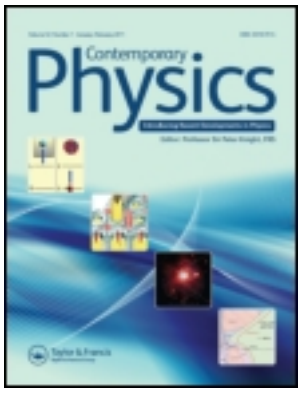

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Introduction to $\mathcal{PT}$-symmetric quantum theory

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In most introductory courses on quantum mechanics one is taught that the Hamiltonian operator must be Hermitian in order that the energy levels be real and that the theory be unitary (probability conserving). To express the Hermiticity of a Hamiltonian, one writes $H = H^{\dagger}$, where the symbol † denotes the usual Dirac Hermitian conjugation; that is, transpose and complex conjugate. In the past few years it has been recognized that the requirement of Hermiticity, which is often stated as an axiom of quantum mechanics, may be replaced by the less mathematical and more physical requirement of space – time reflection symmetry ($\mathcal{PT}$ symmetry) without losing any of the essential physical features of quantum mechanics. Theories defined by non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians exhibit strange and unexpected properties at the classical as well as at the quantum level. This paper explains how the requirement of Hermiticity can be evaded and discusses the properties of some non-Hermitian $\mathcal{PT}$-symmetric quantum theories.

1. Introduction

The field of $\mathcal{PT}$-symmetric quantum theory is only six years old but already hundreds of papers have been published on various aspects of $\mathcal{PT}$-symmetric quantum mechanics and $\mathcal{PT}$-symmetric quantum field theory. Three international conferences have been held (Prague, 2003; Prague, 2004; Shizuoka, 2004) and three more conferences are planned. Work on $\mathcal{PT}$ symmetry began with the investigation of quantum-mechanical models and has now extended into many areas including quasi-exact solvability, supersymmetry and quantum field theory. Recently, it has been recognized that there is a connection between $\mathcal{PT}$-symmetric quantum mechanics and integrable models. The aim of this paper is to introduce the subject at an elementary level and to elucidate the properties of theories described by $\mathcal{PT}$-symmetric Hamiltonians. This paper will make the field of $\mathcal{PT}$ symmetry accessible to students who are interested in exploring this exciting, new, and active area of physics.

The central idea of $\mathcal{PT}$-symmetric quantum theory is to replace the condition that the Hamiltonian of a quantum theory be Hermitian with the weaker condition that it possess space – time reflection symmetry ($\mathcal{PT}$ symmetry). This allows us to construct and study many new kinds of Hamiltonians that would previously have been ignored. These new Hamiltonians have remarkable mathematical properties and it may well turn out that these new Hamiltonians will be useful in describing the physical world. It is crucial, of course, that in replacing the condition of Hermiticity by $\mathcal{PT}$ symmetry we do not give up any of the key physical properties that a quantum theory must have. We will see that if the $\mathcal{PT}$ symmetry of the Hamiltonian is not broken, then the Hamiltonian will exhibit all of the features of a quantum theory described by a Hermitian Hamiltonian. (The word *broken* as used here is a technical term that will be explained in section 2.)

Let us begin by reviewing some basic ideas of quantum theory. For simplicity, in this paper we restrict our attention to one-dimensional quantum-mechanical systems. Also, we work in units where Planck's constant $\hbar = 1$. In elementary courses on quantum mechanics one learns that a quantum theory is specified by the Hamiltonian operator

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that acts on a Hilbert space. The Hamiltonian H does three things.

(i) The Hamiltonian determines the energy eigenstates $|\mathrm{En}\rangle$. These states are the eigenstates of the Hamiltonian operator and they solve the time-independent Schrödinger equation $H|E_n\rangle = E_n|E_n\rangle$. The energy eigenstates span the Hilbert space of physical state vectors. The eigenvalues E_n are the energy levels of the quantum theory. In principle, one can observe or measure these energy levels. The outcome of such a physical measurement is a real number, so it is essential that these energy eigenvalues be real.

(ii) The Hamiltonian H determines the time evolution in the theory. States $|t\rangle$ in the Schrödinger picture evolve in time according to the time-dependent Schrödinger equation $H|t\rangle = -\mathrm{i}(\mathrm{d}/\mathrm{d}t)|t\rangle$, whose formal solution is $|t\rangle = \exp(\mathrm{i}Ht)|0\rangle$. Operators $A(t)$ in the Heisenberg picture evolve according to the time-dependent Schrödinger equation $(\mathrm{d}/\mathrm{d}t)A(t) = -\mathrm{i}[A(t),H]$, whose formal solution is $A(t) = \exp(\mathrm{i}Ht)A(0)\exp(-\mathrm{i}Ht)$.

(iii) The Hamiltonian incorporates the symmetries of the theory. A quantum theory may have two kinds of symmetries: continuous symmetries, such as Lorentz invariance, and discrete symmetries, such as parity invariance and time reversal invariance. A quantum theory is symmetric under a transformation represented by an operator A if A commutes with the Hamiltonian that describes the quantum theory: $[A,H] = 0$. Note that if a symmetry transformation is represented by a *linear* operator A and if A commutes with the Hamiltonian, then the eigenstates of H are also eigenstates of A. Two important discrete symmetry operators are parity (space reflection), which is represented by the symbol $\mathcal{P}$, and time reversal, which is represented by the symbol $\mathcal{T}$. The operators $\mathcal{P}$ and $\mathcal{T}$ are defined by their effects on the dynamical variables $\hat{x}$ (the position operator) and $\hat{p}$ (the momentum operator). The operator $\mathcal{P}$ is *linear* and has the effect of changing the sign of the momentum operator $\hat{p}$ and the position operator $\hat{x}$: $\hat{p}\to-\hat{p}$ and $\hat{x}\to-\hat{x}$. The operator $\mathcal{T}$ is antilinear and has the effect $\hat{p}\to-\hat{p}$, $\hat{x}\to\hat{x}$ and $i\to i$. Note that $\mathcal{T}$ changes the sign of i because (like $\mathcal{P}$) $\mathcal{T}$ is required to preserve the fundamental commutation relation $[\hat{x},\hat{p}] = i$ of the dynamical variables in quantum mechanics.

Quantum mechanics is an association between states in a mathematical Hilbert space and experimentally measurable probabilities. The norm of a vector in the Hilbert space must be positive because this norm is a probability and a probability must be real and positive. Furthermore, the inner product between any two different vectors in the Hilbert space must be constant in time because probability is conserved. The requirement that the probability does not change with time is called *unitarity*. Unitarity is a fundamental property of any quantum theory and must not be violated.

To summarize the discussion so far, the two crucial properties of any quantum theory are that the energy levels must be real and that the time evolution must be unitary. There is a simple mathematical condition on the Hamiltonian that guarantees the reality of the energy eigenvalues and the unitarity of the time evolution; namely, that the Hamiltonian be *real and symmetric*. To explain the term *symmetric*, as it is used here, let us first consider the possibility that the quantum system has only a finite number of states. In this case the Hamiltonian is a finite-dimensional symmetric matrix

$$H = \begin{pmatrix} a & b & c & \cdots \\ b & d & e & \cdots \\ c & e & f & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{1}$$

whose entries $a, b, c, d, e, f, \ldots$ are real numbers. For systems having an infinite number of states we express H in terms of the dynamical variables $\hat{x}$ and $\hat{p}$. The $\hat{x}$ operator in coordinate space is a *real* and *symmetric* diagonal matrix, all of whose entries are the real number x. The $\hat{p}$ operator in coordinate space is *imaginary* and *anti-symmetric* because $\hat{p} = -\mathrm{i}(\mathrm{d}/\mathrm{d}x)$ when it acts to the right but, as we can see using integration by parts, $\hat{p}$ changes sign $\hat{p} = \mathrm{i}(\mathrm{d}/\mathrm{d}x)$ when it acts to the left. The operator $\hat{p}^2 = -\mathrm{d}^2/\mathrm{d}x^2$ is real and symmetric. Thus, any Hamiltonian of the form $H = \hat{p}^2 + \mathrm{V}(\hat{x})$ when written in coordinate space is real and symmetric. (In this paper we use units in which $m = \frac{1}{2}$ and we treat $\hat{x}$ and $\hat{p}$ as dimensionless.)

However, the condition that H be real and symmetric is not the most general condition that guarantees the reality of the energy levels and the unitarity of the time evolution because it excludes the possibility that the Hamiltonian matrix might be complex. Indeed, there are many physical applications which require that the Hamiltonian be complex. There is a more general condition that guarantees spectral reality and unitary time evolution and which includes real, symmetric Hamiltonians as a special case. This condition is known as *Hermiticity*. To express the condition that a complex Hamiltonian H is Hermitian we write $H = H^\dagger$. The symbol † represents *Dirac Hermitian conjugation*; that is, combined transpose and complex conjugation. The condition that H must exhibit Dirac Hermiticity is often taught as an axiom of quantum mechanics. The Hamiltonians $H = \hat{p}^2 + \hat{p} + V(\hat{x})$ and $H = \hat{p}^2 + \hat{p}\hat{x} + \hat{x}\hat{p} + V(\hat{x})$ are complex and non-symmetric but they are Hermitian.

In this paper we show that while Hermiticity is sufficient to guarantee the two essential properties of quantum mechanics, it is not necessary. We describe here an

alternative way to construct complex Hamiltonians that still guarantees the reality of the eigenvalues and the unitarity of time evolution and which also includes real, symmetric Hamiltonians as a special case. We will maintain the symmetry of the Hamiltonians in coordinate space, but we will allow the matrix elements to become complex in such a way that the condition of space–time reflection symmetry ($\mathcal{PT}$ symmetry) is preserved. The new kinds of Hamiltonians discussed in this paper are symmetric and have the property that they commute with the $\mathcal{PT}$ operator: $[H, \mathcal{PT}] = 0$. In analogy with the property of Hermiticity $H = H^\dagger$, we will express the property that a Hamiltonian is $\mathcal{PT}$ symmetric by using the notation $H = H^{\mathcal{PT}}$. We emphasize that our new kinds of complex Hamiltonians are symmetric in coordinate space but are not Hermitian in the Dirac sense. To reiterate, acceptable complex Hamiltonians may be either Hermitian $H = H^\dagger$ or $\mathcal{PT}$-symmetric $H = H^{\mathcal{PT}}$, but not both. Real symmetric Hamiltonians may be both Hermitian and $\mathcal{PT}$-symmetric.

