

**\mathcal{PT} -symmetric Hamiltonian
systems and Painlevé equations**

Alexander van Spaendonck

Supervisors: Daniël Boer & Holger Waalkens
Bachelor Thesis
University of Groningen
2017

Abstract

This paper explores the quantum mechanics involving \mathcal{PT} -symmetric Hamiltonians and an application of it concerning Painlevé equations. It shows that under an additional condition these Hamiltonians have real eigenvalues and unitary time-evolution, just like regular Hermitian Hamiltonians. Using a WKB approximation we compute the energy spectrum of a class of \mathcal{PT} -symmetric Hamiltonians that is of the form $H = p^2 + a(ix)^N$. Next to that we investigate special solutions of the first, second and fourth Painlevé equation using a method from Carl M. Bender. It involves rewriting these equations to potentially \mathcal{PT} -symmetric Hamiltonians and calculating their energies. From these energies we find the relation that predicts the critical values corresponding to these special solutions. The method is very accurate and the predicted critical values of our resulting relation converge very quickly to the exact values.

Contents

Abstract	3
1 Introduction	7
2 \mathcal{PT}-Symmetric Quantum Theory	9
2.1 Symmetries and Hermiticity	9
2.2 Real energy levels	11
2.3 Unitary time-evolution	14
2.4 WKB approximation	14
3 Separatrix solutions of Painlevé equations	17
3.1 Introduction to Painlevé equations	17
3.2 Painlevé I	18
3.2.1 Behaviour of the solutions	18
3.2.2 Calculating the eigenvalues	20
3.3 Painlevé II	21
3.3.1 Behaviour of the solutions	21
3.3.2 Calculating the eigenvalues	22
3.4 Painlevé IV	23
3.4.1 Behaviour of solutions	23
3.4.2 Calculating the eigenvalues	24
3.5 Discussion of the results	25
4 Conclusion	27
Bibliography	29

Chapter 1

Introduction

In conventional quantum mechanics observables like the Hamiltonian are always Hermitian, because the hermiticity guarantees real expectation values and a unitary time-evolution. But in 1998 Carl. M. Bender published together with his former grad student Stefan Boettcher a paper [1] on Hamiltonians that were not Hermitian, but \mathcal{PT} -symmetric. Bender calculated the periodic orbits of particles under this Hamiltonian and even numerically computed the energy levels. This spectrum appeared to be real and so Bender continued his investigation of \mathcal{PT} -symmetric Hamiltonians to what there was more to see. Now, 19 years later, \mathcal{PT} -symmetric quantum mechanics has become a field on its own with over two thousand papers published. The subject has grown from a mathematical curiosity to a powerful theory with many applications.

The question that naturally arises is whether such Hamiltonians can be useful and if so why do we normally only restrict ourselves to Hermitian ones? For the physics part of this thesis we want to see what changes if we swap the condition of Hermiticity of a Hamiltonian with the condition of \mathcal{PT} -symmetry. Does such a system still work and what are the differences we our Hermitian one. We will review some basics and then investigate these new Hamiltonians.

Now one might also wonder if there is any need for these 'new' Hamiltonians. Are there any physical or mathematical applications where such a system would be helpful? For the mathematics part of this thesis we will examine separatrix solutions of some Painlevé equations using our knowledge of \mathcal{PT} -symmetric Hamiltonians. We will see that our ability to calculate the energies of such a \mathcal{PT} -symmetric system, will aid us in finding these separatrices.

Chapter 2

\mathcal{PT} -Symmetric Quantum Theory

2.1 Symmetries and Hermiticity

In regular quantum mechanics all observables including the Hamiltonian are Hermitian. The Hermiticity guarantees a number of features that are essential for a useful quantum theory. First of all it guarantees that the eigenvalues of an observable are real, and so in the case of a Hamiltonian it yields real energy levels. Secondly, the Hamiltonian also dictates the time evolution of the states and assures that it is unitary: this implies that the probability of a state will be conserved over time.

