Quantum counterpart of spontaneously broken classical $\mathcal{PT}$ symmetry

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Abstract
The classical trajectories of a particle governed by the $\mathcal{PT}$-symmetric Hamiltonian $H = p^2 + x^2 (ix)^\epsilon$ ($\epsilon \geq 0$) have been studied in depth. It was found that almost all trajectories that begin at a classical turning point oscillate periodically between this turning point and the corresponding $\mathcal{PT}$-symmetric turning point. Recently it has been found that, whereas in some regions of $\epsilon$ the period is a smooth function of $\epsilon$, in others it is a rapidly varying and noisy function. The current paper examines the corresponding quantum-mechanical systems. The eigenvalues of these quantum systems exhibit characteristic behaviors that are correlated with those of the associated classical system.

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

1. Introduction

This paper studies the eigenvalues of the non-Hermitian quantum systems defined by the $\mathcal{PT}$-symmetric Hamiltonians

$$H = p^2 + x^2 (ix)^\epsilon \quad (\epsilon \geq 0).$$

(1)

The Hamiltonians (1) can have many different spectra depending on the large-$|x|$ boundary conditions that are imposed on the solutions to the corresponding time-independent Schrödinger eigenvalue equation

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

(2)

The boundary conditions on $\psi(x)$ are imposed in Stokes’ wedges in the complex-$x$ plane. At the edges of the Stokes wedges both linearly independent solutions to (2) are oscillatory as $|x| \to \infty$. However, in the interior of the wedges, one solution decays exponentially and
the linearly independent solution grows exponentially. The eigenvalues $E$ are determined by requiring that the solution $\psi(x)$ decay exponentially in two nonadjacent wedges. Ordinarily, the eigenvalues are complex. However, if the two wedges are $\mathcal{PT}$-symmetric reflections of one another, then there is a possibility that all the eigenvalues will be real. (The $\mathcal{PT}$ reflection of the complex number $x$ is the number $-x^*.$)

If $\epsilon$ is not a rational number, there are infinitely many Stokes’ wedges, which we label by the integer $K$. The center of the $K$th Stokes wedge lies at the angle

$$\theta_{\text{center}} = \frac{(4K + 2)\pi}{4 + \epsilon} - \frac{\pi}{2}. \quad (3)$$

The upper edge of the wedge lies at the angle

$$\theta_{\text{upper}} = \frac{(4K + 3)\pi}{4 + \epsilon} - \frac{\pi}{2}, \quad (4)$$

and the lower edge lies at the angle

$$\theta_{\text{lower}} = \frac{(4K + 1)\pi}{4 + \epsilon} - \frac{\pi}{2}. \quad (5)$$

The opening angles $\Delta\theta$ of all wedges are the same:

$$\Delta\theta = \frac{2\pi}{4 + \epsilon}. \quad (6)$$

The $\mathcal{PT}$ reflection of the wedge $K$ is the wedge $-K - 1$.

The $\mathcal{PT}$-symmetric eigenvalue problem posed in the wedges $K = 0$ and $K = -1$ has been studied in depth in [1–3]. The spectrum for this problem is real when $\epsilon \geq 0$, as illustrated in figure 1. For these boundary conditions the quantum theory specified by the Hamiltonian exhibits unitary time evolution [4].

The classical system corresponding to this quantum system has also been examined carefully [2]. Without loss of generality, one can take the classical energy to be unity. One can then graph the classical trajectories by solving numerically the system of Hamilton’s differential equations.
\[ \dot{x} = \frac{\partial H}{\partial p} = 2p, \quad \dot{p} = -\frac{\partial H}{\partial x} = -(2 + \epsilon)x(i\epsilon)^k \tag{7} \]

for an initial condition \( x(0); p(0) \) is determined from the equation \( H = E = 1 \). Since \( x(0) \) and \( p(0) \) are not necessarily real and the differential equations (7) are complex, the classical trajectories are curves in the complex-\( x \) plane. For \( \epsilon \geq 0 \) nearly all trajectories are closed curves. (When \( \epsilon \) is a positive integer, trajectories originating at some turning points can run off to infinity, but these are special isolated cases. When \( \epsilon < 0 \), all trajectories are open curves.) If \( \epsilon \) is noninteger, there is a branch cut in the complex-\( x \) plane, and to be consistent with \( \mathcal{PT} \) symmetry we take this cut to run from 0 to \( \infty \) along the positive-imaginary axis. A closed trajectory may cross this branch cut and visit many sheets of the Riemann surface before returning to its starting point.

