonian (93) must be large.

The result demonstrated here does not violate the uncertainty principle. Indeed, Hermitian and non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonians share the properties that (i) the evolution time is given by  $2\pi\hbar/\omega$  and (ii)  $\Delta H \leq \omega/2$ . The key difference is that a pair of states such as  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  are orthogonal in a Hermitian theory, but have separation  $\delta = \pi - 2|\alpha|$  in the  $\mathcal{PT}$ -symmetric theory. This is because the Hilbert-space metric of the  $\mathcal{PT}$ -symmetric quantum theory depends on the Hamiltonian. Hence, it is possible to choose the parameter  $\alpha$  to create a wormhole-like effect in the Hilbert space.

A *gedanken* experiment to realize this effect in a laboratory might work as follows: a Stern–Gerlach filter creates a beam of spin-up electrons. The beam then passes through a ‘black box’ containing a device governed by a  $\mathcal{PT}$ -symmetric Hamiltonian that flips the spins unitarily in a very short time. The outgoing beam then enters a second Stern–Gerlach device which verifies that the electrons are now in spin-down states. In effect, the black-box device is applying a magnetic field in the complex direction  $(s, 0, ir \sin \theta)$ . If the field strength is sufficiently strong, then spins can be flipped unitarily in virtually no time because the complex path joining these two states is arbitrary short without violating the energy constraint. The arbitrarily short alternative complex pathway from a spin-up state to a spin-down state, as illustrated by this thought experiment, is reminiscent of the short alternative distance between two widely separated space–time points as measured through a wormhole in general relativity.

The results established here provide the possibility of performing experiments that distinguish between Hermitian and  $\mathcal{PT}$ -symmetric Hamiltonians. If practical implementation of complex  $\mathcal{PT}$ -symmetric Hamiltonians were feasible, then identifying the optimal unitary transformation would be particularly important in the design and implementation of fast quantum communication and computation algorithms. Of course, the wormhole-like effect we have discussed here can only be realized if it is possible to switch rapidly between Hermitian and  $\mathcal{PT}$ -symmetric Hamiltonians by means of similarity transformations. It is conceivable that so much quantum noise would be generated that there is a sort of quantum protection mechanism that places a lower bound on the time required to switch Hilbert spaces. If so, this would limit the applicability of a Hilbert-space wormhole to improve quantum algorithms.

#### 7.4. Supersymmetric $\mathcal{PT}$ -symmetric Hamiltonians

After the discovery of  $\mathcal{PT}$ -symmetric Hamiltonians in quantum mechanics, it was proposed that  $\mathcal{PT}$  symmetry might be combined with supersymmetry [117] in the context of quantum field theory. In [117] it was shown that one can easily construct two-dimensional supersymmetric quantum field theories by introducing a  $\mathcal{PT}$ -symmetric superpotential of the form  $S(\phi) = -ig(i\phi)^{1+\epsilon}$ . The resulting quantum field theories exhibit a broken parity symmetry for all  $\delta > 0$ . However, supersymmetry remains unbroken, which is verified by showing that the ground-state energy density vanishes and that the fermion-boson mass ratio is unity. Many papers have subsequently been written on  $\mathcal{PT}$ -symmetric supersymmetric quantum mechanics. (See [118].) A particularly interesting paper by Dorey *et al* examines the connection between supersymmetry and broken  $\mathcal{PT}$  symmetry in quantum mechanics [119].

#### 7.5. Other quantum-mechanical applications

There are many additional quantum-mechanical applications of non-Hermitian  $\mathcal{PT}$ -invariant Hamiltonians. In condensed matter physics Hamiltonians rendered non-Hermitian by an imaginary external field have been introduced to study delocalization transitions in condensed matter systems such as vortex flux-line depinning in type-II superconductors [120]. In this Hatano–Nelson model there is a critical value of the anisotropy (non-Hermiticity) parameter below which all eigenvalues are real [121]. In the theory of reaction–diffusion systems, many models have been constructed for systems described by matrices that can be non-Hermitian [122, 123] and with the appropriate definition of the  $\mathcal{P}$  and  $\mathcal{T}$  operators, these systems can be shown to be  $\mathcal{PT}$  symmetric. Finally, we mention a recent paper by Hibberd *et al* who found a transformation that maps a Hamiltonian describing coherent superpositions of Cooper pairs and condensed molecular bosons to one that is  $\mathcal{PT}$ -symmetric [124].

### 8. $\mathcal{PT}$ -symmetric quantum field theory

Quantum-mechanical theories have only a finite number of degrees of freedom. Most of the  $\mathcal{PT}$ -symmetric quantum-mechanical models discussed so far in this paper have just one degree of freedom; that is, the Hamiltonians for these theories are constructed from just one pair of dynamical variables,  $\hat{x}$  and  $\hat{p}$ . In a quantum field theory the operators  $\hat{x}(t)$  and  $\hat{p}(t)$  are replaced by the quantum fields  $\varphi(\mathbf{x}, t)$  and  $\pi(\mathbf{x}, t)$ , which represent a continuously infinite number of degrees of freedom, one for each value of the spatial variable  $\mathbf{x}$ . Such theories are vastly more complicated than quantum-mechanical theories, but constructing quantum field theories that are non-Hermitian and  $\mathcal{PT}$  symmetric is straightforward. For example, the quantum-field-theoretic Hamiltonians that are analogous to the quantum-mechanical Hamiltonians in (10) and (11) are

$$\mathcal{H} = \frac{1}{2}\pi^2(\mathbf{x}, t) + \frac{1}{2}[\nabla_{\mathbf{x}}\varphi(\mathbf{x}, t)]^2 + \frac{1}{2}\mu^2\varphi^2(\mathbf{x}, t) + ig\varphi^3(\mathbf{x}, t) \quad (158)$$

and

$$\mathcal{H} = \frac{1}{2}\pi^2(\mathbf{x}, t) + \frac{1}{2}[\nabla_{\mathbf{x}}\varphi(\mathbf{x}, t)]^2 + \frac{1}{2}\mu^2\varphi^2(\mathbf{x}, t) - \frac{1}{4}g\varphi^4(\mathbf{x}, t). \quad (159)$$

As in quantum mechanics, where the operators  $\hat{x}$  and  $\hat{p}$  change sign under parity reflection  $\mathcal{P}$ , we assume that the fields in these Hamiltonians are *pseudoscalars* so that they also change sign:

$$\mathcal{P}\varphi(\mathbf{x}, t)\mathcal{P} = -\varphi(-\mathbf{x}, t), \quad \mathcal{P}\pi(\mathbf{x}, t)\mathcal{P} = -\pi(-\mathbf{x}, t). \quad (160)$$

Quantum field theories like these that possess  $\mathcal{PT}$  symmetry exhibit a rich variety of behaviours. Cubic field-theory models like that in (158) are of interest because they arise in



the study of the Lee–Yang edge singularity [93–95] and in Reggeon field theory [97, 98]. In these papers it was asserted that an  $i\varphi^3$  field theory is nonunitary. However, by constructing the  $\mathcal{C}$  operator, we argue in section 8.1 that this quantum field theory is, in fact, unitary. We show in section 8.3 how  $\mathcal{PT}$  symmetry eliminates the ghosts in the Lee model, another cubic quantum field theory. The field theory described by (159) is striking because it is asymptotically free, as explained in section 8.4. We also examine  $\mathcal{PT}$ -symmetric quantum electrodynamics in section 8.5, the  $\mathcal{PT}$ -symmetric Thirring and sine-Gordon models in section 8.6, and gravitational and cosmological theories in section 8.7. Last, we look briefly at  $\mathcal{PT}$ -symmetric classical field theories in section 8.8.

### 8.1. $i\varphi^3$ quantum field theory

In courses on quantum field theory, a scalar  $g\varphi^3$  theory is used as a pedagogical example of perturbative renormalization even though this model is not physically realistic because the energy is not bounded below. However, by calculating  $\mathcal{C}$  perturbatively for the case when the coupling constant  $g = i\epsilon$  is pure imaginary, one obtains a fully acceptable Lorentz invariant quantum field theory. This calculation shows that it is possible to construct perturbatively the Hilbert space in which the Hamiltonian for this cubic scalar field theory in  $(D+1)$ -dimensional Minkowski space–time is *self-adjoint*. Consequently, such theories have positive spectra and exhibit unitary time evolution.

