$\mathcal{PT}$-symmetric potentials having continuous spectra

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Received 18 February 2020, revised 29 June 2020
Accepted for publication 9 July 2020
Published 17 August 2020

Abstract

One-dimensional $\mathcal{PT}$-symmetric quantum-mechanical Hamiltonians having continuous spectra are studied. The Hamiltonians considered have the form $H = p^2 + V(x)$, where $-\infty < x < \infty$. The potential $V(x)$ is odd in $x$, pure imaginary, and vanishes as $|x| \to \infty$. Five $\mathcal{PT}$-symmetric potentials are studied: the Scarf-II potential $V_1(x) = iA_1 \text{sech}(x)\tanh(x)$, which decays exponentially for large $|x|$; the rational potentials $V_2(x) = iA_2 x/(1 + x^4)$ and $V_3(x) = iA_3 x/(1 + |x|^3)$, which decay algebraically for large $|x|$; the step-function potential $V_4(x) = iA_4 \text{sgn}(x)\theta(2.5 - |x|)$, which has compact support; the regulated Coulomb potential $V_5(x) = iA_5 x/(1 + x^2)$, which decays slowly as $|x| \to \infty$ and thus may be viewed as a long-range potential. The real parameters $A_n$ measure the strengths of these potentials. Numerical techniques for solving the time-independent Schrödinger eigenvalue problems associated with these potentials reveal that, in general, the spectra of these Hamiltonians are partly real and partly complex. The real eigenvalues form the continuous part of the spectrum and the complex eigenvalues form the discrete part of the spectrum. The real eigenvalues range continuously in value from 0 to $+\infty$. The complex eigenvalues occur in discrete complex-conjugate pairs and for $V_n(x)$ ($1 \leq n \leq 4$) the number of these pairs is finite and increases as the value of the strength parameter $A_n$ increases. However, for $V_5(x)$ there is an infinite sequence of discrete eigenvalues with a limit point at the origin. While this sequence is complex, it resembles the Balmer series for the hydrogen atom because it has inverse-square convergence.
Keywords: PT symmetry, continuous spectra, long-range potentials, non-Hermitian

(Some figures may appear in colour only in the online journal)

1. Introduction

A \( \mathcal{PT} \)-symmetric quantum theory is defined by a Hamiltonian that is invariant under combined space reflection (parity) \( \mathcal{P} \) and time reversal \( \mathcal{T} \). An early class of non-Hermitian \( \mathcal{PT} \)-symmetric Hamiltonians that has been studied in depth is

\[
H = p^2 + x^2(ix)^\varepsilon \quad (\varepsilon \text{ real}).
\]

(1)

These Hamiltonians are \( \mathcal{PT} \)-invariant because \( x \rightarrow -x \) under \( \mathcal{P} \) and \( i \rightarrow -i \) under \( \mathcal{T} \). It was shown in references \([1, 2]\) that the eigenvalues of this class of Hamiltonians are real, discrete, and positive for all \( \varepsilon \geq 0 \); the reality of these eigenvalues was attributed to the \( \mathcal{PT} \) symmetry of \( H \). Subsequently, the reality of the spectrum was established at a mathematically rigorous level \([3, 4]\).

In general, the eigenvalues of a \( \mathcal{PT} \)-symmetric Hamiltonian are either real or come in complex-conjugate pairs. If the eigenvalue spectrum is entirely real, the \( \mathcal{PT} \) symmetry of the Hamiltonian is said to be unbroken, but if some of the eigenvalues are complex, the \( \mathcal{PT} \) symmetry of the Hamiltonian is said to be broken. In studies of model \( \mathcal{PT} \)-invariant Hamiltonians it has been observed that such Hamiltonians often exhibit a transition from a parametric region of unbroken \( \mathcal{PT} \) symmetry to a region of broken \( \mathcal{PT} \) symmetry. This \( \mathcal{PT} \) transition occurs in both the classical and in the quantized versions of a \( \mathcal{PT} \)-symmetric Hamiltonian \([2]\) and this transition has been observed in numerous laboratory experiments \([5, 6]\).

There are many papers on \( \mathcal{PT} \)-symmetric Hamiltonians having discrete spectra but very few studies of \( \mathcal{PT} \)-symmetric Hamiltonians having continuous spectra. This paper examines one-dimensional \( \mathcal{PT} \)-invariant Hamiltonians \( H = p^2 + V(x) \ ( -\infty < x < \infty ) \) that possess continuous spectra. The potentials \( V(x) \) considered here are \( \mathcal{PT} \) symmetric because they are odd under \( x \rightarrow -x \) and are pure imaginary. Thus, the eigenvalues of \( H \) are either real or occur in complex-conjugate pairs \([5]\).