As \( \epsilon \) increases from 0, the harmonic oscillator turning points at \( x = 1 \) (and at \( x = -1 \)) rotate downward and clockwise (anticlockwise) into the complex-\( x \) plane. These turning points are solutions to the equation \( 1 + (ix)^{2+\epsilon} = 0 \). When \( \epsilon > 0 \) is irrational, this equation has infinitely many solutions; all solutions lie on the unit circle and have the form

\[ x = e^{i\theta_{\text{turning point}}}, \tag{8} \]

where

\[ \theta_{\text{turning point}} = \frac{(2K + 1)\pi}{2 + \epsilon} - \frac{\pi}{2}. \tag{9} \]

These turning points occur in \( \mathcal{PT} \)-symmetric pairs (pairs that are symmetric when reflected through the imaginary axis) corresponding to the \( K \) values \((K = -1, K = 0), (K = -2, K = 1), (K = -3, K = 2), (K = -4, K = 3) \) and so on. When \( \epsilon \) is rational, there are only a finite number of turning points in the complex-\( x \) Riemann surface. For example, when \( \epsilon = \frac{12}{5} \), the Riemann surface consists of five sheets and there are eleven pairs of turning points.

The period \( T \) of a 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 explained in \([5, 6]\), any 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 oscillate between the \( K = -1, K = 0 \) pair of turning points, the period \([2]\) of the closed orbit is a smoothly decreasing function of \( \epsilon \):

\[ T(\epsilon) = 2\sqrt{\pi} \frac{\Gamma(3 + \epsilon)/(2 + \epsilon)}{\Gamma(4 + \epsilon)/(4 + 2\epsilon)} \cos \left( \frac{\epsilon\pi}{4 + 2\epsilon} \right), \tag{10} \]

valid for all \( \epsilon \geq 0 \). This smooth classical behavior mirrors the smooth behavior of the quantum eigenvalues shown in figure 1.

However, for \( \epsilon < 0 \) there exist orbits with infinite period, and this behavior again finds a qualitative counterpart in the quantum problem. As can be seen from figure 1, the real eigenvalues progressively merge into complex conjugate pairs, exhibiting broken \( \mathcal{PT} \) symmetry, and at the limiting point \( \epsilon = -1 \) the remaining real ground-state energy goes off to infinity.

This is the well-established situation for the \( K = 0 \) and \( K = -1 \) turning points. More recently the classical situation for other pairs of turning points has been investigated in \([5]\) and \([6]\), where a remarkable pattern of regular and irregular behavior of the period was found. However, as yet the corresponding quantum situation has not been investigated, and that is the purpose of the present paper. In the following section we summarize the classical results of \([5]\) and \([6]\) and then in section 3 we investigate the pattern of eigenvalues in the corresponding quantum problems. In section 4 we discuss the extent to which the behavior of the classical system finds an echo in the quantum system.
2. Classical trajectories for other pairs of turning points

Complex trajectories that begin at turning points other than the $K = 0$ and $K = -1$ turning points are more interesting. For these trajectories it was shown in [5] and [6] that there are three qualitatively distinct regions of $\epsilon$. For the $K > 0$ turning point and the corresponding $-K - 1$ turning point, region I extends from $\epsilon = 0$ to $\epsilon = 1/K$. As $\epsilon$ increases from 0 in region I, the period of the classical trajectory is a smooth monotone decreasing function of $\epsilon$ like that in (10). In region II, where $\epsilon$ ranges from $1/K$ up to $4K$, the period $T(\epsilon)$ of the classical trajectories is a noisy function of $\epsilon$ and the classical orbits in this region are acutely 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 the value of $\epsilon$, some orbits have short periods and others have long and possibly even arbitrarily long periods. In this region there are isolated values of $\epsilon$ for which the orbits are not symmetric when reflected through the imaginary axis, and thus these orbits are not $\mathcal{PT}$ symmetric; such orbits are said to have spontaneously broken classical $\mathcal{PT}$ symmetry. In region III, $\epsilon$ ranges from $4K$ up to $\infty$ and the period of the orbits is again a smooth monotone decreasing function of $\epsilon$.