In this section we explain how to calculate perturbatively the  $\mathcal{C}$  operator for the quantum-field-theoretic Hamiltonian in (158) [83]. We apply the powerful algebraic techniques explained in sections 6.1 and 6.2 for the calculation of the  $\mathcal{C}$  operator in quantum mechanics. As in quantum mechanics, we express  $\mathcal{C}$  in the form  $\mathcal{C} = \exp(\epsilon Q_1 + \epsilon^3 Q_3 + \dots) \mathcal{P}$ , where now  $Q_{2n+1}$  ( $n = 0, 1, 2, \dots$ ) are real functionals of the fields  $\varphi_x$  and  $\pi_x$ . To find  $Q_n$  for  $\mathcal{H}$  in (158) we must solve a system of operator equations.

We begin by making an ansatz for  $Q_1$  analogous to the ansatz used in (120):

$$Q_1 = \iiint d\mathbf{x} d\mathbf{y} d\mathbf{z} (M_{(xyz)} \pi_x \pi_y \pi_z + N_{x(yz)} \varphi_y \pi_x \varphi_z). \quad (161)$$

In quantum mechanics  $M$  and  $N$  are constants, but in field theory they are functions. The notation  $M_{(xyz)}$  indicates that this function is totally symmetric in its three arguments, and the notation  $N_{x(yz)}$  indicates that this function is symmetric under the interchange of the second and third arguments. The unknown functions  $M$  and  $N$  are form factors; they describe the spatial distribution of three-point interactions of the field variables in  $Q_1$ . The non-local spatial interaction of the fields is an intrinsic property of  $\mathcal{C}$ . (Note that we have suppressed the time variable  $t$  in the fields and that we use subscripts to indicate the spatial dependence.)

To determine  $M$  and  $N$  we substitute  $Q_1$  into the first equation in (119), namely  $[H_0, Q_1] = -2H_1$ , which now takes the form

$$\left[ \int d\mathbf{x} \pi_x^2 + \int d\mathbf{x} d\mathbf{y} \varphi_x G_{xy}^{-1} \varphi_y, Q_1 \right] = -4i \int d\mathbf{x} \varphi_x^3, \quad (162)$$

where the inverse Green's function is given by  $G_{xy}^{-1} \equiv (\mu^2 - \nabla_x^2) \delta(\mathbf{x} - \mathbf{y})$ . We obtain the following coupled system of partial differential equations:

$$\begin{aligned} (\mu^2 - \nabla_x^2) N_{x(yz)} + (\mu^2 - \nabla_y^2) N_{y(xz)} + (\mu^2 - \nabla_z^2) N_{z(xy)} &= -6\delta(\mathbf{x} - \mathbf{y})\delta(\mathbf{x} - \mathbf{z}), \\ N_{x(yz)} + N_{y(xz)} &= 3(\mu^2 - \nabla_z^2) M_{(wxy)}. \end{aligned} \quad (163)$$

We solve these equations by Fourier transforming to momentum space and get

$$M_{(xyz)} = -\frac{4}{(2\pi)^{2D}} \int d\mathbf{p} d\mathbf{q} \frac{e^{i(\mathbf{x}-\mathbf{y})\cdot\mathbf{p} + i(\mathbf{x}-\mathbf{z})\cdot\mathbf{q}}}{D(\mathbf{p}, \mathbf{q})}, \quad (164)$$

where  $D(\mathbf{p}, \mathbf{q}) = 4[\mathbf{p}^2 \mathbf{q}^2 - (\mathbf{p} \cdot \mathbf{q})^2] + 4\mu^2(\mathbf{p}^2 + \mathbf{p} \cdot \mathbf{q} + \mathbf{q}^2) + 3\mu^4$  is positive, and

$$N_{\mathbf{x}(\mathbf{yz})} = -3 \left( \nabla_{\mathbf{y}} \cdot \nabla_{\mathbf{z}} + \frac{1}{2}\mu^2 \right) M_{(\mathbf{xyz})}. \quad (165)$$

For the special case of a  $(1+1)$ -dimensional quantum field theory the integral in (165) evaluates to  $M_{(\mathbf{xyz})} = -K_0(\mu R) / (\sqrt{3}\pi\mu^2)$ , where  $K_0$  is the associated Bessel function and  $R^2 = \frac{1}{2}[(\mathbf{x} - \mathbf{y})^2 + (\mathbf{y} - \mathbf{z})^2 + (\mathbf{z} - \mathbf{x})^2]$ . This completes the calculation of  $\mathcal{C}$  to first order in perturbation theory.

We mention finally that the  $\mathcal{C}$  operator for this cubic quantum field theory transforms as a scalar under the action of the homogeneous Lorentz group [125]. In [125] it was argued that because the Hamiltonian  $H_0$  for the unperturbed theory ( $g = 0$ ) commutes with the parity operator  $\mathcal{P}$ , the intrinsic parity operator  $\mathcal{P}_1$  in the non-interacting theory transforms as a Lorentz scalar. (The *intrinsic* parity operator  $\mathcal{P}_1$  and the parity operator  $\mathcal{P}$  have the same effect on the fields, except that  $\mathcal{P}_1$  does not reverse the sign of the spatial argument of the field. In quantum mechanics  $\mathcal{P}$  and  $\mathcal{P}_1$  are indistinguishable.) When the coupling constant  $g$  is non-zero, the parity symmetry of  $H$  is broken and  $\mathcal{P}_1$  is no longer a scalar. However,  $\mathcal{C}$  is a scalar. Since  $\lim_{g \rightarrow 0} \mathcal{C} = \mathcal{P}_1$ , one can interpret the  $\mathcal{C}$  operator in quantum field theory as the complex extension of the intrinsic parity operator when the imaginary coupling constant is turned on. This means that  $\mathcal{C}$  is frame-invariant and it shows that the  $\mathcal{C}$  operator plays a truly fundamental role in non-Hermitian quantum field theory.

### 8.2. Other quantum field theories having cubic interactions

We can repeat the calculations done in section 8.1 for cubic quantum field theories having several interacting scalar fields [83, 84]. For example, consider the case of *two* scalar fields  $\varphi_{\mathbf{x}}^{(1)}$  and  $\varphi_{\mathbf{x}}^{(2)}$  whose interaction is governed by

$$H = H_0^{(1)} + H_0^{(2)} + i\epsilon \int d\mathbf{x} [\varphi_{\mathbf{x}}^{(1)}]^2 \varphi_{\mathbf{x}}^{(2)}, \quad (166)$$

which is the analog of the quantum-mechanical theory described by  $H$  in (123). Here,

$$H_0^{(j)} = \frac{1}{2} \int d\mathbf{x} [\pi_{\mathbf{x}}^{(j)}]^2 + \frac{1}{2} \iint d\mathbf{x} d\mathbf{y} [G_{\mathbf{xy}}^{(j)}]^{-1} \varphi_{\mathbf{x}}^{(j)} \varphi_{\mathbf{y}}^{(j)}. \quad (167)$$