The potentials \( V(x) \) discussed here decay to 0 as \( x \rightarrow \pm \infty \). Thus, we are not surprised to find what we expect intuitively: in general, the real part of the spectrum ranges continuously from 0 to \( +\infty \). The eigenfunctions \( \psi(x) \) associated with these real eigenvalues are \( \mathcal{PT} \) symmetric; that is, \( \psi^\ast(-x) = \psi(x) \). These eigenfunctions are not localized and do not decay exponentially as \( |x| \rightarrow \infty \).

What is interesting is that even though the potential \( V(x) \) vanishes as \( |x| \rightarrow \infty \) it still confines localized states whose energies are discrete and occur in complex-conjugate pairs. The eigenfunctions associated with these energies vanish exponentially as \( |x| \rightarrow \infty \) and are not \( \mathcal{PT} \) symmetric. It is especially interesting that while short-range potentials have a finite number of these discrete complex eigenvalues, long-range potentials have an infinite number of discrete complex eigenvalues.

An interesting question is whether the localized eigenfunctions represent bound states. In conventional Hermitian quantum mechanics a particle in a bound state has a discrete real energy \( E \) and is described by a normalizable eigenfunction \( \psi(x) \) of the time-independent Schrödinger equation

\[
-\psi''(x) + V(x)\psi(x) = E\psi(x).
\]

(2)
The time evolution of the bound state is expressed by the wave-function solution \( \Psi(x, t) = \psi(x) e^{-iEt} \) to the time-dependent Schrödinger equation

\[
i \frac{\partial}{\partial t} \Psi(x, t) = H \Psi(x, t).
\]  

(3)

Since \( E \) is real, the norm of the eigenfunction, which represents the total probability of the confined particle, is constant in time.

However, for the potentials considered in this paper, the discrete eigenvalues of the time-independent Schrödinger equation are complex, and thus the time-dependent wave function \( \Psi(x, t) \) grows or decays exponentially in time. This seems to imply that the norm of the localized state, and thus the probability of finding a particle in the localized state, grows or decays in time. This suggests that the localized state is not a bound state. This may be correct, but the problem with this argument is that because the energy eigenvalue is complex the \( \mathcal{PT} \) symmetry of \( H \) is broken, so we do not know how to calculate the norm of the localized state. In fact, while \( \Psi(x, t) \) is growing or decaying in time, the norm of \( \Psi \) might even be time-independent, which would lead to the interpretation that the localized state is indeed a bound state!

Although this possibility may seem unlikely, the simple classical example of a damped harmonic oscillator, whose equation of motion is

\[
y''(t) + \epsilon y'(t) + \omega^2 y(t) = 0,
\]  

(4)

suggests a mechanism that could explain how the norm of a localized quantum state might be constant in time even if the wave function of the state grows or decays with time. As \( t \) increases, all solutions to (4) are damped exponentially if \( \epsilon > 0 \) and grow exponentially if \( \epsilon < 0 \). Therefore, it might appear that the energy of the damped harmonic oscillator is time dependent if \( \epsilon \neq 0 \). Thus, one might conclude that (4) cannot be derived from a time-independent Hamiltonian. However, as is shown in reference [7], the dynamical equation (4) can in fact be derived by using Hamilton’s equations

\[
\dot{x} = \partial H / \partial p, \quad \dot{p} = -\partial H / \partial x
\]

for a simple time-independent classical Hamiltonian of the form

\[
H(x, p) = axp + f(p),
\]  

(5)

where \( a \) is a constant and \( f(p) \) is a function of \( p \) only. If one calculates the energy by solving (4) and evaluating \( H(x, p) \), one finds that the energy is exactly conserved in time even though the solution \( y(t) \) is growing or decaying exponentially. The classical energy is conserved because exponentially growing and exponentially decaying terms are multiplied together leaving an energy that is independent of time.

We believe that the appropriate norm for a \( \mathcal{PT} \)-symmetric Hamiltonian in a region of broken \( \mathcal{PT} \) symmetry must be constructed from both members of a complex-conjugate pair of localized states, and therefore it is possible that the growing and decaying components can cancel to give a time-independent norm. This conjecture is supported by the physical argument that a decaying localized state loses probability that flows outward to infinity and that a growing localized state gains probability that flows inward from infinity. But, because the eigenstates of the Hamiltonians discussed in this paper are exponentially damped at infinity, there cannot be any measurable flow of probability into or out of the localized states.
For the reasons given above, we conjecture that the complex-conjugate pairs of energy eigenstates studied in this paper are actually bound states. However, lacking a proof of this, we henceforth refer to such states as localized states.

In this paper we study five Hamiltonians of the form $H_n = p^2 + V_n(x)$, where

$$
\begin{align*}
V_1(x) &= iA_1 \sech(x) \tanh(x), \\
V_2(x) &= iA_2 \frac{x}{1 + x^4}, \\
V_3(x) &= iA_3 \frac{x}{1 + |x|^3}, \\
V_4(x) &= iA_4 \text{sgn}(x) \theta(2.5 - |x|), \\
V_5(x) &= iA_5 \frac{x}{1 + x^2},
\end{align*}
$$

where $\theta$ is the Heaviside step function. Because the potentials $V_n(x)$ are odd in $x$ and pure imaginary and we take the strength parameters $A_n$ to be real, the Hamiltonians $H_n$ are all $\mathcal{PT}$ symmetric.