Using $\mathcal{PT}$ symmetry as an alternative condition to Hermiticity, we can construct infinitely many new Hamiltonians that would have been rejected in the past because they are not Hermitian. An example of such a $\mathcal{PT}$-symmetric Hamiltonian is

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

We do not regard the condition of Hermiticity as wrong. Rather, the condition of $\mathcal{PT}$ symmetry offers the possibility of studying new quantum theories that may even describe measurable physical phenomena. Indeed, non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians have already been used to describe such phenomena as the ground state of a quantum system of hard spheres [1], Reggeon field theory [2] and the Lee–Yang edge singularity [3]. Although at the time that they were written these papers were criticized for using Hamiltonians that were not Hermitian, we now understand that these Hamiltonians have spectral positivity and that the associated quantum theories are unitary because these Hamiltonians are $\mathcal{PT}$-symmetric. In physics we should keep an open mind regarding the kinds of theories that we are willing to consider. Gell-Mann's 'totalitarian principle' states that among the possible physical theories 'Everything which is not forbidden is compulsory'.

This paper is organized as follows: I discuss in a personal way my discovery of $\mathcal{PT}$-symmetric quantum mechanics and give a brief history of the early days of this subject in section 2. Section 3 explains how to calculate the energy levels of a $\mathcal{PT}$-symmetric Hamiltonian. Section 4 describes the classical mechanics of $\mathcal{PT}$-symmetric Hamiltonians. Next, in section 5 we show that a Hamiltonian having an unbroken $\mathcal{PT}$ symmetry defines a *unitary* quantum theory. The demonstration of unitarity is based on showing that $\mathcal{PT}$-symmetric Hamiltonians that have an unbroken $\mathcal{PT}$ symmetry also possess a new parity-like symmetry; this symmetry is represented by a new operator that we call $\mathcal{C}$. We give in section 6 a simple 2×2 matrix illustration of the procedures used in section 5. In section 7 we discuss the nature of observables in $\mathcal{PT}$-symmetric quantum-mechanical theories. We show how to calculate the $\mathcal{C}$ operator in section 8. In section 9 we explain why one may regard $\mathcal{PT}$-symmetric quantum mechanics as a complex version of ordinary quantum mechanics. Finally, in section 10 we discuss some possible physical applications of $\mathcal{PT}$-symmetric quantum mechanics.

2. A personal history of $\mathcal{PT}$ symmetry

My first encounter with a non-Hermitian complex Hamiltonian dates back to the summer of 1993. In the course of a private conversation with D. Bessis at CEN Saclay, I learned that he and J. Zinn-Justin had noticed that the eigenvalues of the Hamiltonian operator in (2) seemed to be real and they wondered if the spectrum (the set of energy eigenvalues of the Hamiltonian) might be entirely real. (Their interest in the Hamiltonian (2) was inspired by early work on the Lee–Yang edge singularity [3].) At the time I did not plan to pursue this conjecture further because it seemed absurd that a complex non-Hermitian Hamiltonian might have real energy levels.

I did not know it at the time, but Bessis and Zinn-Justin were not the first to notice that a complex cubic quantum-mechanical Hamiltonian might have real eigenvalues. For example, early studies of Reggeon field theory in the late 1970s led a number of investigators to observe that model cubic quantum-mechanical Hamiltonians like that in (2) might have real eigenvalues [2]. Also, Caliceti *et al.* observed in 1980 that on the basis of Borel summability arguments the spectrum of a Hamiltonian related to (2) is real [4]. In each of these cases the possibility that a complex non-Hermitian Hamiltonian might have real energy levels was viewed as an isolated curiosity. It was believed that such a Hamiltonian could not describe a valid theory of quantum mechanics because the non-Hermiticity of the Hamiltonian would result in non-unitary time evolution [3].

I did not forget about the remarkable Hamiltonian in (2) and in 1997 I decided to investigate it. I suspected that if the spectrum of this Hamiltonian was real, it was probably due to the presence of a symmetry and I realized that (2) does possess $\mathcal{PT}$ symmetry because any real function of $\mathrm{i}\hat{x}$ is $\mathcal{PT}$-symmetric. I decided that a simple and natural way to determine the spectrum of (2) would be to use the delta expansion, a perturbative technique that I had developed several years earlier for solving nonlinear problems [5]. I asked my former graduate student S. Boettcher to join me in this investigation.

The delta expansion is an extremely simple technique for solving nonlinear problems perturbatively (approximately).

The idea of the delta expansion is to introduce a small perturbation parameter δ into a nonlinear problem in such a way that δ is a measure of the nonlinearity of the problem. To illustrate how the delta expansion is used, consider the Thomas–Fermi equation, a difficult nonlinear boundary-value problem that describes the approximate electric charge distribution in an atom:

$$y''(x) = y^{3/2}x^{-1/2}\ , \quad y(0) = 1\ , \quad y(\infty) = 0\ . \tag{3}$$

There is no exact closed-form solution to this problem. However, a nice way to solve this problem perturbatively is to introduce the parameter δ in the exponent:

$$y''(x) = y(y/x)^{\delta}, \quad y(0) = 1\ , \quad y(\infty) = 0\ . \tag{4}$$

When $\delta = \frac{1}{2}$, (4) reduces to (3). However, in (4) we treat the parameter δ as small ($\delta << 1$). When $\delta = 0$, the problem becomes *linear* and therefore it can be solved exactly; the solution is $y_0(x) = \exp(-x)$. This is the leading term in the perturbation expansion for $y(x)$, which has the form $y(x) = \sum_{n=0}^{\infty} y_n(x)\delta^n$. It is easy to calculate the coefficients of the higher powers of δ. At the end of the calculation one sets $\delta = 1/2$, and from just the first few terms in the perturbation series one obtains a good numerical approximation to the solution to the Thomas–Fermi equation.

I was eager to find out what would happen if we applied delta-expansion methods to (2). We replaced the Hamiltonian (2) by the one-parameter family of Hamiltonians

$$H = \hat{p}^2 + \hat{x}^2(\mathrm{i}\hat{x})^{\delta}\ , \tag{5}$$

where δ is regarded as a small real parameter. There are two advantages in inserting δ in this fashion: first, the new Hamiltonian remains $\mathcal{PT}$-symmetric for *all* real δ. Thus, the insertion of δ maintains the $\mathcal{PT}$ symmetry of the original problem. Second, when $\delta = 0$, the Hamiltonian (5) reduces to that of the harmonic oscillator, which can be solved exactly because the underlying classical equations of motion are linear. Each of the energy levels of (5) have a delta expansion of the general form

$$E = \sum_{n=0}^{\infty} a_n\delta^n\ . \tag{6}$$

The series coefficients are easy to calculate and they are real. Thus, assuming that this delta expansion converges, the eigenvalues of H in (5) must be real. At the end of the calculation we set $\delta = 1$ in (6) to recover the eigenvalues of the original Hamiltonian in (2).

The problem with the delta expansion is that it is difficult to prove rigorously that the expansion converges. We were able to conclude only that for every n there is always a neighbourhood about $\delta = 0$ in which the delta expansion for the first n eigenvalues of (5) converges and thus these eigenvalues are real when δ is real. Our discovery that the first n eigenvalues of the complex Hamiltonian (5) were real for a small range of real δ near $\delta = 0$ was astonishing to us, but we were disappointed that the delta expansion was not powerful enough to determine whether all of the eigenvalues of the original complex Hamiltonian (2) are real. However, our delta-expansion analysis inspired us to perform detailed perturbative and numerical studies of the spectrum of H in (5). To our amazement we found that *all of the eigenvalues of H remain real for all $\delta \geqslant 0$* [6]. We coined the term $\mathcal{PT}$-symmetric to describe these new non-Hermitian complex Hamiltonians having real energy levels†.

To present the results of our numerical studies, we rewrite the Hamiltonian (5) as

$$H = \hat{p}^2 - (\mathrm{i}\hat{x})^N\ , \tag{7}$$

where N is a continuous real parameter‡. The eigenvalues of this Hamiltonian are entirely real for all $N \geqslant 2$, while for $N < 2$ the spectrum is partly real and partly complex. Clearly, the Hamiltonian $H = \hat{p}^2 + i\hat{x}^3$ in (2) is just one member of a huge and remarkable class of complex Hamiltonians whose energy levels are real and positive. The spectrum of H exhibits three distinct behaviors as a function of N (see figure 1).

(i) When $N \geqslant 2$ the spectrum is infinite, discrete, and entirely real and positive. This region includes the case $N = 4$ for which $H = \hat{p}^2 - \hat{x}^4$. Amazingly, the spectrum of this wrong-sign potential is positive and discrete. (Also, $\langle\hat{x}\rangle \neq 0$ in the ground state because H breaks parity symmetry!) At the lower bound $N = 2$ of this region lies the harmonic oscillator. (ii) A transition occurs at $N = 2$. When $1 < N < 2$ there are only a *finite* number of positive real eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. We say that in this region the $\mathcal{PT}$ symmetry is *broken* and that $N \geqslant 2$ is a region of *unbroken* $\mathcal{PT}$ symmetry. (We explain the notion of broken and unbroken $\mathcal{PT}$ symmetry in greater detail below.) As N decreases from 2 to 1, adjacent energy levels merge into complex conjugate pairs beginning at the high end of the

†Other examples of complex Hamiltonians having $\mathcal{PT}$ symmetry are $H = \hat{p}^2 + \hat{x}^4(\mathrm{i}\hat{x})^{\delta}$, $H = \hat{p}^2 + \hat{x}^6(\mathrm{i}\hat{x})^{\delta}$, and so on (see [7]). These classes of Hamiltonians are all *different*. For example, the Hamiltonian obtained by continuing H in (5) along the path δ:0→8 has a different spectrum from the Hamiltonian that is obtained by continuing $H = \hat{p}^2 + \hat{x}^6(\mathrm{i}\hat{x})^{\delta}$ along the path δ:0→4. This is because the boundary conditions on the eigenfunctions are different.