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 a relatively small and 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 have shown that there are only a finite number of these special values of $\epsilon$ and that these values of $\epsilon$ are rational [5, 6]. Some special values of $\epsilon$ at which spontaneously broken $\mathcal{PT}$-symmetric orbits occur are indicated in figures 2 and 3 by short vertical lines below the horizontal axis.

Figure 2. Period of a classical trajectory beginning at the $K = 1$ 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 is a rapidly varying and noisy function of $\epsilon$. For $\epsilon > 4$ (region III) the period is once again a smoothly decaying function of $\epsilon$. 
3. Behavior of eigenvalues as $\epsilon$ passes through regions I–III

3.1. Eigenvalues corresponding with $K = 1$ and $K = -2$ turning points

In [5] and [6], the behavior of the classical trajectories was studied and the period of the classical trajectories was found to have a remarkably complicated dependence on $\epsilon$ (see figure 2). In figure 4 we plot the eigenvalues for the corresponding eigenvalue problem for $0 \leq \epsilon \leq 7$. (By the corresponding eigenvalue problem, we mean the eigenvalues for the eigenvalue problem associated with the $K = 1$ and $K = -2$ Stokes wedges.) These eigenvalues were calculated by numerically integrating the Schrödinger equation from large $|x|$ into the origin along the centers of the two Stokes wedges and then applying the appropriate matching condition on $\psi(x)$ and $\psi'(x)$ at $x = 0$. At the origin, $\psi(x)$ is continuous, but the matching condition on $\psi'(x)$ incorporates the angle of rotation between the two wedges. These matching conditions are reminiscent of the techniques used by Znojil in his discussion of 'quantum toboggans' [7].

The eigenvalues in figure 4 exhibit the following features: at $\epsilon = 0$ the spectrum is that of the harmonic oscillator, $E_n = 2n + 1$ ($n = 0, 1, 2, \ldots$), and the entire spectrum is real, positive and discrete. As soon as $\epsilon$ increases from 0, the eigenvalues begin to coalesce into complex conjugate pairs; the process of combining into complex-conjugate pairs starts at the high-energy part of the spectrum. (This disappearance of real eigenvalues qualitatively resembles that shown in figure 1 as $\epsilon$ decreases below 0.) When $\epsilon$ reaches the value 0.5, only one real eigenvalue (the ground-state eigenvalue) remains. This eigenvalue becomes infinite at $\epsilon = 1$. Between $\epsilon = 1$ and $\epsilon = 3$ there are no real eigenvalues at all. The real ground-state eigenvalue reappears when $\epsilon$ increases past 3, and as $\epsilon$ approaches 4, more and more real
Figure 4. Real eigenvalues associated with the $K = 1$ and $K = -2$ pair of turning points plotted as functions of $\epsilon$. (The periods of the classical orbits that begin at the $K = 1$ turning point are shown in figure 2 for regions I–III.)

Eigenvalues appear. At the isolated point $\epsilon = 4$ the spectrum is again entirely real\(^3\) and agrees exactly with the spectrum of figure 1 when extended to $\epsilon = 4$. At the isolated point $\epsilon = 5$ the spectrum is once again entirely real, but just above and below this value of $\epsilon$ the spectrum becomes complex again. Finally, as $\epsilon$ reaches a value near $\epsilon = 5.5$, the spectrum is again entirely real, positive and discrete and it remains so for all larger values of $\epsilon$.

Note that some of the qualitative changes in figures 2 and 4 occur at the same value of $\epsilon$. For example, the noisy fluctuations in figure 2 begin at $\epsilon = 1$, just as the real ground-state eigenvalue blows up, and the fluctuations stop temporarily at $\epsilon = 3$, just as the real ground-state eigenvalue reappears in figure 4. The noisy classical fluctuations cease completely at $\epsilon = 4$, just as the real eigenvalues begin to reappear in figure 4.