We solve the time-independent Schrödinger equation associated with $H_n$ on the interval $-L \leq x \leq L$ and require that the eigenfunctions satisfy the boundary condition

$$
\psi(\pm L) = 0.
$$

We then examine what happens as $L \to \infty$. Since the potentials all vanish as $|x| \to \infty$, it follows from an asymptotic analysis of (2) that for large $|x|$ the eigenfunctions are either oscillatory or vanish exponentially.

We find that for all $n$ the Hamiltonians $H_n$ have real eigenvalues that range continuously from 0 to $+\infty$ and that the associated eigenfunctions are oscillatory for large $|x|$. However, the universal property of the five Hamiltonians studied here is that in addition to the real continuous part of the spectra, there are complex-conjugate pairs of discrete eigenvalues for sufficiently large strength parameters $A_n$. The eigenfunctions associated with the discrete eigenvalues vanish exponentially for large $|x|$. Thus, in all cases the $\mathcal{PT}$ symmetry of the Hamiltonians $H_n$ is broken.

The five potentials $V_n(x)$ vanish at different rates for large $|x|$: the Scarf-II potential $V_1(x)$ decays exponentially for $|x| \gg 1$. Because it is analytically solvable, we have used it to verify that our numerical work is accurate to at least 9 decimal places. Exponentially decaying potentials have previously been studied in references [8–10]. The rational potentials $V_2(x)$ and $V_3(x)$ decay algebraically like $|x|^{-3}$ and $|x|^{-2}$ for large $|x|$ and are not analytically solvable. The step-function potential $V_4(x)$ has compact support; potentials with imaginary steps have been examined in reference [11–13] and odd-$\mathcal{PT}$-symmetric step-function potentials were studied in reference [14]. These are all short-range potentials and such potentials confine a finite number of discrete complex localized states. The number and magnitudes of these complex eigenvalues increase as the strength parameters $A_n$ increase.

The potential $V_5(x)$ is special; it vanishes like $1/|x|$ for large $|x|$. Because it vanishes slowly, it is a long-range potential like the Coulomb potential. Even though this potential is bounded (unlike the Coulomb potential, which blows up at the origin), the property that it is long range allows it to confine infinitely many discrete complex localized states. Like the Balmer series for the hydrogen atom, the sequence of complex-conjugate pairs of eigenvalues converges to a limit, which happens to be at 0, and the $k$th pair of eigenvalues approaches 0 like $1/k^2$. 

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Figure 1. Eigenvalues in the complex plane for $V_1(x)$ in (6) with strength parameter $A_1 = 30$ for $L = 10$ in panel (a) and for $L = 100$ in panel (b). Continuum eigenvalues are indicated by red crosses in panel (a) and by green dots in panel (b). Discrete localized-state eigenvalues are indicated by black circles. Note that as $L$ increases, the locations of the localized states stabilize but the continuum eigenvalues all collapse onto the real axis. As they do so, a new complex-conjugate pair of localized states is uncovered. Observe that the continuum eigenvalues come in complex-conjugate pairs until the real parts of these eigenvalues exceed about 28. Above this critical value the continuum eigenvalues are all real.

1.1. Earlier studies of complex Hamiltonians having continuous spectra

In the 1960s a prominent mathematical analysis of complex Hamiltonians was done by Naimark [15]. In this long theorem-and-proof paper the time-independent Schrödinger equation (2) with a complex potential was examined in detail and it was shown that the eigenvalue spectrum can have continuous real eigenvalues and discrete complex eigenvalues. However, in Naimark’s paper (2) was examined on the positive real axis $x \geq 0$, rather than the whole real line, as in the current paper, and (2) was solved subject to the boundary condition $\psi'(0) = \Theta \psi(0)$, where $\Theta$ is complex number. In the current paper we impose the boundary condition (7) and then examine the behavior of the spectrum in the limit $L \to \infty$. Unlike the exposition here, no illustrative numerical examples are presented. Furthermore, throughout reference [15] special emphasis is given to potentials $V(x)$ that satisfy the condition

$$\int_0^\infty dx |V(x)| e^\epsilon x < \infty \quad (\epsilon > 0).$$

(8)

This strong constraint excludes potentials that vanish algebraically as $x \to \infty$, whereas we find that algebraically vanishing potentials, such as $V_2(x)$, $V_3(x)$, and $V_5(x)$, which decay like $|x|^{-3}$, $|x|^{-2}$, and $|x|^{-1}$, have the most interesting eigenvalue spectra.