‡An important technical issue concerns the definition of the operator $(i\hat{x})^N$ when N is noninteger. This operator is defined in coordinate space and is used in the Schrödinger equation $H\phi = E\phi$, which reads $-\phi(x) + (ix)N\phi(x) = E\phi(x)$. The term $(\mathrm{i}x)^{\mathrm{N}} \equiv \exp[N \log(\mathrm{i}x)]$ uses the complex logarithm function $\log(ix)$, which is defined with a branch cut that runs up the imaginary axis in the complex-x plane. This is explained more fully in section 3.

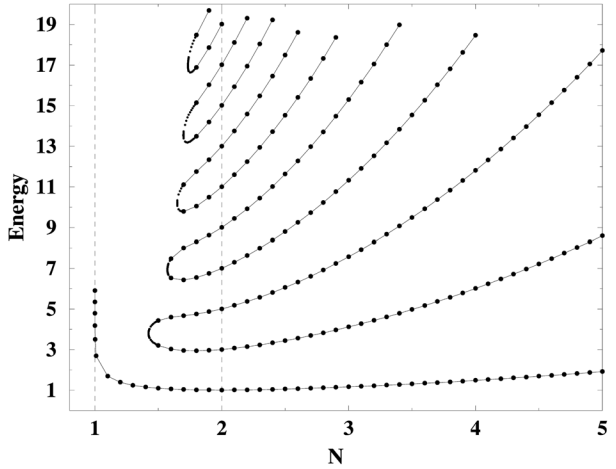

Figure 1. Real energy levels of the Hamiltonian $H = \hat{p}^2 - (\mathrm{i}\hat{x})^N$ as a function of the parameter N. When $N \geqslant 2$, the entire spectrum is real and positive. The lower bound of this region, $N = 2$, corresponds to the harmonic oscillator, whose energy levels are $E_n = 2n + 1$. When $1 < N < 2$, there are a finite number of positive real eigenvalues and infinitely many complex conjugate pairs of eigenvalues. As N decreases from 2 to 1, the number of real eigenvalues decreases and when $\mathrm{N} \leqslant 1.42207$, the only real eigenvalue is the ground-state energy. As $N \to 1^+$, the ground-state energy diverges. For $\mathrm{N} \leqslant 1$ there are no real eigenvalues.

spectrum. Ultimately, the only remaining real eigenvalue is the ground-state energy, which diverges as $N \to 1^+$ (the spectrum of $H = \hat{p}^2 - \mathrm{i}\hat{x}$ is null: [8]). (iii) When $\mathrm{N} \leqslant 1$ there are no real eigenvalues.

It is apparent that the reality of the spectrum of (7) when $N \geqslant 2$ is connected with its $\mathcal{PT}$ symmetry. The association between $\mathcal{PT}$ symmetry and the reality of spectra can be understood as follows: we say that the $\mathcal{PT}$ symmetry of a Hamiltonian H is *unbroken* if all of the eigenfunctions of H are simultaneously eigenfunctions of $\mathcal{PT}$§.

Here is a proof that if the $\mathcal{PT}$ symmetry of a Hamiltonian H is unbroken, then the spectrum of H is real: assume that a Hamiltonian H possesses $\mathcal{PT}$ symmetry (i.e. that H commutes with the $\mathcal{PT}$ operator) and that if ϕ is an eigenstate of H with eigenvalue E, then it is simultaneously an eigenstate of $\mathcal{PT}$ with eigenvalue λ:

$$H\phi = E\phi \quad \text{and} \quad \mathcal{PT}\phi = \lambda\phi\,. \tag{8}$$

We begin by showing that the eigenvalue λ is a pure phase. Multiply $\mathcal{PT}\phi = \lambda\phi$ on the left by $\mathcal{PT}$ and use the fact that $\mathcal{P}$ and $\mathcal{T}$ commute and that $\mathcal{P}^2 = \mathcal{T}^2 = 1$ to conclude that $\phi = \lambda^*\lambda\phi$ and thus $\lambda = \exp(\mathrm{i}\alpha)$ for some real α. Next, introduce a convention that we use throughout this paper. Without loss of generality we replace the eigenfunction ϕ by $\exp(-\mathrm{i}\alpha/2)\phi$ so that its eigenvalue under the operator $\mathcal{PT}$ is unity:

$$\mathcal{PT}\phi = \phi\,. \tag{9}$$

Next, we multiply the eigenvalue equation $H\phi = E\phi$ on the left by $\mathcal{PT}$ and use $[\mathcal{PT},\ H] = 0$ to obtain $E\phi = E^*\phi$. Hence, $E = E^*$ and the eigenvalue E is real.

The crucial assumption in this argument is that ϕ is simultaneously an eigenstate of H and of $\mathcal{PT}$. In quantum mechanics if a linear operator X commutes with the Hamiltonian H, then the eigenstates of H are also eigenstates of X. However, we emphasize that the operator $\mathcal{PT}$ is *not linear* (it is antilinear) and thus we must make the extra assumption that the $\mathcal{PT}$ symmetry of H is unbroken; that is, ϕ is simultaneously an eigenstate of H and $\mathcal{PT}$. This extra assumption is non-trivial because it is hard to determine *a priori* whether the $\mathcal{PT}$ symmetry of a particular Hamiltonian H is broken or unbroken. For H in (7) the $\mathcal{PT}$ symmetry is unbroken when $N \geqslant 2$ and it is broken when $N < 2$. The conventional Hermitian Hamiltonian for the quantum-mechanical harmonic oscillator lies at the boundary of the unbroken and the broken regimes.

I am delighted at the research activity that my work has inspired. In 2001 Dorey *et al.* proved rigorously that the spectrum of H in (7) is real and positive [9] in the region $N \geqslant 2$. Dorey *et al.* used techniques such as the Bethe *ansatz* and the Baxter-TQ relation, which are used in the study of integrable models and conformal quantum field theory. In doing so they have helped to establish a remarkable connection between the ordinary differential equation (the Schrödinger equation) that describes $\mathcal{PT}$-symmetric quantum mechanics and the study of integrable models. This connection, which has become known as the ODE/IM correspondence, is rich and profound and will lead to a much deeper understanding of both types of theories. Many other $\mathcal{PT}$-symmetric Hamiltonians for which space–time reflection symmetry is not broken have been investigated, and the spectra of these Hamiltonians have also been shown to be real and positive [4,10–12]. Evidently, the phenomenon of $\mathcal{PT}$ symmetry is quite widespread and arises in many contexts.

§If a system is defined by an equation that possesses a discrete symmetry, the solution to this equation need not exhibit that symmetry. For example, the differential equation $\ddot{y}(t) = y(t)$ is symmetric under time reversal $t \to -t$. The solutions $y(t) = \exp(t)$ and $y(t) = \exp(-t)$ do not exhibit time-reversal symmetry while the solution $y(t) = \cosh(t)$ is time-reversal symmetric. The same is true of a system whose Hamiltonian is $\mathcal{PT}$-symmetric. Even if the Schrödinger equation and corresponding boundary conditions are $\mathcal{PT}$ symmetric, the solution to the Schrödinger equation boundary value problem may not be symmetric under space–time reflection. When the solution exhibits $\mathcal{PT}$ symmetry, we say that the $\mathcal{PT}$ symmetry is unbroken. Conversely, if the solution does not possess $\mathcal{PT}$ symmetry, we say that the $\mathcal{PT}$ symmetry is broken.

3. Energy levels of a $\mathcal{PT}$-symmetric Hamiltonian

The purpose of this section is to explain how to calculate the eigenvalues of the complex Hamiltonian operator in (6). To calculate the energy levels of a $\mathcal{PT}$-symmetric Hamiltonian we adopt the techniques that are used for calculating the energy levels of conventional Hermitian Hamiltonians. These techniques involve converting the formal eigenvalue problem $H\phi = E\phi$ to a Schrödinger differential equation whose solutions satisfy appropriate boundary conditions. This Schrödinger equation is then solved numerically or by using approximate methods such as WKB.

The Schrödinger eigenvalue problem for the $\mathcal{PT}$-symmetric Hamiltonian (7) is

$$-\phi_n''(x) - (ix)^N\phi_n(x) = E_n\phi_n(x)\ , \qquad (10)$$

where E_n is the nth eigenvalue. For a Hermitian Hamiltonian the boundary conditions that give quantized energy levels E_n are that the eigenfunctions $\phi_n(x)\to 0$ as $|x|\to\infty$ on the real axis. This condition suffices for (10) when $1 < N < 4$, but for $N \geqslant 4$ we must continue the eigenvalue problem for (10) into the complex-x plane. Thus, we replace the real-x axis by a contour in the complex plane along which the differential equation holds. The boundary conditions that lead to quantization are imposed at the endpoints of this contour. (The rest of this brief section is somewhat technical and may be skipped by those without a background in complex differential equations. See [13] for more information on how to solve such problems.)

The endpoints of this contour lie in regions in the complex-x plane in which the eigenfunctions $\phi_n\ (x)\to 0$ exponentially as $|\ x\ |\to\infty$. These regions are known as *Stokes wedges* (see figure 2). The Stokes wedges are bounded by the lines along which the solution to the differential equation is oscillatory [14]. There are many wedges in which we can require that $\phi(x)\to 0$ as $|\ x\ |\to\infty$. Thus, there are many eigenvalue problems associated with a given differential equation [13]. For a given value of N we must first identify which one of these eigenvalue problems is associated with (10). To do so we start with the harmonic oscillator problem at $N = 2$ and smoothly vary the parameter N until it reaches the given value. At $N = 2$ the eigenfunctions vanish in wedges of angular opening $\frac{1}{2}\pi$ centred about the negative-real and positive-real x axes. For any $N \geqslant 1$ the centres of the left and right wedges lie at the angles

$$\theta_{\text{left}} = -\pi + \frac{N-2}{2N+4}\pi \quad \text{and} \quad \theta_{\text{right}} = -\frac{N-2}{2N+4}\pi\ . \qquad (11)$$

The opening angle of these wedges is $\Delta = [2/(N+2)]\pi$. The differential equation (10) may be integrated on any path in the complex-x plane so long as the path approaches complex infinity inside the left wedge and inside the right wedge. These wedges contain the real-x axis when $1 < N < 4$.