Is Hermiticity however absolutely necessary? No it is not. As it appears, one can construct Hamiltonians that despite being non-Hermitian will still produce real and positive energy levels and have a unitary time-evolution. These Hamiltonians share the characteristic of being ' \mathcal{PT} -symmetric'. Some examples will be discussed and more importantly this part of the thesis aims to see whether a viable quantum theory can be build around \mathcal{PT} -symmetric Hamiltonians. As mentioned before, there are a number of sought-after properties that the new Hamiltonian must guarantee, but before getting into that, we first look at what it means for a Hamiltonian to be \mathcal{PT} -symmetric?

Before answering that question we will briefly mention some essential definitions and characteristics from quantum mechanics. In a quantum theory states live in a space \mathcal{H} that is a *Hilbert space*. It consists of all square-integrable functions, that is all $\psi(x)$ for which:

$$\int_a^b |\psi(x)|^2 dx < \infty. \quad (2.1)$$

This space is endowed with the positive-definite inner product $\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ defined as

$$\langle \phi | \psi \rangle = \int_a^b \phi^* \cdot \psi dx, \quad (2.2)$$

and all operators act as linear transformations within our Hilbert space \mathcal{H} . Our states can also be represented by vectors in a complex vectorspace. In that case the innerproduct of two states is simply the dot product with the complex conjugate: $\langle \phi | \psi \rangle = \phi^* \cdot \psi$. An operator A will always have a *Hermitian adjoint* A^\dagger that is defined by

$$\langle A\phi, \psi \rangle = \langle \phi, A^\dagger\psi \rangle \quad (2.3)$$

If we have the equality $A^\dagger = A$ then we say A is Hermitian.

A Hamiltonian will be symmetric under a transformation X if the operator X commutes with the Hamiltonian: $[H, X] = 0$. This can easily be seen if one looks at the corresponding eigenstates of the Hamiltonian. Let $|\psi\rangle$ be an eigenstate of H and let X be a time-independent operator that transforms our state $|\psi\rangle$ like $|\psi'\rangle = X|\psi\rangle$. Now the Schrödinger equation for the new state $|\psi'\rangle$ can be written as

$$i\hbar \frac{d}{dt} |\psi'\rangle = i\hbar \frac{d}{dt} X|\psi\rangle = XH|\psi\rangle = XHX^{-1}|\psi'\rangle \equiv H'|\psi'\rangle \quad (2.4)$$

So $H' = XHX^{-1}$ is the corresponding Hamiltonian of the new state. For the transformed system to be equivalent to the old one H' must be equal to H and so writing $H = XHX^{-1}$ implies $[H, X] = 0$. The Hamiltonians that this thesis considers will therefore all commute with the \mathcal{PT} operator.

This operator is the combination of parity transformation (\mathcal{P}) and time-reversal (\mathcal{T}). The first one mirrors the spatial coordinates ($x \mapsto -x$) and the second one, as the name suggests, reverses time ($t \mapsto -t$). Both \mathcal{P} and \mathcal{T} therefore also map the momentum p to $-p$. Using the commutation relation $[x, p]$ we observe another property of the time-reversal operator:

$$\mathcal{T}[x, p]\mathcal{T}^{-1} = \mathcal{T}xp\mathcal{T}^{-1} - \mathcal{T}px\mathcal{T}^{-1} = x(-p) - (-p)x = [p, x] = -i\hbar. \quad (2.5)$$

Because $[x, p] = i\hbar$ our time-reversal operation \mathcal{T} must transform $i \rightarrow -i$ such that $\mathcal{T}i\hbar\mathcal{T}^{-1} = -i\hbar$. We say that \mathcal{T} is an 'antiunitary operator': a bijective map on our Hilbert space \mathcal{H} such that

$$\langle \mathcal{T}\psi, \mathcal{T}\phi \rangle = \langle \psi, \phi \rangle^*, \quad (2.6)$$

for all $\psi, \phi \in \mathcal{H}$. An example of a \mathcal{PT} -symmetric Hamiltonian is given in [2]:

$$H_1 = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix}, \quad (2.7)$$

where r, s and θ are real. Here states live in the complex vector space \mathbb{C}^2 and this Hamiltonian is not Hermitian but does commute with the \mathcal{PT} operator. To see this note that $\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ in this space and it can be checked that H_1 commutes with \mathcal{PT} . An example of a Hermitian Hamiltonian that is not \mathcal{PT} -symmetric is:

$$H_2 = \begin{pmatrix} s & a + bi \\ a - bi & t \end{pmatrix}, \quad (2.8)$$

where r, s, a and b are real and $s \neq t$. If we would set t equal to s we would have a Hamiltonian that is both Hermitian and \mathcal{PT} -symmetric. So in a nutshell we can draw a Venn diagram like in figure 2.1. For this thesis to be non-trivial we will look at Hamiltonians that are in section 2 of that figure.