There are several recent mathematical studies that were inspired by reference [15] (see, for example, references [16, 17]). In these papers the constraint (8) was imposed from the very beginning and indeed is stated in the abstract. Furthermore, in reference [13] there is a similar integral constraint that excludes the $V_3(x)$ and $V_5(x)$ potentials.

1.2. Numerical analysis used in this paper

In previous studies of $\mathcal{PT}$-symmetric Hamiltonians accurate numerical calculations of real discrete eigenvalues were done by using the shooting method [1]. However, if the discrete eigenvalues are complex, the shooting method becomes unwieldy and alternative techniques based on the finite-element and variational methods were used. Recently a numerical technique known as the Arnoldi algorithm was used in reference [18].
Figure 2. Eigenvalues in the complex plane for $V_1(x)$ in (6) with strength parameter $A_1 = 30$ for the case $L = 1000$. The discrete localized-state eigenvalues (black circles) have not shifted but the continuum eigenvalues (blue dots) are now very close to the real axis.

Figure 3. Logarithmic plot of the eigenvalue data in figures 1 and 2. This plot presents dramatic evidence that the transition from slightly complex continuum eigenvalues to exactly real continuum eigenvalues near $x = 28$ is sharp. There is a jump at the dashed line of about ten orders of magnitude at this transition point. The location of the transition does not change as $L$ increases from 10 to 100 to 1000.

In this paper we used a different numerical technique. Since we cannot work directly on the infinite $x$ axis, we reduce the problem to that of solving the Schrödinger equation on a large but finite interval. Consequently, numerical techniques used to calculate eigenvalues can only return discrete values and one must determine whether a given eigenvalue belongs to a discrete or a continuous part of the spectrum. To distinguish between these two possibilities we examine the associated eigenfunctions and observe how they satisfy the boundary conditions. As explained in detail in reference [18], the eigenfunctions associated with discrete eigenvalues are localized in space (like bound states) and decay to 0 smoothly and exponentially as $x$ approaches the boundary points of the interval. However, the eigenfunctions for eigenvalues that belong to the continuous part of the spectrum drop abruptly to 0 at one or both endpoints of the finite interval.

The technique used here to compute the eigenvalues of $H_n$ is called Chebyshev spectral collocation. This technique relies on the properties of Chebyshev polynomials and Chebyshev series and is explained in detail in reference [19]. To calculate the spectra of the Hamiltonians

\[ V_1(x) = A_1 \delta(x-L/2) \]
Figure 4. Plots of absolute values of eigenfunctions associated with some eigenvalues in figure 1. Panels (a)–(c) display eigenfunctions of the three discrete localized-state eigenvalues in panel (b) of figure 1: panel (a) shows the eigenfunction for the eigenvalue $2.374\,999\,999\,702\,702 + 12.272\,301\,129\,148\,877i$ for $L = 10$; panel (b) shows the eigenfunction for the eigenvalue $5.875\,000\,000\,021\,835 + 6.817\,945\,071\,620\,461i$ for $L = 10$; panel (c) shows the eigenfunction for the eigenvalue $7.374\,999\,997\,301\,000 + 1.363\,589\,013\,462\,076i$ for $L = 100$. The next three plots show the behavior of the eigenfunctions for some continuum eigenvalues: panel (d) shows the eigenfunction for the continuum eigenvalue $7.361\,943\,725\,638\,523 + 2.501\,634\,415\,578\,858i$ for $L = 10$; panel (e) shows the eigenfunction for the continuum eigenvalue $0.277\,713\,365\,597\,523 + 0.009\,073\,644\,654\,185i$ for $L = 100$; panel (f) shows the eigenfunction for the (real) continuum eigenvalue $30.234\,638\,465\,149\,410 + 0.000\,000\,000\,526\,705i$ for $L = 10$. Unlike the eigenfunctions in panels (a)–(e), this eigenfunction is $PT$ symmetric. The localized eigenfunctions in panels (a)–(c) decay smoothly and exponentially as $x$ approaches the endpoints but the continuum eigenfunctions in panels (d)–(f) abruptly and sharply drop to 0 at one or both endpoints.

$H_n$ by using Chebyshev spectral collocation we replace the infinite $x$ axis by the finite interval $-L \leq x \leq L$. We then decompose the interval $[-L, L]$ into $N$ subintervals bounded by grid points at $x_j$, where $j = 0, 1, 2, 3, \ldots, N$. These subintervals are not of equal length, rather, the subintervals shorten as we approach the endpoints at $x = -L$ and $x = L$. To determine the positions of the grid points, we construct a semicircle of radius $L$ centered at the origin $x = 0$ and divide the circle into equal sectors. We then project onto the $x$ axis. Thus, the grid points are located at $x_j = L \cos(\pi j / N)$. For all computations done in this paper we take $N = 2^{14} - 1$. The first and last grid points lie at $x = \pm L$, but since $N$ is odd there is no grid point at the origin. This choice is convenient because the potential $V_4(x)$ is discontinuous at $x = 0$. To find the eigenvalues we impose homogeneous boundary conditions at the endpoints $\pm L$ and finally let $L$ tend to infinity. In all cases we take $L = 10, 100,$ and $1000$, and we find that the eigenvalues converge rapidly to their $L = \infty$ values. We have verified the accuracy of our numerical work by comparing our results with the earlier analytical studies of the Scarf-II potential.