To determine  $\mathcal{C}$  to order  $\epsilon$  we introduce the ansatz

$$\begin{aligned} \mathcal{Q}_1 = & \iiint d\mathbf{x} d\mathbf{y} d\mathbf{z} [N_{\mathbf{x}(\mathbf{yz})}^{(1)} (\pi_{\mathbf{z}}^{(1)} \varphi_{\mathbf{y}}^{(1)} + \varphi_{\mathbf{y}}^{(1)} \pi_{\mathbf{z}}^{(1)}) \varphi_{\mathbf{x}}^{(2)} \\ & + N_{\mathbf{x}(\mathbf{yz})}^{(2)} \pi_{\mathbf{x}}^{(2)} \varphi_{\mathbf{y}}^{(1)} \varphi_{\mathbf{z}}^{(1)} + M_{\mathbf{x}(\mathbf{yz})} \pi_{\mathbf{x}}^{(2)} \pi_{\mathbf{y}}^{(1)} \pi_{\mathbf{z}}^{(1)}], \end{aligned} \quad (168)$$

where  $M_{\mathbf{x}(\mathbf{yz})}$ ,  $N_{\mathbf{x}(\mathbf{yz})}^{(1)}$  and  $N_{\mathbf{x}(\mathbf{yz})}^{(2)}$  are unknown functions and the parentheses indicate symmetrization. We get

$$\begin{aligned} M_{\mathbf{x}(\mathbf{yz})} &= -G_m(R_1) G_{\mu_2}(R_2), \\ N_{\mathbf{x}(\mathbf{yz})}^{(1)} &= -\delta(2\mathbf{x} - \mathbf{y} - \mathbf{z}) G_m(R_1), \\ N_{\mathbf{x}(\mathbf{yz})}^{(2)} &= \frac{1}{2} \delta(2\mathbf{x} - \mathbf{y} - \mathbf{z}) G_m(R_1) - \delta(\mathbf{y} - \mathbf{z}) G_{\mu_2}(R_2), \end{aligned} \quad (169)$$

where  $G_{\mu}(r) = \frac{r}{\mu} \left( \frac{\mu}{2\pi r} \right)^{D/2} K_{-1+D/2}(\mu r)$  with  $r = |\mathbf{r}|$  is Green's function in  $D$ -dimensional space,  $m^2 = \mu_1^2 - \frac{1}{4}\mu_2^2$ ,  $R_1^2 = (\mathbf{y} - \mathbf{z})^2$  and  $R_2^2 = \frac{1}{4}(2\mathbf{x} - \mathbf{y} - \mathbf{z})^2$ .

For *three* interacting scalar fields whose dynamics is described by

$$H = H_0^{(1)} + H_0^{(2)} + H_0^{(3)} + i\epsilon \int d\mathbf{x} \varphi_{\mathbf{x}}^{(1)} \varphi_{\mathbf{x}}^{(2)} \varphi_{\mathbf{x}}^{(3)}, \quad (170)$$

which is the analog of  $H$  in (125), we make the ansatz

$$\begin{aligned} Q_1 = \iiint dx dy dz [ & N_{xyz}^{(1)} \pi_x^{(1)} \varphi_y^{(2)} \varphi_z^{(3)} + N_{xyz}^{(2)} \pi_x^{(2)} \varphi_y^{(3)} \varphi_z^{(1)} + N_{xyz}^{(3)} \pi_x^{(3)} \varphi_y^{(1)} \varphi_z^{(2)} \\ & + M_{xyz} \pi_x^{(1)} \pi_y^{(2)} \pi_z^{(3)} ]. \end{aligned} \quad (171)$$

The solutions for the unknown functions are as follows:  $M_{xyz}$  is given by the integral (164) with the more general formula  $D(\mathbf{p}, \mathbf{q}) = 4[\mathbf{p}^2 \mathbf{q}^2 - (\mathbf{p} \cdot \mathbf{q})^2] + 4[\mu_1^2 (\mathbf{q}^2 + \mathbf{p} \cdot \mathbf{q}) + \mu_2^2 (\mathbf{p}^2 + \mathbf{p} \cdot \mathbf{q}) - \mu_3^2 \mathbf{p} \cdot \mathbf{q}] + \mu^4$  with  $\mu^4 = 2\mu_1^2 \mu_2^2 + 2\mu_1^2 \mu_3^2 + 2\mu_2^2 \mu_3^2 - \mu_1^4 - \mu_2^4 - \mu_3^4$ . The  $N$  coefficients are expressed as derivatives acting on  $M$ :

$$\begin{aligned} N_{xyz}^{(1)} &= [4\nabla_y \cdot \nabla_z + 2(\mu_2^2 + \mu_3^2 - \mu_1^2)] M_{xyz}, \\ N_{xyz}^{(2)} &= [-4\nabla_y \cdot \nabla_z - 4\nabla_z^2 + 2(\mu_1^2 + \mu_3^2 - \mu_2^2)] M_{xyz}, \\ N_{xyz}^{(3)} &= [-4\nabla_y \cdot \nabla_z - 4\nabla_y^2 + 2(\mu_1^2 + \mu_2^2 - \mu_3^2)] M_{xyz}. \end{aligned} \quad (172)$$

Once again, the calculation of  $\mathcal{C}$  shows that these cubic field theories are fully consistent quantum theories<sup>9</sup>.

### 8.3. The Lee model

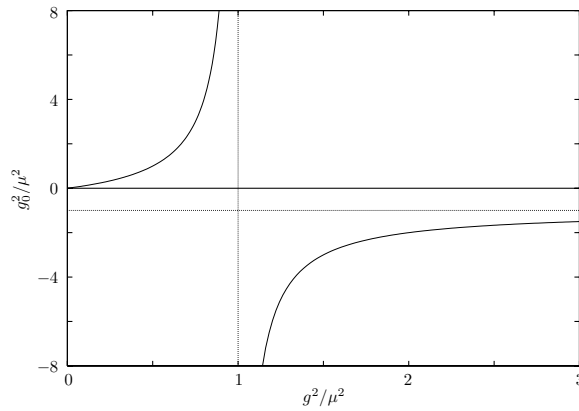
In this section we will show how to use the tools that we have developed to study non-Hermitian  $\mathcal{PT}$ -symmetric quantum theories to examine a famous model quantum field theory known as the *Lee model*. In 1954 the Lee model was proposed as a quantum field theory in which mass, wave function and charge renormalization could be performed exactly and in closed form [1, 126–128]. We discuss the Lee model here because when the renormalized coupling constant is taken to be larger than a critical value, the Hamiltonian becomes non-Hermitian and a (negative-norm) ghost state appears. The appearance of the ghost state was assumed to be a fundamental defect of the Lee model. However, we show that the non-Hermitian Lee-model Hamiltonian is actually  $\mathcal{PT}$  symmetric. When the states of this model are examined using the  $\mathcal{C}$  operator, the ghost state is found to be an ordinary physical state having positive norm [129].

The idea for studying the Lee model as a non-Hermitian Hamiltonian is due to Kleefeld, who was the first to point out this transition to  $\mathcal{PT}$  symmetry [130]. His work gives a comprehensive history of non-Hermitian Hamiltonians.

The Lee model has a cubic interaction term that describes the interaction of three spinless particles called  $V$ ,  $N$  and  $\theta$ . The  $V$  and  $N$  particles are fermions and behave roughly like nucleons, and the  $\theta$  particle is a boson and behaves roughly like a pion. In the model a  $V$  may emit a  $\theta$ , but when it does so it becomes an  $N$ :  $V \rightarrow N + \theta$ . Also, an  $N$  may absorb a  $\theta$ , but when it does so it becomes a  $V$ :  $N + \theta \rightarrow V$ .

The solvability of the Lee model is based on the fact that there is no crossing symmetry. That is, the  $N$  is forbidden to emit an anti- $\theta$  and become a  $V$ . Eliminating crossing symmetry makes the Lee model solvable because it introduces two conservation laws. First, *the number of  $N$  quanta plus the number of  $V$  quanta is fixed*. Second, *the number of  $N$  quanta minus the number of  $\theta$  quanta is fixed*. These two highly constraining conservation laws decompose the Hilbert space of states into an infinite number of non-interacting sectors. The simplest sector is the vacuum sector. Because of the conservation laws, there are no vacuum graphs and the bare vacuum is the physical vacuum. The next two sectors are the one- $\theta$ -particle and

<sup>9</sup> In [125, 129] it is shown that the  $\mathcal{C}$  operator in quantum field theory has the form  $\mathcal{C} = e^{\mathcal{Q}} \mathcal{P}_1$ , where  $\mathcal{P}_1$  is the *intrinsic* parity-reflection operator. The difference between  $\mathcal{P}$  and  $\mathcal{P}_1$  is that  $\mathcal{P}_1$  does not reflect the spatial arguments of the fields. For a cubic interaction Hamiltonian this distinction is technical. It does not affect the final result for the  $\mathcal{Q}$  operator in (161), (168) and (171).