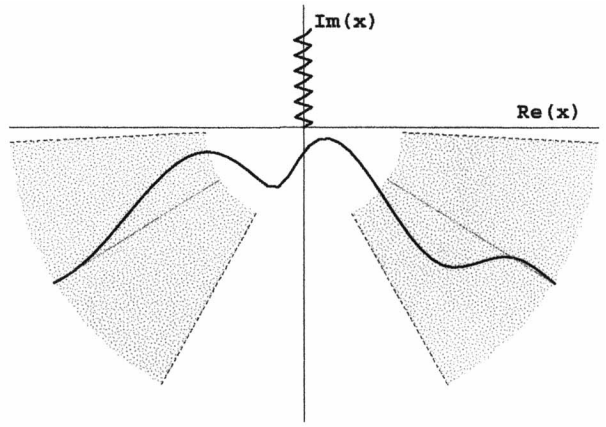

Figure 2. Wedges in the complex-x plane containing the contour on which the eigenvalue problem for the differential equation (10) for $N = 4.2$ is posed. In these wedges $\phi(x)$ vanishes exponentially as $|x|\to\infty$. The wedges are bounded by lines along which the solution to the differential equation is oscillatory.

As N increases from 2, the left and right wedges rotate downward into the complex-x plane and become thinner. We can see on figure 1 that the eigenvalues grow with N as $N\to\infty$. At $N = \infty$ the differential equation contour runs up and down the negative imaginary axis, and this leads to an interesting limiting eigenvalue problem. Because all of the eigenvalues of (7) diverge like N^2 as $N\to\infty$, for large N we replace H by the rescaled Hamiltonian H/N^2. In the limit $N\to\infty$ this new Hamiltonian becomes exactly solvable in terms of Bessel functions. The eigenvalue problem at $N = \infty$ is the $\mathcal{PT}$-symmetric equivalent of the square well in ordinary Hermitian quantum mechanics [15].

As N decreases below 2, the wedges become wider and rotate into the upper-half x plane. At $N = 1$ the angular opening of the wedges is $\frac{2}{3}\pi$ and the wedges are centred at $\frac{5}{6}\pi$ and $\frac{1}{6}\pi$. Thus, the wedges become contiguous at the positive-imaginary x axis, and the differential equation contour can be pushed off to infinity. Hence, there is no eigenvalue problem when $N = 1$ and, as we would expect, the ground-state energy diverges as $N\to 1^+$ (see figure 1).

Having defined the eigenvalue problem for the Hamiltonian in (7), we can solve the differential equation by using numerical methods. We can also can use approximate analytical methods such as WKB [14]. WKB gives a good approximation to the eigenvalues in figure 1 when $N \geqslant 2$. The novelty of this WKB calculation is that it must be performed in the complex plane. The turning points $x_\pm$ are those roots of $E + (ix)^N = 0$ that *analytically continue* off the real axis as N moves away from $N = 2$:

$$x_- = E^{1/N} \exp\left[i\pi(3/2 - 1/N)\right] ,$$
$$x_+ = E^{1/N} \exp\left[-i\pi(1/2 - 1/N)\right] . \quad (12)$$

These points lie in the lower (upper) x plane in figure 2 when $N > 2$ ($N < 2$).

The WKB quantization condition is $(n + 1/2)\pi = \int_{x_-}^{x_+} dx[E + (ix)^N]^{1/2}$. It is crucial that the integration path be such that this *integral is real*. When $N > 2$ this path lies entirely in the lower-half x plane, and when $N = 2$ the path lies on the real axis. When $N < 2$ the path is in the upper-half x plane; it crosses the cut on the positive-imaginary axis and thus is *not a continuous path joining the turning points*. Hence, WKB fails when $N < 2$.

When $N \geqslant 2$, the WKB calculation gives

$$E_n \sim \left[\frac{\Gamma(3/2 + 1/N)\pi^{1/2}(n + 1/2)}{\sin(\pi/N)\Gamma(1 + 1/N)}\right]^{2N/(N+2)} \quad (n \to \infty) . \quad (13)$$

This result is quite accurate. The fourth exact eigenvalue (obtained using Runge-Kutta) for the case $N = 3$ is 11.3143 while WKB gives 11.3042, and the fourth exact eigenvalue for the case $N = 4$ is 18.4590 while WKB gives 18.4321.

4. $\mathcal{PT}$-symmetric classical mechanics

In the study of classical mechanics the objective is to describe the motion of a particle satisfying Newton's law $F = ma$. The trajectory $x(t)$ of the particle is a *real* function of time t. The classical equation of motion for the complex $\mathcal{PT}$-symmetric Hamiltonian (7) describes a particle of energy E subject to *complex* forces. Thus, we have the surprising result that classical $\mathcal{PT}$-symmetric Hamiltonians describe motion that is not limited to the real-x axis. The classical path $x(t)$ may lie in the complex-x plane. The purpose of this section is to describe this remarkable possibility [7].

An intriguing aspect of figure 1 is the transition at $N = 2$. As N goes below 2, the eigenvalues begin to merge into complex conjugate pairs. The onset of eigenvalue merging can be thought of as a phase transition. We show in this section that the underlying cause of this quantum transition can be understood by studying the theory at *classical* level.

The trajectory $x(t)$ of a classical particle governed by the $\mathcal{PT}$-symmetric Hamiltonian (7) obeys $\pm dx[E + (ix)^N]^{-1/2} = 2dt$. While E and dt are real, $x(t)$ lies in the complex plane in figure 2. When $N = 2$ (the harmonic oscillator), there is one classical path that terminates at the classical turning points $x_\pm$ in (12). Other paths are nested ellipses with foci at the turning points (see figure 3). All these paths have the same period.

When $N = 3$, there is again a classical path that joins the left and right turning points and an infinite class of paths enclosing the turning points (see figure 4). As these paths increase in size, they approach a cardioid shape (see figure 5). The indentation in the limiting cardioid occurs because paths may not cross, and thus all periodic paths must avoid the path in figure 4 that runs up the imaginary axis. When N is noninteger, we obtain classical paths that move off onto *different sheets* of the Riemann surface (see figure 6).

In general, whenever $N \geqslant 2$, the trajectory joining $x_\pm$ is a smile-shaped arc in the lower complex plane. The motion is *periodic*. Thus, the equation describes a *complex pendulum* whose (real) period T is given by

$$T = 2E^{(2-N)/2N} \cos\left[\frac{(N-2)\pi}{2N}\right] \frac{\Gamma(1 + 1/N)\pi^{1/2}}{\Gamma(1/2 + 1/N)} . \quad (14)$$

Below the transition at $N = 2$ a path starting at one turning point, say x_-, moves toward but *misses* the turning point x_+. This path spirals outward, crossing from sheet to sheet on the Riemann surface, and eventually veers off to infinity. Hence, the period abruptly becomes infinite. The total angular rotation of the spiral is finite for all $N < 2$, but it becomes infinite as $N \to 2^-$ (see figure 7).

5. $\mathcal{PT}$-symmetric quantum mechanics

The discovery that the eigenvalues of many $\mathcal{PT}$-symmetric Hamiltonians are real and positive raises an urgent question: does a non-Hermitian Hamiltonian such as H in (7) define a physical theory of quantum mechanics or is the positivity of the spectrum merely an intriguing mathematical property of special classes of complex eigenvalue problems? A *physical* quantum theory (i) must possess a Hilbert space of state vectors and this Hilbert

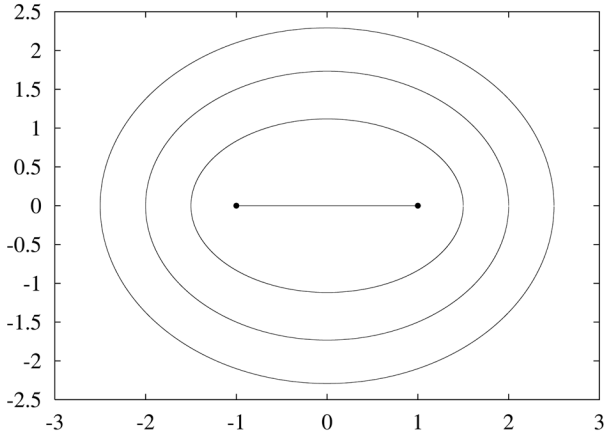

Figure 3. Classical paths in the complex-x plane for the $N = 2$ oscillator. The paths form a set of nested ellipses. These closed periodic orbits occur when the $\mathcal{PT}$ symmetry is unbroken.

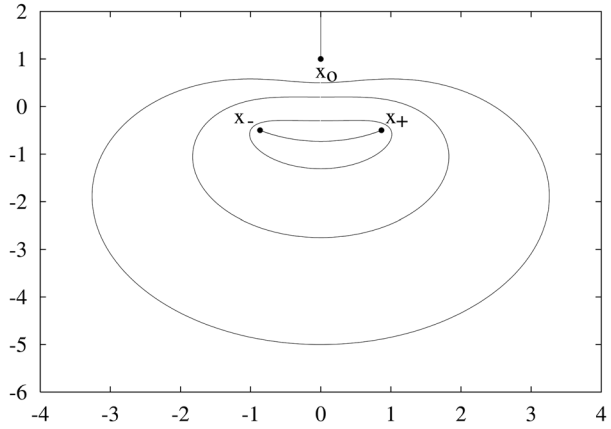

Figure 4. Classical paths in the complex-x plane for the $N = 3$ oscillator. In addition to the periodic orbits, one path runs off to $i\infty$ from the turning point on the imaginary axis.

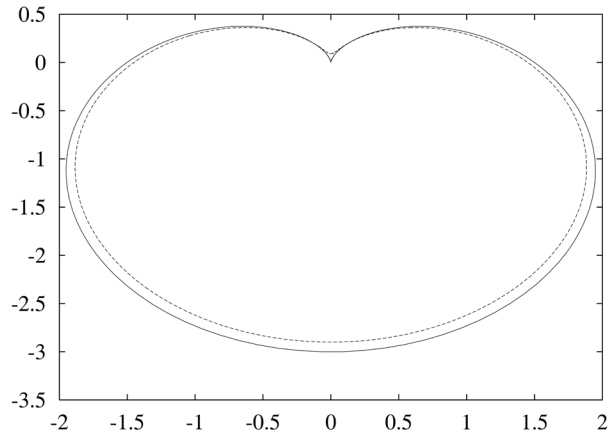

Figure 5. Classical paths in the complex-x plane for the $N = 3$ oscillator. As the paths get larger, they approach a shape resembling a cardioid. We have plotted the *rescaled* paths.

space must have an inner product with a positive norm; (ii) the time evolution of the theory must be unitary; that is, the norm must be preserved in time.