The most important qualitative changes in figure 4 appear to be caused by the classical turning points entering and leaving the Stokes wedges inside of which the eigenvalue problem is specified (see figure 5). For the case $K = 1$ the upper and lower edges of the wedge are given by

$$
\theta_{\text{upper}} = \frac{7\pi}{4 + \epsilon} - \frac{\pi}{2} \quad \text{and} \quad \theta_{\text{lower}} = \frac{5\pi}{4 + \epsilon} - \frac{\pi}{2}.
$$

(11)

At $\epsilon = 0$ the $K = 1$ classical turning point lies in the center of the wedge. However, as $\epsilon$ increases, the turning point rotates faster than the wedge rotates, and at $\epsilon = 1$ this turning point leaves the wedge, as shown in figure 5(a). There are no turning points in the wedge between $\epsilon = 1$ and $\epsilon = 3$, which corresponds with the total nonexistence of real eigenvalues. At $\epsilon = 3$ a turning point re-enters the wedge, as shown in figure 5(b), but this is the $K = 2$

\(^3\) This is not entirely clear from the diagram. What can be seen near $\epsilon = 4$ is actually the beginning of a vertical spiral of rapidly decreasing width centered on $\epsilon = 4$. The calculation becomes technically rather difficult at this point. However, we can be assured that the eigenvalues are indeed entirely real by reference to figure 7 and the commentary that follows. The figure would be exactly the same for $K = 1$, with just the upper left- and right-hand wedges interchanged.
Figure 5. Turning points entering and leaving the $K = 1$ wedge as $\epsilon$ increases. As $\epsilon$ increases past 1, the $K = 1$ turning point, whose angle is indicated by a dotted line, leaves the wedge (panel (a)). Then, as $\epsilon$ increases past 3, a new turning point enters the wedge (panel (b)).

turning point and not the $K = 1$ turning point. The re-entry of a classical turning point is strongly correlated with the reappearance of real eigenvalues.

When the turning point leaves the wedge, WKB quantization is no longer possible. Thus, the high-energy portion of the spectrum is no longer real. In fact, we believe that there are no eigenvalues at all, real or complex, when $1 < \epsilon < 3$.

3.2. Eigenvalues corresponding with $K = 2$ and $K = -3$ turning points

For a classical trajectory beginning at the $K = 2$ turning point, the period as a function of $\epsilon$ again exhibits three types of behaviors. The period decreases smoothly for $0 \leq \epsilon < 1/2$ (region I). When $1/2 \leq \epsilon \leq 8$ (region II), the period becomes a rapidly varying and noisy function of $\epsilon$. When $\epsilon > 8$ (region III), the period is once again a smoothly decaying function of $\epsilon$. These behaviors are shown in figure 3. As in figure 2, the period in regions I and III is very small compared with the period in region II. The classical trajectory that begins at the $K = 2$ turning point terminates at the $K = -3$ turning point except when $\mathcal{PT}$ symmetry is spontaneously broken. Broken-symmetry orbits occur at isolated points in region II.

Figure 6 displays the eigenvalues of the corresponding quantum problem. Observe that the eigenvalues are all real at $\epsilon = 0$ (the harmonic oscillator spectrum), but they begin to become complex as $\epsilon$ increases from 0. There are no real eigenvalues when $\epsilon$ reaches the value $1/2$, just at the onset of noisy fluctuations in figure 3. There are several isolated values of $\epsilon$ at 2, 4, 5, 7, 8 and 9, where the spectrum is entirely real. There are also two regions, $1/2 \leq \epsilon \leq 3/2$ and $5 \leq \epsilon \leq 7$, where there are no real eigenvalues at all. Between 2 and 3 there appears to be a patch where the eigenvalues are all (or almost all) real. (This patch corresponds with a temporary disappearance of noise in figure 3.) Real eigenvalues begin to reappear at $\epsilon = 9$, and the spectrum appears to be completely real beyond $\epsilon = 21/2$.