This paper is organized very simply. In sections 2–6 we describe in turn the spectra of $V_n(x)$ for $n = 1, 2, 3, 4,$ and $5$, and then in section 7 we give some concluding remarks.
Figure 5. Energy spectra for $V_2(x)$ with $A_2 = 30$. Panel (a) shows the eigenvalues for $L = 10$ and panel (b) shows the eigenvalues for $L = 100$. Like the case for the Scarf-II potential $V_1(x)$, the continuum part of the spectrum is slightly complex until the critical point near 21, after which the continuum eigenvalues are real. One pair of localized-state eigenvalues (black circles) is visible in panel (a) but as $L$ is increased to 100 in panel (b), a new pair of localized-state eigenvalues is uncovered.

Figure 6. Eigenvalues for the $V_2(x)$ potential for $A_2 = 30$. For this calculation $L = 1000$. Note that the discrete localized-state energies have not changed from their values in figure 5(b). However, the continuum part of the spectrum has moved closer to the real axis.

2. Eigenvalues for the Scarf-II potential $V_1(x)$

For the potential $V_1(x)$ in (6) we chose $A_1 = 30$. In figure 1 we plot the eigenvalues in the complex plane for $L = 10$ in panel (a) and for $L = 100$ in panel (b). We observe two kinds of eigenvalues, localized-state eigenvalues, which are indicated by circles, and continuum eigenvalues, which are indicated by crosses in (a) and by dots in (b). As we will see in figure 4, we can distinguish between localized-state and continuum eigenvalues by examining the corresponding eigenfunctions. This plot of the absolute values of the eigenfunctions as functions of $x$ shows that the eigenfunctions for localized-state eigenvalues decay smoothly and exponentially to 0 as $x$ approaches the boundaries at $\pm L$ while the continuum eigenfunctions abruptly drop to 0 at one or both boundaries. Note that as $L$ increases from 10 in (a) to 100 in (b), the positions of the localized-state eigenvalues stabilize rapidly but the continuum eigenvalues approach the real axis.

We observe two kinds of continuum eigenvalues in figure 1. Above a critical value near 28 the continuum eigenvalues are real, but below this critical value the continuum eigenvalues come in complex-conjugate pairs that lie slightly above and below the real axis. These pairs
Figure 7. Logarithmic plot of the energy eigenvalues for the potential $V_2(x)$ plotted for $L = 10, 100, $ and $1000$. Like the eigenvalues in figure 3, the continuum eigenvalues here undergo an abrupt jump at the dashed line near the critical value close to 21, where the imaginary parts of the continuum eigenvalues suddenly drop by about 10 orders of magnitude. The location of this line is insensitive to the value of $L$.

Figure 8. Eigenvalues for $V_3(x)$ with $A_3 = 30$. In panel (a) we display the data for $L = 10$ and in panel (b) we display the data for $L = 100$. Observe that as $L$ increases, the continuous eigenvalues approach the real axis. However the discrete complex-conjugate localized-state eigenvalues (black circles) remain fixed.

of eigenvalues approach the real axis as $L$ increases but the position of the critical value near $x = 28$ does not change. With increasing $L$ each member of the complex-conjugate pair of eigenvalues approaches the real axis vertically, but as they reach the real axis, one member of the pair moves slightly rightward and the other moves slightly leftward along the real axis, thus doubling the density of points. (This behavior of the continuum eigenvalues is in exact analogy to the motion of the roots of the famous Wilkinson polynomial [20].) For $L = 1000$, the continuum eigenvalues below $x = 28$ are extremely close to the real axis, but the positions of the complex localized states do not move, as we can see in figure 2.

Figure 3 is a logarithmic plot of the eigenvalues shown in figures 1 and 2. Observe that the critical point at $x = 28$ at which the continuum eigenvalues jump from being complex-conjugate pairs to real numbers remains fixed as $L$ is increased.

We emphasize that to distinguish between discrete and continuum eigenvalues we investigate the behavior of the associated eigenfunctions. Six possible behaviors of the eigenfunctions are displayed in figure 4. In general, the eigenfunctions of discrete eigenvalues decay smoothly to 0 at the endpoints of the interval but the eigenfunctions of continuum eigenvalues abruptly drop to 0 at one or both endpoints.
3. Eigenvalue behavior of $V_2(x)$

While the potential $V_1(x)$ decays exponentially for large $|x|$, the potential $V_2(x)$ decays algebraically like $|x|^{-3}$ for large $|x|$. Nevertheless, the spectral properties of $V_2(x)$ are strikingly similar to those of $V_1(x)$. For $V_2(x)$ the analog of figure 1 is figure 5. Again, we take the strength parameter $A_2$ to be 30 and observe one complex-conjugate pair of localized-state eigenvalues for $L = 10$ in panel (a) and two complex-conjugate pairs of localized-state eigenvalues for $L = 100$ in panel (b). The new pair of localized-state eigenvalues is uncovered as the continuum eigenvalues collapse toward the real axis.