A definitive answer to this question has been found [16,17]. For a complex non-Hermitian Hamiltonian having an *unbroken* $\mathcal{PT}$ symmetry, a linear operator $\mathcal{C}$ that commutes with both H and $\mathcal{PT}$ can be constructed. We denote the operator representing this symmetry by $\mathcal{C}$ because the properties of $\mathcal{C}$ are similar to those of the charge conjugation operator in ordinary particle physics. The inner product with respect to $\mathcal{T}$ conjugation is

$$\langle\psi|\chi\rangle^{\mathcal{CPT}} = \int \mathrm{d}x\, \psi^{\mathcal{CPT}}(x)\chi(x)\ , \tag{15}$$

where $\psi^{\mathcal{CPT}}(x) = \int \mathrm{d}y \mathcal{C}(x,y)\psi^*(-y)$. 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.

To explain the construction of the $\mathcal{C}$ operator we begin by summarizing the mathematical properties of the solution to the eigenvalue problem (10) associated with the Hamiltonian H in (7). Recall from figure 2 that this differential equation is imposed on an infinite contour in the complex-x plane and that for large $|x|$ this contour lies in wedges placed symmetrically with respect to the imaginary-x axis as in figure 2. When $N \geqslant 2$, H has an unbroken $\mathcal{PT}$ symmetry. Thus, the eigenfunctions $\phi_n(x)$ are simultaneously eigenstates of the $\mathcal{PT}$ operator: $\mathcal{PT}\phi_n(x) = \lambda_n\phi_n(x)$. As we argued in section 2, λ_n can be absorbed into $\phi_n(x)$ so that $\mathcal{PT}\phi_n(x) = \phi_n^*(-x) = \phi_n(x)$ (see (9)).

The eigenstates of a conventional Hermitian Hamiltonian are complete. There is strong evidence that the eigenfunctions $\phi_n(x)$ for the $\mathcal{PT}$-symmetric Hamiltonian (7) are also complete. The coordinate-space statement of completeness is

$$\sum_{n=0}^{\infty}(-1)^n\phi_n(x)\phi_n(y) = \delta(x-y) \quad (x, y \text{ real})\ . \tag{16}$$

This non-trivial result has been verified numerically to extremely high accuracy (twenty decimal places) [18,19]. The unusual factor of $(-1)^-$ in this sum does not appear in conventional quantum mechanics. This factor is explained in the following discussion.

We must now try to find the inner product associated with our $\mathcal{PT}$-symmetric Hamiltonian and it is here that we can see the difficulty connected with its non-Hermiticity. In conventional Hermitian quantum mechanics the Hilbert space inner product is specified even before we begin to look for the eigenstates of H. For our non-Hermitian Hamiltonian we must try to guess the inner product. A reasonable guess for the inner product of two functions $f(x)$ and $g(x)$ might be

$$(f,g) \equiv \int \mathrm{d}x\, [\mathcal{PT}f(x)]g(x)\ , \tag{17}$$

where $\mathcal{PT}f(x) = [f(-x)]^*$ and the path of integration in the complex-x plane follows the contour described in section 3. The apparent advantage of this choice for the inner product is that the associated $\mathcal{PT}$ norm (f,f) is independent of the overall phase of $f(x)$ and is conserved in time. With respect to this inner product the eigenfunctions $\phi_m(x)$ and $\phi_n(x)$ of H in (7) are orthogonal for $n \neq m$. However, when $m = n$ we see that the $\mathcal{PT}$ norms of the eigenfunctions are *not positive*:

$$(\phi_m, \phi_n) = (-1)^n\delta_{mn}\ . \tag{18}$$

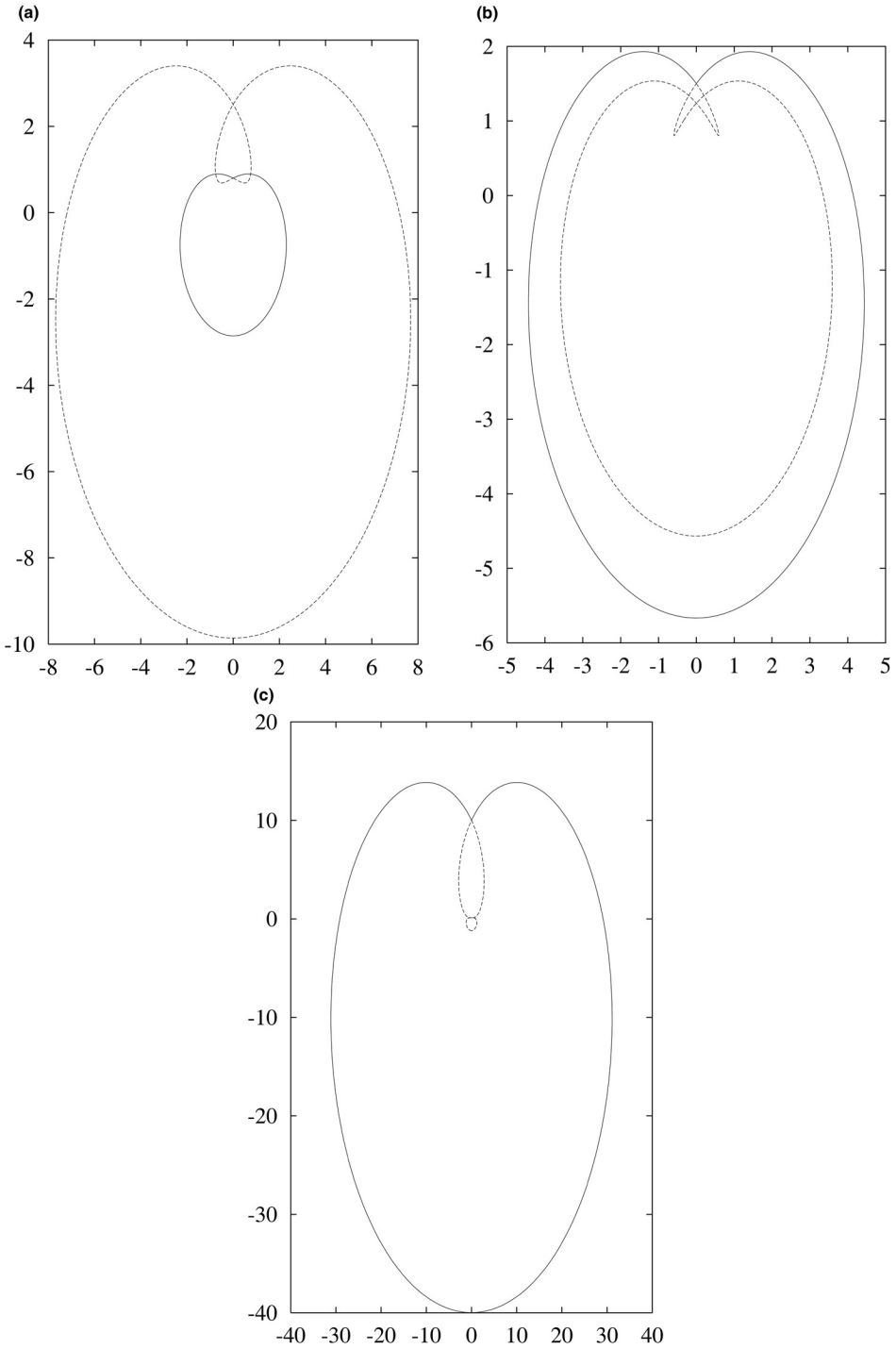

Figure 6. Classical paths for the case $N = 2.5$. These paths do not intersect. The graph shows the projection of the parts of the path that lie on three different sheets of the Riemann surface. As the size of the paths increases, a limiting cardioid appears on the principal sheet. On the remaining sheets of the surface the path exhibits a knot-like topological structure.

This result is apparently true for all values of N in (7) and it has been verified numerically to extremely high precision. Because the norms of the eigenfunctions alternate in sign, the metric associated with the $\mathcal{PT}$ inner product $(\cdot,\cdot)$ is indefinite. This sign alternation is a *generic* feature of the $\mathcal{PT}$ inner product. Extensive numerical calculations verify that (18) holds for all $N \geqslant 2$.