**Figure 26.** Square of the unrenormalized coupling constant,  $g_0^2$ , plotted as a function of the square of the renormalized coupling constant  $g^2$ . Note that  $g^2 = 0$  when  $g_0^2 = 0$ , and as  $g^2$  increases from 0 so does  $g_0^2$ . However, as  $g^2$  increases past a critical value,  $g_0^2$  abruptly becomes negative. In this regime  $g_0$  is imaginary and the Hamiltonian is non-Hermitian.

the one- $N$ -particle sector. These two sectors are also trivial because the two conservation laws prevent any dynamical processes from occurring there. As a result, the masses of the  $N$  particle and of the  $\theta$  particle are not renormalized; that is, the physical masses of these particles are the same as their bare masses.

The lowest non-trivial sector is the  $V/N\theta$  sector. The physical states in this sector of the Hilbert space are linear combinations of the bare  $V$  and the bare  $N\theta$  states, and these states consist of the one-physical- $V$ -particle state and the physical  $N$ - $\theta$ -scattering states. To find these states one can look for the poles and cuts of Green's functions. The renormalization in this sector is easy to perform. Following the conventional renormalization procedure, one finds that the mass of the  $V$  particle is renormalized; that is, the mass of the physical  $V$  particle is different from its bare mass. In the Lee model one calculates the unrenormalized coupling constant as a function of the renormalized coupling constant in closed form. There are many ways to define the renormalized coupling constant. For example, in an actual scattering experiment one could define the square of the renormalized coupling constant  $g^2$  as the value of the  $N\theta$  scattering amplitude at threshold.

The intriguing aspect of the Lee model is the appearance of a ghost state in the  $V/N\theta$  sector. This state appears when one performs coupling-constant renormalization. Expressing  $g_0^2$ , the square of the unrenormalized coupling constant, in terms of  $g^2$ , the square of the renormalized coupling constant, one obtains the graph in figure 1. In principle, the  $g$  is a physical parameter whose numerical value is determined by a laboratory experiment. If  $g^2$  is measured to be near 0, then from figure 26 we see that  $g_0^2$  is also small. However, if the experimental value of  $g^2$  is larger than this critical value, then the square of the unrenormalized coupling constant is negative. In this regime  $g_0$  is imaginary and the Hamiltonian is non-Hermitian. Moreover, a new state appears in the  $V/N\theta$  sector, and because its norm is negative, the state is called a *ghost*. Ghost states are unacceptable in quantum theory because their presence signals a violation of unitarity and makes a probabilistic interpretation impossible.

There have been many unsuccessful attempts to make sense of the Lee model as a physical quantum theory in the ghost regime [1, 127, 128]. However, the methods of  $\mathcal{PT}$ -symmetric quantum theory enable us to give a physical interpretation for the  $V/N\theta$  sector of the Lee model when  $g_0$  becomes imaginary and  $H$  becomes non-Hermitian. The Lee model is a

cubic interaction and we have already shown in sections 8.1 and 8.2 how to make sense of a Hamiltonian in which there is a cubic interaction multiplied by an imaginary coupling constant. The procedure is to calculate the  $\mathcal{C}$  operator and to use it to define a new inner product when the Hamiltonian is non-Hermitian.

For simplicity, we focus here on the *quantum-mechanical* Lee model; the results for the field-theoretic Lee model in [129] are qualitatively identical. The Hamiltonian for the quantum-mechanical Lee model is

$$H = H_0 + g_0 H_1 = m_{V_0} V^\dagger V + m_N N^\dagger N + m_\theta a^\dagger a + \left( V^\dagger N a + a^\dagger N^\dagger V \right). \quad (173)$$

The bare states are the eigenstates of  $H_0$  and the physical states are the eigenstates of the full Hamiltonian  $H$ . The mass parameters  $m_N$  and  $m_\theta$  represent the *physical* masses of the one- $N$ -particle and one- $\theta$ -particle states because these states do not undergo mass renormalization. However,  $m_{V_0}$  is the *bare* mass of the  $V$  particle.

We treat the  $V$ ,  $N$  and  $\theta$  particles as pseudoscalars. To understand why, recall that in quantum mechanics the position operator  $x = (a + a^\dagger)/\sqrt{2}$  and the momentum operator  $p = i(a^\dagger - a)/\sqrt{2}$  both change sign under parity reflection  $\mathcal{P}$ :

$$\mathcal{P}x\mathcal{P} = -x, \quad \mathcal{P}p\mathcal{P} = -p. \quad (174)$$

Thus,  $\mathcal{P}V\mathcal{P} = -V$ ,  $\mathcal{P}N\mathcal{P} = -N$ ,  $\mathcal{P}a\mathcal{P} = -a$ ,  $\mathcal{P}V^\dagger\mathcal{P} = -V^\dagger$ ,  $\mathcal{P}N^\dagger\mathcal{P} = -N^\dagger$ ,  $\mathcal{P}a^\dagger\mathcal{P} = -a^\dagger$ . Under time reversal  $\mathcal{T}$ ,  $p$  and  $i$  change sign but  $x$  does not:

$$\mathcal{T}p\mathcal{T} = -p, \quad \mathcal{T}i\mathcal{T} = -i, \quad \mathcal{T}x\mathcal{T} = x. \quad (175)$$

Thus,  $\mathcal{T}V\mathcal{T} = V$ ,  $\mathcal{T}N\mathcal{T} = N$ ,  $\mathcal{T}a\mathcal{T} = a$ ,  $\mathcal{T}V^\dagger\mathcal{T} = V^\dagger$ ,  $\mathcal{T}N^\dagger\mathcal{T} = N^\dagger$ ,  $\mathcal{T}a^\dagger\mathcal{T} = a^\dagger$ .

When the bare coupling constant  $g_0$  is real,  $H$  in (173) is Hermitian:  $H^\dagger = H$ . When  $g_0$  is imaginary,  $g_0 = i\lambda_0$  ( $\lambda_0$  real),  $H$  is not Hermitian, but by virtue of the above transformation properties,  $H$  is  $\mathcal{PT}$ -symmetric:  $H^{\mathcal{PT}} = H$ .

We assume first that  $g_0$  is real so that  $H$  is Hermitian and we examine the simplest non-trivial sector of the quantum-mechanical Lee model; namely, the  $V/N\theta$  sector. We look for the eigenstates of the Hamiltonian  $H$  in the form of linear combinations of the bare one- $V$ -particle and the bare one- $N$ -one- $\theta$ -particle states. There are two eigenfunctions. We interpret the eigenfunction corresponding to the lower-energy eigenvalue as the physical one- $V$ -particle state, and we interpret the eigenfunction corresponding with the higher-energy eigenvalue as the physical one- $N$ -one- $\theta$ -particle state. (In the field-theoretic Lee model this higher-energy state corresponds to the continuum of physical  $N$ - $\theta$  scattering states.) Thus, we make the ansatz

$$|V\rangle = c_{11}|1, 0, 0\rangle + c_{12}|0, 1, 1\rangle, \quad |N\theta\rangle = c_{21}|1, 0, 0\rangle + c_{22}|0, 1, 1\rangle, \quad (176)$$

and demand that these states be eigenstates of  $H$  with eigenvalues  $m_V$  (the renormalized  $V$ -particle mass) and  $E_{N\theta}$ . The eigenvalue problem reduces to a pair of elementary algebraic equations:

$$c_{11}m_{V_0} + c_{12}g_0 = c_{11}m_V, \quad c_{21}g_0 + c_{22}(m_N + m_\theta) = c_{22}E_{N\theta}. \quad (177)$$

The solutions to (177) are

$$m_V = \frac{1}{2} \left( m_N + m_\theta + m_{V_0} - \sqrt{\mu_0^2 + 4g_0^2} \right), \\ E_{N\theta} = \frac{1}{2} \left( m_N + m_\theta + m_{V_0} + \sqrt{\mu_0^2 + 4g_0^2} \right), \quad (178)$$

where  $\mu_0 \equiv m_N + m_\theta - m_{V_0}$ . Notice that  $m_V$ , the mass of the physical  $V$  particle, is different from  $m_{V_0}$ , the mass of the bare  $V$  particle, because the  $V$  particle undergoes mass renormalization.