If we increase $L$ to 1000, we observe in figure 6 that the localized-state eigenvalues do not move. However, the continuum eigenvalues lie very close to the real axis.

As with the Scarf-II potential $V_1(x)$, there is a transition in the continuum part of the spectrum that for this model occurs near 21. To examine this transition, we plot the eigenvalues on a logarithmic scale in figure 7. Observe that near 21 the continuum eigenvalues undergo an abrupt jump in their imaginary parts of 10 orders of magnitude.

4. Eigenvalue behavior of $V_3(x)$

The spectral structure associated with the potential $V_3(x)$ is qualitatively similar to that of $V_2(x)$. We take the strength parameter $A_3 = 30$ and plot the eigenvalues for $L = 10$ in figure 8, panel (a), and for $L = 100$ in figure 8, panel (b).

Observe that as $L$ is increased from 10 to 100, the discrete localized-state eigenvalues do not move but the continuum part of the spectrum rapidly approaches the real axis. In figure 9 we increase the value of $L$ to 1000. This higher-accuracy calculation shows that the continuum eigenvalues are extremely close to the real axis. However, there is still a critical point where the continuum eigenvalues go from having a small imaginary part to a vanishing imaginary part. This transition point is near 27 and the transition is indicated in figure 10 by a dashed line. Once again, the logarithmic plot shows that at the transition the imaginary parts of the continuum eigenvalues abruptly drop by about ten orders of magnitude.

5. Eigenvalue behavior of $V_4(x)$

The pattern of eigenvalues associated with $V_4(x)$ is similar to that of $V_1(x)$, $V_2(x)$, and $V_3(x)$. For this potential we take the strength parameter $A_4 = 3$ and plot the spectra for $L = 10$ and
Figure 10. Logarithmic plot of the data in figures 8 and 9. As in figures 3 and 7 we see once again that there is a transition point, in this case near 27, at which the imaginary parts of the continuum eigenvalues suddenly drop by about ten orders of magnitude. The location of this transition, which is indicated by a dashed line, appears to be independent of the choice of $L$.

Figure 11. Eigenvalues associated with $V_4(x)$ for $L = 10$ in panel (a) and for $L = 100$ in panel (b). The strength parameter $A_4 = 3$. One pair of localized-state energies (black circles) can be seen in panel (a) but a new pair becomes visible in panel (b).

$L = 100$ in figure 11 and for $L = 1000$ in figure 12. These figures show no qualitatively new features.

A logarithmic plot of the eigenvalue data in figures 11 and 12 is shown in figure 13. Once again we see a transition, in this case near 9.5, at which the continuum eigenvalues abruptly drop in magnitude by about ten orders of magnitude. The location of the transition is again insensitive to the value of $L$.

6. Eigenvalue behavior of $V_5(x)$

The most interesting and surprising results that we have obtained concern the eigenspectrum associated with $V_5(x)$. For this potential we take the strength parameter $A_5 = 10$. Because this is a long-range potential, it is not easy to obtain accurate and trustworthy numerical results, and we have had to do the $L = 1000$ calculation in quadruple precision (for all other results in this paper double precision is sufficient). In figure 14 we plot the eigenvalues for $L = 10$ in panel (a) and $L = 100$ in panel (b). There is one pair of localized-state eigenvalues in panel (a). When we increase the size of the interval, we see in panel (b) that the continuum spectrum has dropped much closer to the real axis and has uncovered three new pairs of localized-state eigenvalues.
Figure 12. Eigenvalues for $V_4(x)$ with $A_4 = 3$ for $L = 1000$. Note that the localized-state eigenvalues have not changed their positions from those in panel (b) of figure 11.

Figure 13. Logarithmic plot of the eigenvalue data in figures 11 and 12. The data in this figure, like the data in figures 3, 7, and 10, indicates that the sharp transition, which in this case is close to 9.5 is not sensitive to the value of $L$.

Figure 14 reveals two new effects that we have not observed in our studies of short-range potentials. First, the sequence of localized-state eigenvalues has turned around and is heading backward toward the origin. In figures 1, 5, 8, and 11 the real parts of the eigenvalues are increasing, not decreasing. Second, the transition in the continuum part of the spectrum at which the eigenvalues become real is no longer a fixed point on the real axis; rather, the transition point is moving up the real axis as $L$ increases. In panel (a) the transition is near 16 but in panel (b) it is near 28.