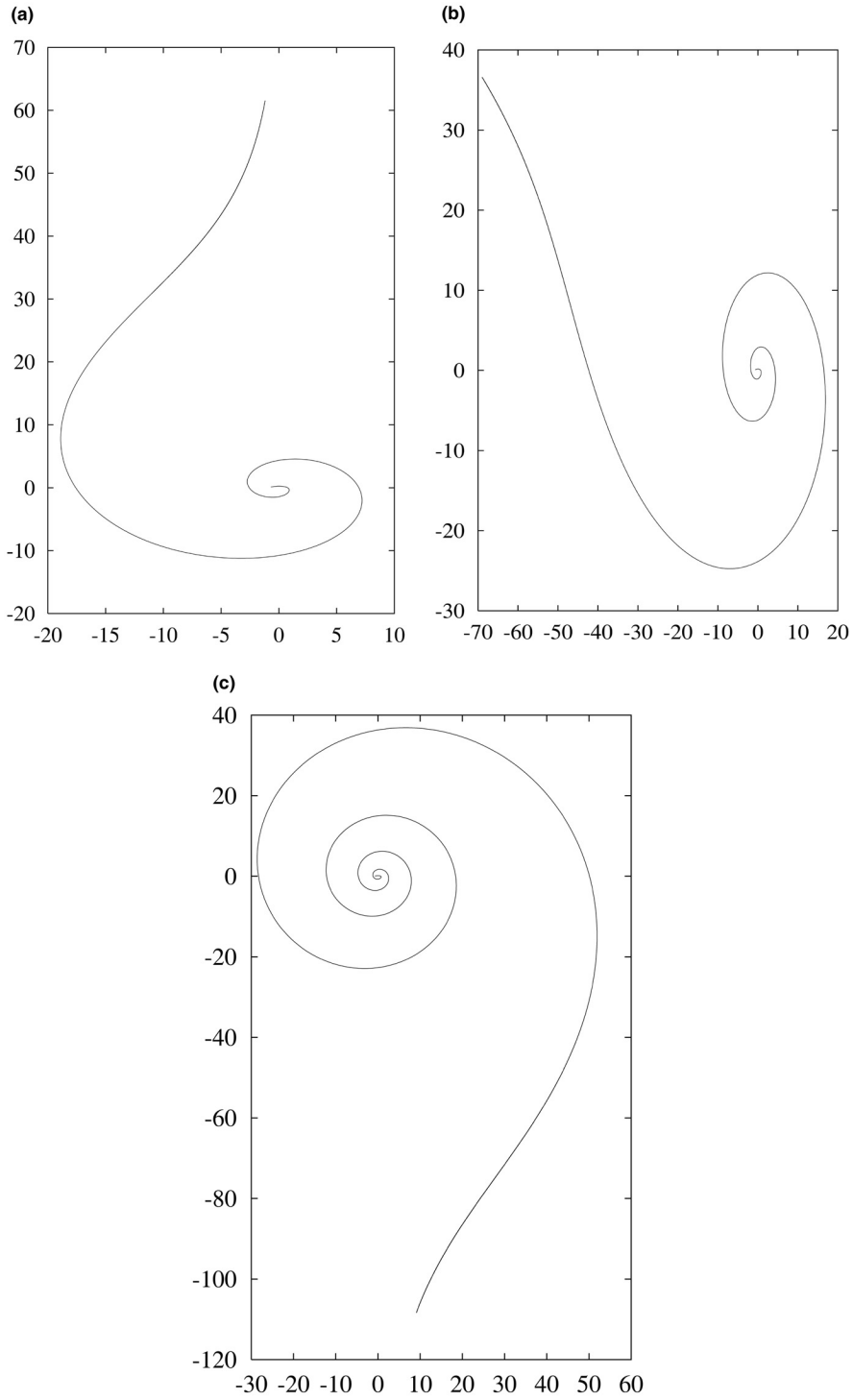

Figure 7. Classical paths in the complex-x plane for $N = 1.8$, $N = 1.85$ and $N = 1.9$. These non-periodic paths spiral outward to infinity. As $N \to 2$ from below, the number of turns in the spiral increases. The lack of periodic orbits corresponds to a broken $\mathcal{PT}$ symmetry.

Despite the existence of a non-positive inner product, we can still do some of the analysis that one would normally perform for a conventional Schrödinger equation $H\phi_n = E_n\phi_n$. For example, we can use the inner product formula (18) to verify that (16) is the representation of the unity operator by showing that $\mathrm{d}y\delta(x-y)\delta(y-z) = \delta(x-z)$.

We can use completeness to reconstruct the parity operator $\mathcal{P}$ in terms of the eigenstates. The parity operator in position space is

$$\mathcal{P}(x,y) = \sum_{n=0}^{\infty} (-1)^n \phi_n(x)\phi_n(-y) = \delta(x+y) \; . \qquad (19)$$

By virtue of (18) the square of the parity operator is unity: $\mathcal{P}^2 = 1$. We can also reconstruct H in coordinate space: $H(x,y) = \Sigma_n(-1)^n E_n \phi_n(x)\phi_n(y)$. Using (16)–(18) we can see that this Hamiltonian satisfies $H\phi_n(x) = E_n\phi_n(x)$.

We now address the question of whether a $\mathcal{PT}$-symmetric Hamiltonian defines a physically viable quantum mechanics. The difficulty with formulating a $\mathcal{PT}$-symmetric quantum theory is that the vector space of quantum states is spanned by the energy eigenstates, of which half have norm $+1$ and half have norm -1. In quantum theory the norms of states carry a probabilistic interpretation, so the indefinite metric (18) is unacceptable.

The situation here in which half of the energy eigenstates have positive norm and half have negative norm is analogous to the problem that Dirac encountered in formulating the spinor wave equation in relativistic quantum theory [20]. Following Dirac, we attack the problem of an indefinite norm by finding an interpretation of the negative-norm states. We claim that in *any* theory having an unbroken $\mathcal{PT}$ symmetry there exists a symmetry of the Hamiltonian connected with the fact that there are equal numbers of positive- and negative-norm states. To describe this symmetry we construct the aforementioned linear operator $\mathcal{C}$ in position space as a sum over the eigenstates of the Hamiltonian [16]:

$$C(x,y) = \sum_{n=0}^{\infty} \phi_n(x)\phi_n(y) \; . \qquad (20)$$

The properties of this new operator $\mathcal{C}$ resemble those of the charge conjugation operator in quantum field theory. For example, we can use (16)–(18) to verify that the square of $\mathcal{C}$ is unity ($\mathcal{C}^2 = 1$): $\mathrm{d}y\mathcal{C}(x,y)\mathcal{C}(y,z) = \delta(x-z)$. Thus, the eigenvalues of $\mathcal{C}$ are ± 1. Also, $\mathcal{C}$ commutes with the Hamiltonian H. Therefore, since $\mathcal{C}$ is linear, the eigenstates of H have definite values of $\mathcal{C}$. Specifically, if the energy eigenstates satisfy (18), then we have

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

Thus, $\mathcal{C}$ represents the measurement of the sign of the $\mathcal{PT}$ norm of an eigenstate in (18).

The operators $\mathcal{P}$ and $\mathcal{C}$ are distinct square roots of the unity operator $\delta(x-y)$. That is, $\mathcal{P}^2 = \mathcal{C}^2 = 1$, but $\mathcal{P} \neq \mathcal{C}$. Indeed, $\mathcal{P}$ 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, as we see in (20). The two operators $\mathcal{P}$ and $\mathcal{C}$ do not commute. However, $\mathcal{C}$ *does* commute with $\mathcal{PT}$.

Finally, having obtained the operator $\mathcal{C}$ we define the new inner product structure given in (15). This inner product has a *positive definite* norm. Like the $\mathcal{PT}$ inner product (17) this new inner product is phase independent. Also, it is conserved in time because the time evolution operator (just as in ordinary quantum mechanics) is exp ($\mathrm{i}Ht$). The fact that H commutes with $\mathcal{PT}$ and with $\mathcal{CPT}$ implies that both inner products, (17) and (15), remain time independent as the states evolve. However, unlike (17), the inner product (15) is positive definite because $\mathcal{C}$ contributes -1 when it acts on states with negative $\mathcal{PT}$ norm. In terms of the $\mathcal{CPT}$ conjugate, the completeness condition (16) reads

$$\sum_{n=0}^{\infty} \phi_n(x)[\mathcal{CPT}\phi_n(y)] = \delta(x-y) \; . \qquad (21)$$

To review, in the mathematical formulation of a conventional quantum theory the Hilbert space of physical states is specified first. The inner product in this vector space is defined with respect to ordinary 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 is thus determined *dynamically*. One can view this new kind of quantum theory as a 'bootstrap' theory because one must solve for the eigenstates of H before knowing what the Hilbert space and the associated inner product of the theory are. The Hilbert space and the $\mathcal{CPT}$ inner product (15) are then determined by these eigenstates via (20).

The operator $\mathcal{C}$ does not exist as a distinct entity in ordinary Hermitian quantum mechanics. Indeed, if we allow the parameter N in (7) to tend to 2, the operator $\mathcal{C}$ in this limit becomes identical to $\mathcal{P}$. Thus, in this limit the $\mathcal{CPT}$ operator becomes $\mathcal{T}$, which is just complex conjugation. As a consequence, the inner product (15) defined with respect to the $\mathcal{CPT}$ conjugation reduces to the complex conjugate inner product of conventional quantum mechanics when $N \to 2$. Similarly, in this limit (21) reduces to the usual statement of completeness $\sum_n \phi_n(x)\phi_n^*(y) = \delta(x-y)$.

The $\mathcal{CPT}$ inner-product (15) is independent of the choice of integration contour $\mathcal{C}$ as long as $\mathcal{C}$ lies inside the asymptotic wedges associated with the boundary conditions for the eigenvalue problem (10). In ordinary quantum

mechanics, where the positive-definite inner product has the form $dx\, f^*(x)g(x)$, the integral must be taken along the real axis and the path of the integration cannot be deformed into the complex plane because the integrand is not analytic†. The $\mathcal{PT}$ inner product (17) shares with (15) 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 $\mathcal{PT}$ conjugation without disturbing the path independence of the inner-product integral.

We can now explain why $\mathcal{PT}$-symmetric theories are unitary. Time evolution is expressed by the operator $\exp(-iHt)$, 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 a prescribed initial wave function belonging to the Hilbert space spanned by the energy eigenstates, then it evolves into the state $\psi_1(x)$ at time t according to $\psi_t(x) = \exp(-iHt)\psi_0(x)$. With respect to the $\mathcal{CPT}$ inner product defined in (15), the norm of the vector $\psi_t(x)$ does not change in time, $\langle\psi_t|\psi_t\rangle = \langle\psi_0|\psi_0\rangle$, because the Hamiltonian H commutes with the $\mathcal{CPT}$ operator.

6. Illustrative example: a 2 × 2 matrix Hamiltonian

The 2 × 2 matrix Hamiltonian

$$H = \begin{pmatrix} r\exp(i\theta) & s \\ s & r\exp(-i\theta) \end{pmatrix}, \tag{22}$$

where the three parameters r, s and θ are real, illustrates the above results on $\mathcal{PT}$-symmetric quantum mechanics. This Hamiltonian is not Hermitian, but it is $\mathcal{PT}$ symmetric, where the parity operator is $\mathrm{P} = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ and $\mathcal{T}$ performs complex conjugation [21].