Next, we perform wave-function renormalization. Following Barton [1] we define the wave-function renormalization constant  $Z_V$  by  $\sqrt{Z_V} = \langle 0|V|V \rangle$ . This gives

$$Z_V^{-1} = \frac{1}{2}g_0^{-2}\sqrt{\mu_0^2 + 4g_0^2}\left(\sqrt{\mu_0^2 + 4g_0^2} - \mu_0\right). \quad (179)$$

Finally, we perform coupling-constant renormalization. Again, following Barton we note that  $\sqrt{Z_V}$  is the ratio between the renormalized coupling constant  $g$  and the bare coupling constant  $g_0$  [1]. Thus,  $g^2/g_0^2 = Z_V$ . Elementary algebra gives the bare coupling constant in terms of the renormalized mass and coupling constant:

$$g_0^2 = g^2/(1 - g^2/\mu^2), \quad (180)$$

where  $\mu$  is defined as  $\mu \equiv m_N + m_\theta - m_V$ . We cannot freely choose  $g$  because the value of  $g$  is, in principle, taken from experimental data. Once  $g$  has been determined experimentally, we can use (21) to determine  $g_0$ . The relation in (21) is plotted in figure 26. This figure reveals a surprising property of the Lee model: if  $g$  is larger than the critical value  $\mu$ , then the square of  $g_0$  is negative and  $g_0$  is imaginary.

As  $g$  approaches its critical value from below, the two energy eigenvalues in (178) vary accordingly. The energy eigenvalues are the two zeros of the secular determinant  $f(E)$  obtained from applying Cramer's rule to (177). As  $g$  (and  $g_0$ ) increase, the energy of the physical  $N\theta$  state increases. The energy of the  $N\theta$  state becomes infinite as  $g$  reaches its critical value. As  $g$  increases past its critical value, the upper energy eigenvalue goes around the bend; it abruptly jumps from being large and positive to being large and negative. Then, as  $g$  continues to increase, this energy eigenvalue approaches the energy of the physical  $V$  particle from below.

When  $g$  increases past its critical value, the Hamiltonian  $H$  in (173) becomes non-Hermitian, but its eigenvalues in the  $V/N\theta$  sector remain real. (The eigenvalues remain real because  $H$  becomes  $\mathcal{PT}$  symmetric. All cubic  $\mathcal{PT}$ -symmetric Hamiltonians that we have studied have been shown to have real spectra.) However, in the  $\mathcal{PT}$ -symmetric regime it is no longer appropriate to interpret the lower eigenvalue as the energy of the physical  $N\theta$  state. Rather, it is the energy of a new kind of state  $|G\rangle$  called a *ghost*. As is shown in [1, 127, 128], the Hermitian norm of this state is *negative*.

A physical interpretation of the ghost state emerges easily when we use the procedure developed in [129]. We begin by verifying that in the  $\mathcal{PT}$ -symmetric regime, where  $g_0$  is imaginary, the states of the Hamiltonian are eigenstates of the  $\mathcal{PT}$  operator, and we then choose the multiplicative phases of these states so that their  $\mathcal{PT}$  eigenvalues are unity:

$$\mathcal{PT}|G\rangle = |G\rangle, \quad \mathcal{PT}|V\rangle = |V\rangle. \quad (181)$$

It is then straightforward to verify that the  $\mathcal{PT}$  norm of the  $V$  state is positive, while the  $\mathcal{PT}$  norm of the ghost state is negative.

We now follow the procedures described in section 6 to calculate  $\mathcal{C}$ . We express the  $\mathcal{C}$  operator as an exponential of a function  $Q$  multiplying the parity operator:  $\mathcal{C} = \exp[Q(V^\dagger, V; N^\dagger, N; a^\dagger, a)]\mathcal{P}$ . We then impose the operator equations  $\mathcal{C}^2 = \mathbf{1}$ ,  $[\mathcal{C}, \mathcal{PT}] = 0$ , and  $[\mathcal{C}, H] = 0$ . The condition  $\mathcal{C}^2 = \mathbf{1}$  gives

$$Q(V^\dagger, V; N^\dagger, N; a^\dagger, a) = -Q(-V^\dagger, -V; -N^\dagger, -N; -a^\dagger, -a). \quad (182)$$

Thus,  $Q(V^\dagger, V; N^\dagger, N; a^\dagger, a)$  is an odd function in total powers of  $V^\dagger, V, N^\dagger, N, a^\dagger$ , and  $a$ . Next, we impose the condition  $[\mathcal{C}, \mathcal{PT}] = 0$  and obtain

$$Q(V^\dagger, V; N^\dagger, N; a^\dagger, a) = Q^*(-V^\dagger, -V; -N^\dagger, -N; -a^\dagger, -a), \quad (183)$$

where  $*$  denotes complex conjugation.

Last, we impose the condition that  $\mathcal{C}$  commutes with  $H$ , which requires that

$$[e^Q, H_0] = g_0 [e^Q, H_1]_+. \quad (184)$$

Although in sections 8.1 and 8.2 we were only able to find the  $\mathcal{C}$  operator to leading order in perturbation theory, for the Lee model one can calculate  $\mathcal{C}$  exactly and in closed form. To do so, we seek a solution for  $Q$  as a formal Taylor series in powers of  $g_0$ :

$$Q = \sum_{n=0}^{\infty} g_0^{2n+1} Q_{2n+1}. \quad (185)$$

Only odd powers of  $g_0$  appear in this series, and  $Q_{2n+1}$  are all anti-Hermitian:  $Q_{2n+1}^\dagger = -Q_{2n+1}$ . From (185) we get

$$Q_{2n+1} = (-1)^n \frac{2^{2n+1}}{(2n+1)\mu_0^{2n+1}} (V^\dagger N a n_\theta^n - n_\theta^n a^\dagger N^\dagger V), \quad (186)$$

where  $n_\theta = a^\dagger a$  is the number operator for  $\theta$ -particle quanta.

We then sum over all  $Q_{2n+1}$  and obtain the *exact* result that

$$Q = V^\dagger N a \frac{1}{\sqrt{n_\theta}} \arctan\left(\frac{2g_0\sqrt{n_\theta}}{\mu_0}\right) - \frac{1}{\sqrt{n_\theta}} \arctan\left(\frac{2g_0\sqrt{n_\theta}}{\mu_0}\right) a^\dagger N^\dagger V. \quad (187)$$

We exponentiate this result to obtain the  $\mathcal{C}$  operator. The exponential of  $Q$  simplifies considerably because we are treating the  $V$  and  $N$  particles as fermions and therefore we can use the identity  $n_{V,N}^2 = n_{V,N}$ . The *exact* result for  $e^Q$  is

$$e^Q = \left[ 1 - \frac{2g_0\sqrt{n_\theta}}{\sqrt{\mu_0^2 + 4g_0^2 n_\theta}} a^\dagger N^\dagger V + \frac{\mu_0 n_N (1 - n_V)}{\sqrt{\mu_0^2 + 4g_0^2 n_\theta}} + \frac{\mu_0 n_V (1 - n_N)}{\sqrt{\mu_0^2 + 4g_0^2 (n_\theta + 1)}} \right. \\ \left. + V^\dagger N a \frac{2g_0\sqrt{n_\theta}}{\sqrt{\mu_0^2 + 4g_0^2 n_\theta}} - n_V - n_N + n_V n_N \right]. \quad (188)$$

We can also express the parity operator  $\mathcal{P}$  in terms of number operators:

$$\mathcal{P} = e^{i\pi(n_V + n_N + n_\theta)} = (1 - 2n_V)(1 - 2n_N) e^{i\pi n_\theta}. \quad (189)$$

Combining  $e^Q$  and  $\mathcal{P}$ , we obtain the exact expression for  $\mathcal{C}$ :

$$\mathcal{C} = \left[ 1 - \frac{2g_0\sqrt{n_\theta}}{\sqrt{\mu_0^2 + 4g_0^2 n_\theta}} a^\dagger N^\dagger V + \frac{\mu_0 n_N (1 - n_V)}{\sqrt{\mu_0^2 + 4g_0^2 n_\theta}} + \frac{\mu_0 n_V (1 - n_N)}{\sqrt{\mu_0^2 + 4g_0^2 (n_\theta + 1)}} \right. \\ \left. + V^\dagger N a \frac{2g_0\sqrt{n_\theta}}{\sqrt{\mu_0^2 + 4g_0^2 n_\theta}} - n_V - n_N + n_V n_N \right] (1 - 2n_V)(1 - 2n_N) e^{i\pi n_\theta}. \quad (190)$$

Using this  $\mathcal{C}$  operator to calculate the  $\mathcal{CPT}$  norm of the  $V$  state and of the ghost state, we find that these norms are both positive. Furthermore, the time evolution is unitary. This

establishes that with the proper definition of the inner product the quantum-mechanical Lee model is a physically acceptable and consistent quantum theory, even in the ghost regime where the unrenormalized coupling constant is imaginary. The procedure of redefining the inner product to show that the ghost state is a physical state is a powerful technique that has been used by Curtright *et al* and by Ivanov and Smilga for more advanced problems [131, 132].