The regions in which there are no real eigenvalues are exactly correlated with turning points leaving the Stokes wedges. At $\epsilon = 1/2$ the $K = 2$ classical turning point leaves the wedge at the angle $\theta = 3\pi/2$. Then, at $\epsilon = 3/2$ the $K = 3$ classical turning point enters the wedge at the angle $3\pi/2$. Again, at $\epsilon = 5$ the $K = 3$ turning point leaves the wedge at
4. Concluding remarks

Figures 2 and 3 for $K = 1$ and figures 4 and 6 for $K = 2$ illustrate a general pattern that appears to hold for all $K$. For classical orbits that oscillate between the $K$th pair of turning points, there are always three regions, region I for which $0 \leq \epsilon \leq \frac{1}{K}$, region II for which $\frac{1}{K} < \epsilon < 4K$ and region III for which $4K < \epsilon$. When $\epsilon = 0$, the turning points lie on the real axis in the centers of the Stokes wedges. As $\epsilon$ increases, the turning points rotate faster than the wedges rotate and they rotate out of the wedges at $\epsilon = \frac{1}{K}$. At this point there is a patch where there are no real eigenvalues. As $\epsilon$ continues to increase, the $K+1$ turning point rotates into the Stokes wedge and the eigenvalues begin to become real. Eventually, this turning point leaves the wedge and there are again no real eigenvalues. In total, there are $K$ regions where there are no real eigenvalues. Eventually, the $2K$ turning point enters the wedge at the end of region II, and the spectrum begins to become entirely real and remains entirely real in region III.

There are many isolated points at which the eigenvalues are all real. For example, when $K = 2$, real eigenvalues occur at 2, 4, 8 and 9. Some of these points can be analyzed in terms of $\mathcal{PT}$ reflection. Specifically: (i) from (3) we can see that at $\epsilon = 2$ the $K = 2$ wedge is centered at the angle $\pi/6$. The $\mathcal{PT}$ reflection of this wedge lies at the angle $-\pi/6$. Thus, the $K = 2$ spectrum agrees exactly with the $K = 0$ spectrum in figure 1 for this value of $\epsilon$. (ii) At $\epsilon = 4$ the $K = 2$ wedge is centered at $3\pi/4$. The $\mathcal{PT}$ reflection of this wedge is centered at $\pi/4$, and under complex conjugation this angle becomes $-\pi/4$. Thus, the $K = 2$ spectrum is identical to the $K = 0$ spectrum for this value of $\epsilon$. This configuration of wedges is shown in figure 7. Note that the intervening wedges, centered on the real axis, correspond to the angle $\pi/2$ and at $\epsilon = 7$ the $K = 4$ classical turning point enters the wedge at the angle $\theta = \pi/2$. 

Figure 6. Real eigenvalues associated with the $K = 2$ and $K = -3$ pair of turning points plotted as a function of $\epsilon$. (The periods of the classical orbits that begin at the $K = 1$ turning point are shown in figure 3 for regions I–III.)
Figure 7. The Stokes wedges for $\epsilon = 4$ for the cases $K = 0$ and $K = 2$. Because the wedges are complex conjugate pairs the spectra are identical for this value of $\epsilon$.

To the conventional Hermitian $x^{6}$ potential, and of course have an entirely different spectrum.

(iii) At $\epsilon = 8$ the $K = 2$ wedge is centered at $\pi/3$. Under complex conjugation, this wedge is now centered at the angle $-\pi/3$, which corresponds with the wedge for the $K = 0$ case. Thus, once again, the spectra for these two problems are identical at this value of $\epsilon$. (Note that for these three situations $\epsilon$ is integer valued, and hence there is no cut in the complex-$x$ plane.)

While quantum mechanics and classical mechanics are of course different theories with different regimes of applicability, our investigation has shown that there are nonetheless some correlations between the two. Regular classical behavior seems to correspond to a completely real quantum spectrum, while chaotic classical behavior in the complex plane is associated with either a partially complex spectrum or a complete absence of eigenvalues. In the systems we have studied, the onset of rapid and irregular variation in the periods of the classical trajectories correlates precisely with the disappearance of all quantum eigenvalues as the ground-state energy goes to infinity, while the end of the noisy region is associated with the gradual reappearance of a completely real spectrum. Within the region of rapid variation some correlations can be observed, but they are less clear-cut and merit further analysis.

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