There are two parametric regions for this Hamiltonian. 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 $s^2 \geqslant r^2\sin^2\theta$, then 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

$$\begin{aligned} |\epsilon_+\rangle &= \frac{1}{(2\cos\alpha)^{1/2}}\begin{pmatrix} \exp(i\alpha/2) \\ \exp(-i\alpha/2) \end{pmatrix}, \\ |\epsilon_-\rangle &= \frac{i}{(2\cos\alpha)^{1/2}}\begin{pmatrix} \exp(-i\alpha/2) \\ -\exp(i\alpha/2) \end{pmatrix}, \end{aligned} \tag{23}$$

where we set $\sin\alpha = (r/s)\sin\theta$). The $\mathcal{PT}$ inner product gives $(\varepsilon_\pm, \varepsilon_\pm) = \pm 1$ and $(\varepsilon_\pm, \varepsilon_\pm) = 0$, where $(u, v) = (\mathcal{PT}u)\cdot v$. Therefore, with respect to the $\mathcal{PT}$ inner product, the resulting vector space spanned by the energy eigenstates has a metric of signature $(+,-)$. The condition $s^2 > r^2\sin^2\theta$ ensures that the $\mathcal{PT}$ symmetry is not broken. If this condition is violated, the states (23) are no longer eigenstates of $\mathcal{PT}$ because α 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 (20):

$$\mathcal{C} = \frac{1}{\cos\alpha}\begin{pmatrix} i\sin\alpha & 1 \\ 1 & -i\sin\alpha \end{pmatrix}. \tag{24}$$

Note that $\mathcal{C}$ is distinct from H and $\mathcal{P}$ and it has the key property that $\mathcal{C}\,|\,\varepsilon_\pm\,\rangle = \pm\,|\varepsilon_\pm\rangle$. 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 $\langle\varepsilon_\pm|\varepsilon_\pm\rangle = 1$. Thus, the two-dimensional Hilbert space spanned by $|\varepsilon_\pm\rangle$, with inner product $\langle\cdot|\cdot\rangle$, has signature $(+,+)$.

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

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

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, v and v are real. Then

$$\psi|\psi = \frac{1}{\cos\alpha}\left(x^2 + v^2 + 2xv\sin\alpha + y^2 + u^2 - 2yu\sin\alpha\right), \tag{25}$$

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

$$|\epsilon_+\rangle\langle\epsilon_+| + |\epsilon_-\rangle\langle\epsilon_-| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{26}$$

†If a function satisfies a linear ordinary differential equation, then the function is analytic wherever the coefficient functions of the differential equation are analytic. The Schrödinger equation (10) is linear and its coefficients are analytic except for a branch cut at the origin; this branch cut can be taken to run up the imaginary axis. We choose the integration contour for the inner product (18) so that it does not cross the positive imaginary axis. Path independence occurs because the integrand of the inner product (18) is a product of analytic functions.

Furthermore, using the $\mathcal{CPT}$ conjugate $\langle\varepsilon_\pm|$, we get $\mathcal{C}$ as $\mathcal{C} = |\varepsilon_+\rangle\langle\varepsilon_+| - |\varepsilon_-\rangle\langle\varepsilon_-|$.

If we set $\theta = 0$ in this two-state system, the Hamiltonian (22) becomes Hermitian. However, $\mathcal{C}$ then reduces to the parity operator $\mathcal{P}$. As a consequence, $\mathcal{CPT}$ invariance reduces to the standard condition of Hermiticity for a symmetric matrix; namely, that $H = H^*$. This is why the hidden symmetry $\mathcal{C}$ was not noticed previously. The operator $\mathcal{C}$ emerges only when we extend a real symmetric Hamiltonian into the complex domain.

7. Observables in $\mathcal{PT}$-symmetric quantum mechanics

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. Because operators in the Heisenberg picture evolve in time according to $A(t) = \exp(iHt)A(0)\exp(-iHt)$, 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 $A^{\mathrm{T}} = \mathcal{CPT}A\mathcal{CPT}$, where A^{T} is the *transpose* of A. If this condition holds at $t = 0$, then it will continue to hold for all time because we have assumed that H is symmetric ($H = H^{\mathrm{T}}$). This condition also guarantees that the expectation value of A in any state is real.

The operator $\mathcal{C}$ itself satisfies this requirement, so it is an observable. Also the Hamiltonian is an observable. However, the x and p operators are not observables. Indeed, the expectation value of 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 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 of the *energy* of the electron!

One can see why the expectation of the x operator is a negative imaginary number by examining figure 4. Note that the classical trajectories have left–right ($\mathcal{PT}$) symmetry, but not up–down symmetry. Also, the classical paths favour 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 pointlike objects.

8. Calculation of the $\mathcal{C}$ operator

The distinguishing feature of $\mathcal{PT}$-symmetric quantum mechanics is the $\mathcal{C}$ operator. The discovery of $\mathcal{C}$ in [16] raises the question of how to evaluate the formal sum in (20) that represents $\mathcal{C}$. 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 evaluate (20) for a $\mathcal{PT}$-symmetric Hamiltonian that is also Hermitian, the result would be $\mathcal{P}$, which in coordinate space is $\delta(x + y)$ (see (19)).

Calculating $\mathcal{C}$ by direct evaluation of the sum in (20) is not easy in quantum mechanics because it is necessary to calculate all the eigenfunctions $\phi_n(x)$ of H. Such a procedure cannot be used in quantum field theory because there is no simple analogue of the Schrödinger eigenvalue differential equation and its associated coordinate-space eigenfunctions.

Fortunately, there is an easy way to calculate the $\mathcal{C}$ operator, and the procedure circumvents the difficult problem of evaluating the sum in (20). As a result the technique readily generalizes from quantum mechanics to quantum field theory. In this section we use this technique to calculate $\mathcal{C}$ for the $\mathcal{PT}$-symmetric Hamiltonian [22]

$$H = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{x}^2 + i\epsilon\,\hat{x}^3 \ . \tag{27}$$

We will show how to calculate $\mathcal{C}$ perturbatively to high order in powers of ε for this cubic Hamiltonian. Calculating $\mathcal{C}$ for other kinds of interactions is a bit more difficult and requires the use of semiclassical approximations [23].

Our calculation of $\mathcal{C}$ makes use of its three crucial properties. First, $\mathcal{C}$ commutes with the space–time reflection operator $\mathcal{PT}$,

$$[\mathcal{C}, \mathcal{PT}] = 0 \ , \tag{28}$$

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

$$\mathcal{C}^2 = \mathbf{1} \ , \tag{29}$$

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

$$[\mathcal{C}, H] = 0 \ , \tag{30}$$

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

The procedure for calculating $\mathcal{C}$ begins by introducing a general operator representation for $\mathcal{C}$ of the form [24]

$$\mathcal{C} = \exp[Q(\hat{x}, \hat{p})]\mathcal{P} \ , \tag{31}$$

where $\mathcal{P}$ is the parity operator and $Q(\hat{x}, \hat{p})$ is a real function of the dynamical variables $\hat{x}$ and $\hat{p}$. This representation conveniently incorporates the three requirements (28)–(30).

The representation $\mathcal{C} = \exp(Q)\mathcal{P}$ is general. Let us illustrate this simple representation for $\mathcal{C}$ in two elementary cases: 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 ε. Its eigenvalues $E_n = n + \frac{1}{2} + \frac{1}{2}\epsilon^2$ are all real. The $\mathcal{C}$ operator for this theory is given exactly by $\mathcal{C} = \exp(Q)\mathcal{P}$, where $Q = -\varepsilon\hat{p}$. Note that in the limit $\varepsilon \to 0$, where the Hamiltonian becomes Hermitian, $\mathcal{C}$ becomes identical with $\mathcal{P}$.

As a second example, consider the non-Hermitian 2×2 matrix Hamiltonian (22). The $\mathcal{C}$ operator in (24) can be easily rewritten in the form $\mathcal{C} = \exp(Q)\ \mathcal{P}$, where $Q = \frac{1}{2}\sigma_2 \ln[(1 - \sin\alpha)/(1 + \sin\alpha)]$. Here, $\sigma_2 = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$. Again, observe that in the limit $\theta \to 0$, where the Hamiltonian becomes Hermitian, the $\mathcal{C}$ operator becomes identical with $\mathcal{P}$.

We will now calculate $\mathcal{C}$ directly from its operator representation (31) and we will show that $Q(\hat{x}, \hat{p})$ can be found by solving elementary operator equations. To find the operator equations satisfied by Q we substitute $\mathcal{C} = \exp(Q)\ \mathcal{P}$ into the three equations (28)–(30) in turn.

First, we substitute (31) into the condition (28) to obtain

$$\exp[Q(\hat{x}, \hat{p})] = \mathcal{PT}\exp[Q(\hat{x}, \hat{p})]\mathcal{PT} = \exp[Q(-\hat{x}, \hat{p})] ,$$

from which we conclude that $Q(\hat{x}, \hat{p})$ is an *even* function of $\hat{x}$. Second, we substitute (31) into the condition (29) and find that

$$\exp[Q(\hat{x}, \hat{p})]\mathcal{P}\exp[Q(\hat{x}, \hat{p})]\mathcal{P} = \exp[Q(\hat{x}, \hat{p})]\exp[Q(-\hat{x}, -\hat{p})] = 1 ,$$

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 (30) to be imposed is that the operator $\mathcal{C}$ commutes with H. Substituting $\mathcal{C} = \exp[Q(\hat{x}, \hat{p})]\mathcal{P}$ into (30), we get $\exp[Q(\hat{x}, \hat{p})][\mathcal{P}, H] + [\exp[Q(\hat{x}, \hat{p}], H]\mathcal{P} = 0$. We can express the Hamiltonian H in (27) in the form $H = H_0 + \varepsilon H_1$, where 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 *anti-commutes* with $\mathcal{P}$. The above condition becomes

$$2\epsilon\exp[Q(\hat{x}, \hat{p})]H_1 = [\exp[Q(\hat{x}, \hat{p})], H] . \tag{32}$$

The operator $Q(\hat{x}, \hat{p})$ may be expanded as a series in odd powers of ε:

$$Q(\hat{x}, \hat{p}) = \epsilon Q_1(\hat{x}, \hat{p}) + \epsilon^3 Q_3(\hat{x}, \hat{p}) + \epsilon^5 Q_5(\hat{x}, \hat{p}) + \cdots . \tag{33}$$

Substituting the expansion in (33) into the exponential $\exp[Q(\hat{x}, \hat{p})]$, we get after some algebra a sequence of equations that can be solved systematically for the operator-valued functions $Q_n(\hat{x}, \hat{p})$ ($n = 1,3,5, \ldots$) subject to the symmetry constraints that ensure the conditions (28) and (29). The first three of these equations are

$$\begin{aligned} &[H_0, Q_1] = -2H_1 , \\ &[H_0, Q_3] = -\tfrac{1}{6}[Q_1, [Q_1, H_1]] , \\ &[H_0, Q_5] = \tfrac{1}{360}[Q_1, [Q_1, [Q_1, [Q_1, H_1]]]] \\ &\qquad\qquad - \tfrac{1}{6}([Q_1, [Q_3, H_1]] + [Q_3, [Q_1, H_1]]) . \end{aligned} \tag{34}$$

Let us solve these equations for the Hamiltonian in (27), 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 the first of the equations in (34), $[H_0, Q_1] = -2i\hat{x}^3$, we take as an *ansatz* for Q_1 the most general Hermitian cubic polynomial that is even in $\hat{x}$ and odd in p:

$$Q_1(\hat{x}, \hat{p}) = M\hat{p}^3 + N\hat{x}\hat{p}\hat{x} , \tag{35}$$

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

It is straightforward, though somewhat tedious, 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, $S_{0,0} = 1$, $S_{0,3} = \hat{x}^3$, $S_{1,1} = \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x})$, $S_{1,2} = \frac{1}{3}(\hat{x}^2\hat{p} + \hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2)$, and so on. The properties of the operators $S_{m,n}$ are summarized in [25].