#### 8.4. The Higgs sector of the standard model of particle physics

The distinguishing features of the  $-g\varphi^4$  quantum field theory in (159) are that its spectrum is real and bounded below, it is perturbatively renormalizable, it has a dimensionless coupling constant in four-dimensional space–time, and it is *asymptotically free* [133]. The property of asymptotic freedom was established many years ago by Symanzik [134], as has been emphasized in a recent paper by Kleefeld [135]. As Kleefeld explains, a  $+g\varphi^4$  theory in four-dimensional space–time is trivial because it is not asymptotically free. However, Symanzik proposed a ‘precarious’ theory with a negative quartic coupling constant as a candidate for an asymptotically free theory of strong interactions. Symanzik used the term ‘precarious’ because the negative sign of the coupling constant suggests that this theory is energetically unstable. However, as we have argued in this paper, imposing  $\mathcal{PT}$ -symmetric boundary conditions (in this case on the functional-integral representation of the quantum field theory) gives a spectrum that is bounded below. Thus, Symanzik’s proposal of a non-trivial theory is resurrected.

The  $-g\varphi^4$  quantum field theory has another remarkable property. Although the theory seems to be parity invariant, the  $\mathcal{PT}$ -symmetric boundary conditions violate parity invariance, as explained in section 2.7. Hence, the one-point Green’s function (the expectation value of the field  $\varphi$ ) does not vanish. (Techniques for calculating this expectation value are explained in [136].) Thus, a non-zero vacuum expectation value can be achieved without having to have spontaneous symmetry breaking because parity symmetry is *permanently* broken. These properties suggest that a  $-g\varphi^4$  quantum field theory might be useful in describing the Higgs sector of the standard model.

Perhaps the Higgs particle state is a consequence of the field-theoretic parity anomaly in the same way that the quantum-mechanical parity anomaly described in sections 2.7 and 2.8 gives rise to bound states. Recent research in this area has been done by Jones *et al*, who studied transformations of functional integrals [137], and by Meisinger and Ogilvie, who worked on large- $N$  approximations and matrix models [138].

#### 8.5. $\mathcal{PT}$ -symmetric quantum electrodynamics

If the unrenormalized electric charge  $e$  in the Hamiltonian for quantum electrodynamics were imaginary, then the Hamiltonian would be non-Hermitian. However, if one specifies that the potential  $A^\mu$  in this theory transforms as an *axial* vector instead of a vector, then the Hamiltonian becomes  $\mathcal{PT}$  symmetric [139]. Specifically, we assume that the four-vector potential and the electromagnetic fields transform under  $\mathcal{P}$  like

$$\mathcal{P} : \quad \mathbf{E} \rightarrow \mathbf{E}, \quad \mathbf{B} \rightarrow -\mathbf{B}, \quad \mathbf{A} \rightarrow \mathbf{A}, \quad A^0 \rightarrow -A^0. \quad (191)$$

Under time reversal, the transformations are assumed to be conventional:

$$\mathcal{T} : \quad \mathbf{E} \rightarrow \mathbf{E}, \quad \mathbf{B} \rightarrow -\mathbf{B}, \quad \mathbf{A} \rightarrow -\mathbf{A}, \quad A^0 \rightarrow A^0. \quad (192)$$

The Lagrangian of the theory possesses an imaginary coupling constant in order that it be invariant under the product of these two symmetries:

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{1}{2}\psi^\dagger\gamma^0\gamma^\mu\frac{1}{i}\partial_\mu\psi + \frac{1}{2}m\psi^\dagger\gamma^0\psi + ie\psi^\dagger\gamma^0\gamma^\mu\psi A_\mu. \quad (193)$$



The corresponding Hamiltonian density is then

$$\mathcal{H} = \frac{1}{2}(E^2 + B^2) + \psi^\dagger [\gamma^0 \gamma^k (-i\nabla_k + ieA_k) + m\gamma^0] \psi. \quad (194)$$

The Lorentz transformation properties of the fermions are unchanged from the usual ones. Thus, the electric current appearing in the Lagrangian and Hamiltonian densities,  $j^\mu = \psi^\dagger \gamma^0 \gamma^\mu \psi$ , transforms conventionally under both  $\mathcal{P}$  and  $\mathcal{T}$ :

$$\mathcal{P} j^\mu(\mathbf{x}, t) \mathcal{P} = \begin{pmatrix} j^0 \\ -\mathbf{j} \end{pmatrix}(-\mathbf{x}, t), \quad \mathcal{T} j^\mu(\mathbf{x}, t) \mathcal{T} = \begin{pmatrix} j^0 \\ -\mathbf{j} \end{pmatrix}(\mathbf{x}, -t). \quad (195)$$

Because its interaction is cubic, this non-Hermitian theory of ‘electrodynamics’ is the analog of the spinless  $i\phi^3$  quantum field theory discussed in section 8.1.  $\mathcal{PT}$ -symmetric electrodynamics is especially interesting because it is an asymptotically free theory (unlike ordinary electrodynamics) and because the sign of the Casimir force is the opposite of that in ordinary electrodynamics [139, 140]. This theory is remarkable because finiteness conditions enable it to determine its own coupling constant [140].

The  $\mathcal{C}$  operator for  $\mathcal{PT}$ -symmetric quantum electrodynamics has been constructed perturbatively to first order in  $e$  [141]. This construction is too technical to describe here, but it demonstrates that non-Hermitian quantum electrodynamics is a viable and consistent unitary quantum field theory.  $\mathcal{PT}$ -symmetric quantum electrodynamics is more interesting than an  $i\phi^3$  quantum field theory because it possesses many of the features of conventional quantum electrodynamics, including Abelian gauge invariance. The only asymptotically free quantum field theories described by Hermitian Hamiltonians are those that possess a *non-Abelian* gauge invariance;  $\mathcal{PT}$  symmetry allows for new kinds of asymptotically free theories, such as the  $-\phi^4$  theory discussed in section 8.4, that do not possess a non-Abelian gauge invariance.

### 8.6. Dual $\mathcal{PT}$ -symmetric quantum field theories

Until now we have focused on bosonic  $\mathcal{PT}$ -symmetric Hamiltonians, but it is just as easy to construct fermionic  $\mathcal{PT}$ -symmetric Hamiltonians. We look first at free theories. The Lagrangian density for a conventional Hermitian free fermion field theory is

$$\mathcal{L}(\mathbf{x}, t) = \bar{\psi}(\mathbf{x}, t)(i\not{\partial} - m)\psi(\mathbf{x}, t) \quad (196)$$

and the corresponding Hamiltonian density is

$$\mathcal{H}(\mathbf{x}, t) = \bar{\psi}(\mathbf{x}, t)(-i\nabla + m)\psi(\mathbf{x}, t), \quad (197)$$

where  $\bar{\psi}(\mathbf{x}, t) = \psi^\dagger(\mathbf{x}, t)\gamma_0$ .