If we increase $L$ to 1000, figure 15 shows that there are now nine complex-conjugate pairs of localized-state eigenvalues (which are not easy to see clearly). This sequence of localized-state eigenvalues tends toward the origin. To observe the localized-state eigenvalues more clearly we replot in figure 16 the data in figure 15 on a log–log plot. This plot shows that the sequence of localized-state eigenvalues is becoming linear.

To observe the transition points in the continuum part of the eigenspectrum, we have plotted the data in figures 14 and 15 on a logarithmic graph in figure 17. Note that the transition point in the continuum eigenvalues from complex to real is moving up the real axis; it is no longer fixed as it was for finite-range potentials. Observe that at the transition near 40 there is a drop
Figure 14. Eigenvalues associated with $V_5(x)$ with strength parameter $A_5 = 10$. In panel (a) $L = 10$; we observe one complex-conjugate pair of localized-state eigenvalues; in panel (b) $L = 100$ and we see three new pairs of complex localized-state eigenvalues. Unlike the results for short-range potentials, this figure shows that the sequence of localized-state eigenvalues is turning around and heading back toward the origin. Also, the transition points in the continuum part of the spectrum are not fixed but are moving up the real axis from about 16 in panel (a) to about 28 in panel (b).

Figure 15. Eigenvalues associated with $V_5(x)$ with strength parameter $A_5 = 10$. In this figure $L$ is increased from 100 in figure 14 (right panel) to 1000 and there are now nine complex pairs of localized-state energies (not easy to distinguish). The numerical calculations needed to produce this figure required quadruple precision.

of nearly 20 (and not 10) orders of magnitude. To see this effect requires quadruple (and not double) precision for our numerical calculations.

The most interesting aspect of the long-range potential $V_5(x)$ is that it appears to confine an infinite number of localized states and the complex localized-state energies appear to be approaching 0. To verify this we use Richardson extrapolation [20] to study the behavior of the sequence of localized-state energies.

Richardson extrapolation enables one to find the limit of the sequence $\{a_k\}$ as $k \to \infty$ if the limit is a finite number. Given such a sequence we can calculate more and more accurate Richardson extrapolants, which converge faster to the limiting value. The formulas for the first five Richardson extrapolants are given by

\[
R_k^{(1)} = (k + 1)a_{k+1} - ka_k,
\]

\[
R_k^{(2)} = \left[(k + 2)^2a_{k+2} - 2(k + 1)^2a_{k+1} + k^2a_k \right] / 2!,
\]

\[
R_k^{(3)} = \left[(k + 3)^3a_{k+3} - 3(k + 2)^3a_{k+2} + 3(k + 1)^3a_{k+1} - k^3a_k \right] / 3!.
\]
Figure 16. Plot of the eigenvalue data in figure 15 on a log–log graph. In this plot we can now easily see nine localized-state eigenvalues.

Figure 17. Logarithmic plot of the eigenvalue data in figures 14 and 15. Observe that the transition point in the continuum part of the spectrum moves up the real axis as $L$ increases from $L = 10$ to $L = 100$ to $L = 1000$.

\[ R^{(4)}_k = \frac{(k+4)^4 a_{k+4} - 4(k+3)^4 a_{k+3} + 6(k+2)^4 a_{k+2} - 4(k+1)^4 a_{k+1} + k^4 a_k}{4!} \]
\[ R^{(5)}_k = \frac{(k+5)^5 a_{k+5} - 5(k+4)^5 a_{k+4} + 10(k+3)^5 a_{k+3} - 10(k+2)^5 a_{k+2} + 5(k+1)^5 a_{k+1} + k^5 a_k}{5!} \]  

From our numerical analysis, we have determined that the $k$th localized-state energy $E_k$ has the asymptotic form

\[ E_k \sim \alpha k^{-2} \pm i\beta k^{-3} \quad (k \gg 1), \]  

where $\alpha$ and $\beta$ are real numbers. This shows that the localized-state eigenvalues associated with $V_5(x)$ share many of the quantitative features of the Balmer series for the hydrogen atom. As indicated in the tables 1 and 2, we have determined that the numerical value of $\alpha$ is about 25 and the numerical value of $\beta$ is about 61. To obtain these results we have multiplied the real part of $E_k$ by $k^2$ and the imaginary part of $E_k$ by $k^3$ and computed the first five Richardson extrapolations.
Table 1. Real parts of the first nine eigenvalues \( E_k (1 \leq k \leq 9) \) associated with \( V_5(x) \) and the first five Richardson extrapolants constructed from the sequence \( \{ k^2 \text{Re} E_k \} \). Evidently, the real parts of the eigenvalues vanish like \( \alpha k^{-2} \), where \( \alpha \) is roughly 25.