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

$$\begin{aligned} Q_1 &= -\tfrac{4}{3}\hat{p}^3 - 2S_{1,2} , \\ Q_3 &= \tfrac{128}{15}\hat{p}^5 + \tfrac{40}{3}S_{3,2} + 8S_{1,4} - 12\hat{p} , \\ Q_5 &= -\tfrac{320}{3}\hat{p}^7 - \tfrac{544}{3}S_{5,2} - \tfrac{512}{3}S_{3,4} - 64S_{1,6} + \tfrac{24\,736}{45}\hat{p}^3 + \tfrac{6\,368}{15}S_{1,2} . \end{aligned} \tag{36}$$

This completes the calculation of $\mathcal{C}$. Together, (31), (33) and (36) represent an explicit perturbative expansion of $\mathcal{C}$ in terms of the operators $\hat{x}$ and $\hat{p}$, correct to order ε^6.

To summarize, using the *ansatz* (31) we can calculate the $\mathcal{C}$ operator to very high order in perturbation theory. We are able to perform this calculation because this *ansatz* obviates the necessity of calculating the wave functions $\phi_n(x)$.

9. Quantum mechanics in the complex plane

We have seen in section 4 that the classical motion of particles described by $\mathcal{PT}$-symmetric Hamiltonians is not confined to the real-x axis; the classical paths of such particles lie in the complex-x plane. Analogously, the new kinds of quantum theories discussed in this paper may also

be viewed as extensions of ordinary quantum mechanics into the complex domain. This is so because, as we saw in section 3, the Schrödinger equation eigenvalue problem and the corresponding boundary conditions are posed in the complex-x plane.

The idea of extending a Hermitian Hamiltonian into the complex plane was first discussed by Dyson, who argued heuristically that perturbation theory for quantum electrodynamics diverges [26]. Dyson's argument involves rotating the electric charge e into the complex plane $e \to ie$. Applied to the anharmonic oscillator Hamiltonian

$$H = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{x}^2 + \tfrac{1}{4}g\,\hat{x}^4 \quad (g > 0)\,, \tag{37}$$

Dyson's argument would go as follows: rotate the coupling g into the complex-g plane to $-g$. Then the potential is no longer bounded below, so the resulting theory has no ground state. Thus, the energies $E_n(g)$ are singular at $g = 0$ and the perturbation series for $E_n(g)$, which are series in powers of g, must therefore have a zero radius of convergence and must diverge for all $g \neq 0$. These perturbation series do indeed diverge, but there is a flaw in Dyson's argument, and understanding this flaw is necessary to understand how a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian can have a positive real spectrum.

The flaw in Dyson's argument is simply that the eigenvalues of the Hamiltonian

$$H = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{x}^2 - \tfrac{1}{4}g\,\hat{x}^4 \quad (g > 0)\,, \tag{38}$$

are undefined until the boundary conditions on the eigenfunctions are specified. These boundary conditions depend crucially on how this Hamiltonian with negative coupling is obtained. Dyson's way to obtain H in (38) would be to substitute $g = |g|\exp(\mathrm{i}\theta)$ into (37) and to rotate from $\theta = 0$ to $\theta = \pi$. Under this rotation, the energies $E_n(g)$ become complex: the $E_n(g)$ are real and positive when $g > 0$ but complex when $g < 0$. The $\mathcal{PT}$-symmetric way to obtain (38) is to take the limit δ: $0 \to 2$ of $H = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + \frac{1}{4}g\hat{x}^2(\mathrm{i}\hat{x})^\delta$ ($g > 0$). When (38) is obtained by this limiting process, its spectrum is real, positive and discrete.

How can the Hamiltonian (38) possess two such astonishingly different spectra? As we saw in section 3, the answer lies in understanding the boundary conditions satisfied by the wave functions $\phi_n(x)$. Under Dyson's rotation the eigenfunctions $\phi_n(x)$ vanish in the complex-x plane as $|x| \to \infty$ inside the wedges $-\pi/3 < \arg\, x < 0$ and $-4\pi/3 < \arg\, x < -\pi$. Under the $\mathcal{PT}$ limiting process, in which the exponent δ ranges from 0 to 2, $\phi_n(x)$ vanishes in the complex-x plane as $|x| \to \infty$ inside the wedges $\pi/3 < \arg x < 0$ and $-\pi < \arg x < -2\pi/3$. In the latter case the boundary conditions hold in wedges that are symmetric with respect to the imaginary axis (see figure 2); these boundary conditions enforce the $\mathcal{PT}$ symmetry of H and are responsible for the reality of the energy spectrum.

Apart from the differences in the energy levels, there is another striking difference between the two theories corresponding to H in (38). Under Dyson's rotation the expectation value of the operator $\hat{x}$ remains zero. This is because Dyson's rotation preserves the parity symmetry of H in (38). However, under our limiting process, in which δ ranges from 0 to 2, this expectation value becomes non-zero because as soon as δ begins to increase, parity symmetry is violated (and is replaced by $\mathcal{PT}$ symmetry).

The non-vanishing of the expectation value of $\hat{x}$ has important physical consequences. We suggest in the next section that $\mathcal{PT}$ symmetry may be the ideal quantum field theoretic setting to describe the dynamics of the Higgs sector in the standard model of particle physics.

10. Physical applications of $\mathcal{PT}$-symmetric quantum theories

It is not known whether non-Hermitian, $\mathcal{PT}$-symmetric Hamiltonians can be used to describe experimentally observable phenomena. However, non-Hermitian Hamiltonians have *already* been used to describe interesting interacting systems. For example, Wu showed that the ground state of a Bose system of hard spheres is described by a non-Hermitian Hamiltonian [1]. Wu found that the ground-state energy of this system is real and conjectured that all the energy levels were real. Hollowood showed that even though the Hamiltonian of a complex Toda lattice is non-Hermitian, the energy levels are real [27]. Non-Hermitian Hamiltonians of the form $H = \hat{p}^2 + \mathrm{i}\hat{x}^3$ and cubic quantum field theories arise in studies of the Lee–Yang edge singularity [3] and in various Reggeon field theory models [2]. In each of these cases the fact that a non-Hermitian Hamiltonian had a real spectrum appeared mysterious at the time, but now the explanation is simple: in each case the non-Hermitian Hamiltonian is $\mathcal{PT}$-symmetric. In each case the Hamiltonian is constructed so that the position operator $\bar{x}$ or the field operator ϕ is always multiplied by i.

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 $V(x) = i \sin x$. 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*. However, at the edge of the bands the wave function of a particle in such a lattice is always bosonic (2π-periodic), and unlike the case of ordinary crystal lattices, the wave function is never fermionic (4π-periodic) [28]. Direct observation of such a band structure would give unambiguous evidence of a $\mathcal{PT}$-symmetric Hamiltonian.

The quartic $\mathcal{PT}$-symmetric quantum field theory that corresponds to H in (7) with $N = 4$ is described by the 'wrong-sign' Hamiltonian density

$$\mathcal{H} = \tfrac{1}{2}\pi^2(\mathbf{x},t) + \tfrac{1}{2}[\nabla_x\phi(\mathbf{x},t)]^2 + \tfrac{1}{2}\mu^2\phi^2(\mathbf{x},t) - \tfrac{1}{4}g\phi^4(\mathbf{x},t)\ . \tag{39}$$

This theory is remarkable because, in addition to the energy spectrum being real and positive, the one-point Green's function (the vacuum expectation value of ϕ) is *non-zero* [29]. Also, the field theory is renormalizable, and in four dimensions it is asymptotically free and thus non-trivial [30]. Based on these features, we believe that the theory may provide a useful setting in which to describe the dynamics of the Higgs sector in the standard model.

Other field theory models whose Hamiltonians are non-Hermitian and $\mathcal{PT}$-symmetric have also been studied. For example, $\mathcal{PT}$-symmetric electrodynamics is particularly interesting because it is asymptotically free (unlike ordinary electrodynamics) and because the direction of the Casimir force is the negative of that in ordinary electrodynamics [31]. This theory is remarkable because it can determine its own coupling constant. Supersymmetric $\mathcal{PT}$-symmetric quantum field theories have also been studied [32].

How does a $g\phi^3$ theory compare with a $g\phi^4$ theory? A $g\phi^3$ theory has an attractive force. Bound states arising as a consequence of this force can be found by using the Bethe–Salpeter equation. However, the $g\phi^3$ field theory is unacceptable because the spectrum is not bounded below. If we replace g by ig, the spectrum becomes real and positive, but now the force becomes repulsive and there are no bound states. The same is true for a two-scalar theory with interaction of the form $ig\phi^2\chi$, which is an acceptable model of scalar electrodynamics that has no analogue of positronium. It would be truly remarkable if the repulsive force that arises in a $\mathcal{PT}$-symmetric quantum field theory having a three-point interaction could explain the acceleration in the expansion of the universe.

We believe that the concept of $\mathcal{PT}$ symmetry as a generalization of the usual Dirac Hermiticity requirement in conventional quantum mechanics is physically reasonable and mathematically elegant. While the proposal of $\mathcal{PT}$ symmetry is unconventional, we urge the reader to keep in mind the words of Michael Faraday: 'Nothing is too wonderful to be true, if it be consistent with the laws of nature'.

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