In  $(1+1)$ -dimensional space–time we adopt the following conventions:  $\gamma_0 = \sigma_1$  and  $\gamma_1 = i\sigma_2$ , where the Pauli  $\sigma$  matrices are given in (151). With these definitions, we have  $\gamma_0^2 = 1$  and  $\gamma_1^2 = -1$ . We also define  $\gamma_5 = \gamma_0\gamma_1 = \sigma_3$ , so that  $\gamma_5^2 = 1$ . The parity-reflection operator  $\mathcal{P}$  has the effect

$$\mathcal{P}\psi(x, t)\mathcal{P} = \gamma_0\psi(-x, t), \quad \mathcal{P}\bar{\psi}(x, t)\mathcal{P} = \bar{\psi}(-x, t)\gamma_0. \quad (198)$$

The effect of the time-reversal operator  $\mathcal{T}$ ,

$$\mathcal{T}\psi(x, t)\mathcal{T} = \gamma_0\psi(x, -t), \quad \mathcal{T}\bar{\psi}(x, t)\mathcal{T} = \bar{\psi}(x, -t)\gamma_0, \quad (199)$$

is similar to that of  $\mathcal{P}$ , except that  $\mathcal{T}$  is antilinear and takes the complex conjugate of complex numbers. From these definitions the Hamiltonian  $H = \int dx \mathcal{H}(x, t)$ , where  $\mathcal{H}$  is given in (197), is Hermitian:  $H = H^\dagger$ . Also,  $H$  is separately invariant under parity reflection and under time reversal:  $\mathcal{P}H\mathcal{P} = H$  and  $\mathcal{T}H\mathcal{T} = H$ .

We can construct a non-Hermitian fermionic Hamiltonian by adding a  $\gamma_5$ -dependent mass term to the Hamiltonian density in (197):

$$\mathcal{H}(x, t) = \bar{\psi}(x, t)(-i\nabla + m_1 + m_2\gamma_5)\psi(x, t) \quad (m_2 \text{ real}). \quad (200)$$

The Hamiltonian  $H = \int dx \mathcal{H}(x, t)$  associated with this Hamiltonian density is not Hermitian because the  $m_2$  term changes sign under Hermitian conjugation. This sign change occurs because  $\gamma_0$  and  $\gamma_5$  anticommute. Also,  $H$  is not invariant under  $\mathcal{P}$  or under  $\mathcal{T}$  separately because the  $m_2$  term changes sign under each of these reflections. However,  $H$  is invariant under combined  $\mathcal{P}$  and  $\mathcal{T}$  reflection. Thus,  $H$  is  $\mathcal{PT}$ -symmetric.

To see whether the  $\mathcal{PT}$  symmetry of  $H$  is broken or unbroken, we must check to see whether the spectrum of  $H$  is real. We do so by solving the field equations. The field equation associated with  $\mathcal{H}$  in (200) is

$$(i\partial - m_1 - m_2\gamma_5)\psi(x, t) = 0. \quad (201)$$

If we iterate this equation and use  $\partial^2 = \partial^2$ , we obtain

$$(\partial^2 + \mu^2)\psi(x, t) = 0, \quad (202)$$

which is the two-dimensional Klein–Gordon equation with  $\mu^2 = m_1^2 - m_2^2$ . The physical mass that propagates under this equation is real when the inequality

$$m_1^2 \geq m_2^2 \quad (203)$$

is satisfied. This condition defines the two-dimensional parametric region of *unbroken*  $\mathcal{PT}$  symmetry. When (203) is not satisfied,  $\mathcal{PT}$  symmetry is *broken*. At the boundary between the regions of broken and unbroken  $\mathcal{PT}$  symmetry (the line  $m_2 = 0$ ), the Hamiltonian is Hermitian. (The same is true in quantum mechanics. Recall that for the Hamiltonian in (12) the region of broken (unbroken)  $\mathcal{PT}$  symmetry is  $\epsilon < 0$  ( $\epsilon > 0$ ). At the boundary  $\epsilon = 0$  of these two regions the Hamiltonian is Hermitian.)

The  $\mathcal{C}$  operator associated with the  $\mathcal{PT}$ -symmetric Hamiltonian density  $\mathcal{H}$  in (200) is given by  $\mathcal{C} = e^Q \mathcal{P}$ , where [142]

$$\begin{aligned} Q &= -\tanh^{-1}\epsilon \int dx \bar{\psi}(x, t)\gamma_1\psi(x, t) \\ &= -\tanh^{-1}\epsilon \int dx \psi^\dagger(x, t)\gamma_5\psi(x, t). \end{aligned} \quad (204)$$

The inverse hyperbolic tangent in this equation requires that  $|\epsilon| \leq 1$ , or equivalently that  $m_1^2 \geq m_2^2$ , which corresponds to the unbroken region of  $\mathcal{PT}$  symmetry. We use (204) to construct the equivalent Hermitian Hamiltonian  $h$  as in (132):

$$\begin{aligned} h &= \exp\left[\frac{1}{2}\tanh^{-1}\epsilon \int dx \psi^\dagger(x, t)\gamma_5\psi(x, t)\right] H \\ &\times \exp\left[-\frac{1}{2}\tanh^{-1}\epsilon \int dx \psi^\dagger(x, t)\gamma_5\psi(x, t)\right]. \end{aligned} \quad (205)$$

The commutation relations  $[\gamma_5, \gamma_0] = -2\gamma_1$  and  $[\gamma_5, \gamma_1] = -2\gamma_0$  simplify  $h$  in (205):

$$h = \int dx \bar{\psi}(x, t)(-i\nabla + \mu)\psi(x, t), \quad (206)$$

where  $\mu^2 = m^2(1 - \epsilon^2) = m_1^2 - m_2^2$ , in agreement with (202). Replacing  $H$  by  $h$  changes the  $\gamma_5$ -dependent mass term  $m\psi(1 + \epsilon\gamma_5)\psi$  to a conventional fermion mass term  $\mu\bar{\psi}\psi$ . Thus, the non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian density in (200) is equivalent to the Hermitian Hamiltonian density in (197) with  $m$  replaced by  $\mu$ .

If we introduce a four-point fermion interaction term in (196), we obtain the Lagrangian density for the massive Thirring model in (1 + 1) dimensions:

$$\mathcal{L} = \bar{\psi}(i\partial - m)\psi + \frac{1}{2}g(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi), \quad (207)$$

whose corresponding Hamiltonian density is

$$\mathcal{H} = \bar{\psi}(-i\nabla + m)\psi - \frac{1}{2}g(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi). \quad (208)$$

We can then construct the  $\mathcal{PT}$ -symmetric Thirring model

$$\mathcal{H} = \bar{\psi}(-i\nabla + m + \varepsilon m\gamma_5)\psi - \frac{1}{2}g(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \quad (209)$$

by introducing a  $\gamma_5$ -dependent mass term. The additional term is non-Hermitian but  $\mathcal{PT}$ -symmetric because it is odd under both parity reflection and time reversal. Remarkably, the  $Q$  operator for the interacting case  $g \neq 0$  is *identical* to the  $Q$  operator for the case  $g = 0$  because in (1 + 1)-dimensional space the interaction term  $(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi)$  commutes with the  $Q$  in (204) [142]. Thus, the non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian density in (209) is equivalent to the Hermitian Hamiltonian density in (208) with the mass  $m$  replaced by  $\mu$ , where  $\mu^2 = m^2(1 - \varepsilon^2) = m_1^2 - m_2^2$ .

The same holds true for the (3 + 1)-dimensional interacting Thirring model by virtue of the commutation relation  $[\gamma_5, \gamma_0\gamma_\mu] = 0$ , but because this higher-dimensional field theory is non-renormalizable, the  $Q$  operator may only have a formal significance.

In (1 + 1) dimensions the massive Thirring Model (207) is *dual* to the (1 + 1)-dimensional sine-Gordon model [143], whose Lagrangian density is

$$\mathcal{L} = \frac{1}{2}(\hat{p}_\mu\varphi)^2 + m^2\lambda^{-2}(\cos\lambda\varphi - 1), \quad (210)$$

whose corresponding Hamiltonian density is

$$\mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\varphi)^2 + m^2\lambda^{-2}(1 - \cos\lambda\varphi), \quad (211)$$

where  $\pi(x, t) = \partial_0\varphi(x, t)$  and where in (1 + 1)-dimensional space  $\nabla\varphi(x, t)$  is just  $\hat{p}_1\varphi(x, t)$ . The duality between the Thirring model and the sine-Gordon model is expressed as an algebraic relationship between the coupling constants  $g$  and  $\lambda$ :

$$\frac{\lambda^2}{4\pi} = \frac{1}{1 - g/\pi}. \quad (212)$$

Note that the free fermion theory ( $g = 0$ ) is equivalent to the sine-Gordon model with the special value for the coupling constant  $\lambda^2 = 4\pi$ .