| \( k \) | \( \text{Re} E_k \) | \( k^2 \text{Re} E_k \) | \( R_k^{(1)} \) | \( R_k^{(2)} \) | \( R_k^{(3)} \) | \( R_k^{(4)} \) | \( R_k^{(5)} \) |
|---|---|---|---|---|---|---|---|
| 1 | 0.83298288 | 0.83298 | 10.2355 | 29.8431 | 23.8084 | 24.2927 | |
| 2 | 1.38356468 | 5.53426 | 21.1871 | 25.0154 | 24.2120 | 25.5106 | |
| 3 | 1.19465086 | 10.7319 | 25.1176 | 25.5541 | 24.8568 | 25.2049 | |
| 4 | 0.89645517 | 14.3433 | 25.7219 | 25.5541 | 24.8568 | 25.2049 | |
| 5 | 0.66476032 | 16.6190 | 25.6660 | 25.2553 | 25.0258 | 25.1199 | |
| 6 | 0.50352322 | 18.1268 | 25.5486 | 25.1692 | 25.0676 | — | |
| 7 | 0.39157331 | 19.1871 | 25.4538 | 25.1354 | — | — | |
| 8 | 0.31203794 | 19.9704 | 25.3830 | — | — | — | |
| 9 | 0.25397318 | 20.5718 | — | — | — | — | |

Table 2. Imaginary parts of the first nine eigenvalues \( E_k (1 \leq k \leq 9) \) associated with \( V_5(x) \) and the first five Richardson extrapolants constructed from the sequence \( \{ k^3 \text{Im} E_k \} \). The imaginary parts of the eigenvalues vanish like \( \beta k^{-3} \), where \( \beta \) is roughly 61.

| \( k \) | \( \text{Im} E_k \) | \( k^3 \text{Im} E_k \) | \( R_k^{(1)} \) | \( R_k^{(2)} \) | \( R_k^{(3)} \) | \( R_k^{(4)} \) | \( R_k^{(5)} \) |
|---|---|---|---|---|---|---|---|
| 1 | 3.90859038 | 3.90859 | 29.8484 | 63.7004 | 62.5280 | 53.5920 | 61.0166 |
| 2 | 2.10981263 | 16.8785 | 52.4164 | 62.8211 | 55.3792 | 59.7791 | 62.5903 |
| 3 | 1.06386938 | 28.7245 | 57.6188 | 58.3560 | 58.3125 | 61.7871 | 61.3005 |
| 4 | 0.56168819 | 35.9480 | 57.9136 | 58.3342 | 60.2980 | 61.4830 | 60.9267 |
| 5 | 0.32272930 | 40.3412 | 58.0538 | 59.1758 | 60.8905 | 61.1739 | — |
| 6 | 0.20043182 | 43.2933 | 58.3744 | 59.8188 | 61.0165 | — | — |
| 7 | 0.13250064 | 45.4477 | 58.7355 | 60.2180 | — | — | — |
| 8 | 0.09200917 | 47.1087 | 59.0650 | — | — | — | — |
| 9 | 0.06644330 | 48.4372 | — | — | — | — | — |

7. Conclusions

In this paper we have studied numerically the five \( \mathcal{PT} \)-symmetric potentials in (6) that have continuous spectra. Each of these potentials is pure imaginary and vanishes as \( |x| \to \infty \). The interesting feature of these potentials is that even though they vanish at \( \pm \infty \), they still confine localized states. Of course, an imaginary potential can confine localized states. For example, the \( ix^3 \) potential has an infinite number of localized states [1]. However, this potential becomes stronger as \( |x| \to \infty \). It is interesting that even though the potentials that we have studied here decay and vanish as \( |x| \to \infty \), they still confine localized states. Even more remarkable is the fact that the potential \( V_5(x) \), which decays very slowly as \( |x| = \infty \), binds an infinite number of localized states and that the sequence of localized-state energies asymptotically approaches the Balmer series for the hydrogen atom. For large \( |x| \) this potential vanishes like \( x^{-1} \), so its behavior is like that of the Coulomb potential. However this potential is nonsingular; it does not have a singularity at \( x = 0 \).

We emphasize that the numerical analysis done in this paper has been restricted to the real-\( x \) axis. We have not examined the Schrödinger equation in the complex plane. Indeed, two of the potentials we have examined, \( V_3(x) \) and \( V_4(x) \), cannot be analytically continued into the complex plane and the other three potentials have singularities in the complex-\( x \) plane.
In previous studies of $\mathcal{PT}$-symmetric Hamiltonians, the complex plane has played a crucial role. Indeed, the boundary conditions on the Schrödinger equation (1) are imposed in Stokes sectors. If we let $\varepsilon$ approach $−3$ in order to study a $\mathcal{PT}$-symmetric version of the Coulomb potential, the integration path encircles the origin many times and terminates on different sheets in a Riemann surface [18] and we obtain a completely different spectrum from the regulated Coulomb potential $V_5(x)$. Thus, it is particularly surprising to us that the discrete spectrum in both cases is asymptotic to the Balmer series.

Acknowledgments

CMB thanks the Alexander von Humboldt Foundation for partial financial support.

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