The  $\mathcal{PT}$ -symmetric extension (209) of the modified Thirring model is, by the same analysis, dual to a modified sine-Gordon model with the Hamiltonian density

$$\mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\varphi)^2 + m^2\lambda^{-2}(1 - \cos\lambda\varphi - i\varepsilon\sin\lambda\varphi), \quad (213)$$

which is  $\mathcal{PT}$ -symmetric and not Hermitian. The  $Q$  operator for this Hamiltonian is

$$Q = \frac{2}{\lambda} \tanh^{-1}\varepsilon \int dx \pi(x, t). \quad (214)$$

Thus, the equivalent Hermitian Hamiltonian  $h$  is given by

$$h = \exp\left[-\frac{1}{\lambda} \tanh^{-1}\varepsilon \int dx \pi(x, t)\right] H \exp\left[\frac{1}{\lambda} \tanh^{-1}\varepsilon \int dx \pi(x, t)\right]. \quad (215)$$

Note that the operation that transforms  $H$  to  $h$  has the same effect as shifting the boson field  $\varphi$  by an imaginary constant:

$$\varphi \rightarrow \varphi + \frac{i}{\lambda} \tanh^{-1}\varepsilon. \quad (216)$$

Under this transformation the interaction term  $m^2\lambda^{-2}(1 - \cos \lambda\varphi - i\varepsilon \sin \lambda\varphi)$  in (213) becomes  $-m^2\lambda^{-2}(1 - \varepsilon^2) \cos \lambda\varphi$ , apart from an additive constant. Hence,  $h$  is the Hamiltonian for the Hermitian sine-Gordon model, but with mass  $\mu$  given by  $\mu^2 = m^2(1 - \varepsilon^2) = m_1^2 - m_2^2$ . This change in the mass is the same as for the Thirring model. Being Hermitian,  $h$  is even in the parameter  $\varepsilon$  that breaks the Hermiticity of  $H$ .

The idea of generating a non-Hermitian but  $\mathcal{PT}$ -symmetric Hamiltonian from a Hermitian Hamiltonian by shifting the field operator as in (216), first introduced in the context of quantum mechanics in [144], suggests a way to construct solvable fermionic  $\mathcal{PT}$ -invariant models whenever there is a boson-fermion duality.

### 8.7. $\mathcal{PT}$ -symmetric gravitational and cosmological theories

In section 8.5 we showed that to construct a  $\mathcal{PT}$ -symmetric model of quantum electrodynamics, one needs only to replace the electric charge  $e$  by  $ie$  and then replace the vector potential  $A^\mu$  by an axial-vector potential. The result is a non-Hermitian but  $\mathcal{PT}$ -symmetric Hamiltonian. An interesting classical aspect of this model is that the sign of the Colomb force is reversed, so that like charges feel an attractive force and unlike charges feel a repulsive force.

One can use the same idea to construct a  $\mathcal{PT}$ -symmetric model of massless spin-2 particles (gravitons). One simply replaces the gravitational coupling constant  $G$  by  $iG$  and then requires the two-component tensor field to behave like an axial tensor under parity reflection. The result is a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian, which at the classical level describes a *repulsive* gravitational force. It would be interesting to investigate the possible connections between such a model and the notion of dark energy and the recent observations that the expansion of the universe is accelerating.

The connection discussed in section 2.6 between reflectionless potentials and  $\mathcal{PT}$  symmetry may find application in quantum cosmology. There has been much attention given to anti-de Sitter cosmologies [145] and de Sitter cosmologies [146, 147]. In the AdS description the universe propagates reflectionlessly in the presence of a wrong-sign potential ( $-x^6$ , for example). In the dS case the usual Hermitian quantum mechanics must be abandoned and be replaced by a non-Hermitian one in which there are ‘meta-observables’. The non-Hermitian inner product that is used in the dS case is based on the  $\mathcal{CPT}$  theorem in the same way that the  $\mathcal{CPT}$  inner product is used in  $\mathcal{PT}$ -symmetric quantum theory [60]. The condition of reflectionless, which is equivalent to the requirement of  $\mathcal{PT}$  symmetry, is what allows the wrong-sign potential to have a positive spectrum. Calculating the lowest-energy level in this potential would be equivalent to determining the cosmological constant [148].

### 8.8. Classical field theory

The procedure for constructing  $\mathcal{PT}$ -symmetric Hamiltonians is to begin with a Hamiltonian that is both Hermitian and  $\mathcal{PT}$  symmetric, and then to introduce a parameter  $\epsilon$  that extends the Hamiltonian into the complex domain while maintaining its  $\mathcal{PT}$  symmetry. This is the procedure that was used to construct the new kinds of Hamiltonians in (12). We can follow the same procedure for classical nonlinear wave equations because many wave equations are  $\mathcal{PT}$  symmetric.

As an example, consider the Korteweg–de Vries (KdV) equation

$$u_t + uu_x + u_{xxx} = 0. \quad (217)$$

To demonstrate that this equation is  $\mathcal{PT}$  symmetric, we define a classical parity reflection  $\mathcal{P}$  to be the replacement  $x \rightarrow -x$ , and since  $u = u(x, t)$  is a velocity, the sign of  $u$  also changes under  $\mathcal{P}$ :  $u \rightarrow -u$ . We define a classical time reversal  $\mathcal{T}$  to be the replacement  $t \rightarrow -t$ , and again,

since  $u$  is a velocity, the sign of  $u$  also changes under  $\mathcal{T}$ :  $u \rightarrow -u$ . Following the quantum-mechanical formalism, we also require that  $i \rightarrow -i$  under time reversal. Note that the KdV equation is not symmetric under  $\mathcal{P}$  or  $\mathcal{T}$  separately, but that it *is* symmetric under combined  $\mathcal{PT}$  reflection. The KdV equation is a special case of the Camassa–Holm equation [149], which is also  $\mathcal{PT}$  symmetric. Other nonlinear wave equations such as the generalized KdV equation  $u_t + u^k u_x + u_{xxx} = 0$ , the sine-Gordon equation  $u_{tt} - u_{xx} + g \sin u = 0$ , and the Boussinesq equation are  $\mathcal{PT}$  symmetric as well.

The observation that there are many nonlinear wave equations possessing  $\mathcal{PT}$  symmetry suggests that one can generate rich and interesting families of new complex nonlinear  $\mathcal{PT}$ -symmetric wave equations by following the same procedure that was used in quantum mechanics and one can try to discover which properties (conservation laws, solitons, integrability, stochastic behaviour) of the original wave equations are preserved and which are lost. One possible procedure for generating new nonlinear equations from the KdV equation is to introduce the real parameter  $\epsilon$  as follows:

$$u_t - iu(iu_x)^\epsilon + u_{xxx} = 0. \quad (218)$$

Various members of this family of equations have been studied in [150]. Of course, there are other ways to extend the KdV equation into the complex domain while preserving  $\mathcal{PT}$  symmetry; see, for example [151].

## 9. Final remarks

In this paper we have shown how to extend physical theories into the complex domain. The complex domain is huge compared with the real domain, and therefore there are many exciting new theories to explore. The obvious potential problem with extending a real theory into complex space is that one may lose some of the characteristics that a valid physical theory must possess. Thus, it is necessary that this complex extension be tightly constrained. We have shown that the essential physical axioms of a quantum theory are maintained if the complex extension is done in such a way as to preserve  $\mathcal{PT}$  symmetry.

The complex theories that we have constructed are often far more elaborate and diverse than theories that are restricted to the real domain. Upon entering the complex world we have found a gold mine of new physical theories that have strange and fascinating properties. We have just begun to study the vast new panorama that has opened up and we can hardly begin to guess what new kinds of phenomena have yet to be discovered.

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