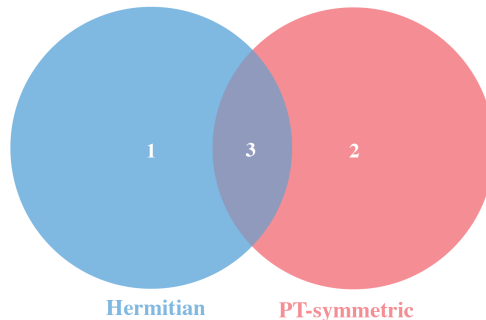


Figure 2.1: Hamiltonians can be Hermitian, \mathcal{PT} -symmetric, both or neither one of them. H_1 corresponds with **1** and H_2 with **2**. A real symmetric Hamiltonian would be an example of **3**.

Another interesting kind of \mathcal{PT} -symmetric Hamiltonians can be constructed by looking at what the effect is of the \mathcal{PT} operator. Momentum is invariant but the spatial coordinate x is not. However the complex quantity ix is invariant and so we can construct a Hamiltonian

$$H = p^2 - (ix)^N, \quad (2.9)$$

which is \mathcal{PT} -symmetric for all $N \in \mathbb{N}$ (and as we will see later for $N \in \mathbb{R}$).

Let us briefly review why Hermitian quantum mechanics work so very well. Recall that our states live in a Hilbert space endowed with a positive-definite inner product as defined in (2.2) and so the inner product of a function with itself is always greater than zero, unless the function is zero. A Hermitian operator A has $A^\dagger = A$ and (2.3) which implies

$$\langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle. \quad (2.10)$$

This mathematically nice property brings a few small benefits with itself. Suppose we have the eigenvalue a corresponding to our observable A for $A\psi = a\psi$. Then note that

$$\langle A\rangle = \langle A\psi|\psi\rangle = a^*\langle\psi|\psi\rangle, \quad (2.11)$$

but because A is Hermitian this is equal to

$$\langle A\rangle = \langle\psi|A\psi\rangle = a\langle\psi|\psi\rangle. \quad (2.12)$$

Unless ψ itself is zero we conclude $a = a^*$ which means our Hermitian operator A has real eigenvalues. Since the Hamiltonian itself is also a Hermitian operator this implies real energy levels as we would like to have.

In quantum mechanics we often have a time-independent potential $V(x)$ that allows for separable solutions of the Schrödinger equation that have the form of $\psi(x, t) = \psi_0(x)e^{-iHt}$. When we want to check the time-evolution of the system for a Hermitian Hamiltonian we see that the norm evolves like:

$$\begin{aligned} \frac{d}{dt}\langle\psi(x, t)|\psi(x, t)\rangle &= \left\langle\frac{d}{dt}\psi(x, t)|\psi(x, t)\right\rangle + \left\langle\psi(x, t)|\frac{d}{dt}\psi(x, t)\right\rangle \\ &= \langle iH\psi(x, t)|\psi(x, t)\rangle + \langle\psi(x, t)|-iH\psi(x, t)\rangle \\ &= i\langle H\psi(x, t)|\psi(x, t)\rangle - i\langle H\psi(x, t)|\psi(x, t)\rangle \\ &= 0. \end{aligned} \quad (2.13)$$

So the norm of our states is conserved.

There can be a dispute about what qualifies as a 'viable' quantum theory, because there seem to be applications in physics where for instance complex eigenvalues are very common. For this thesis however we will look for the following two properties

1. Real energy levels
2. Unitary time-evolution

Both of them are guaranteed by Hermiticity as we just saw, but what happens if we now drop this condition and our Hamiltonian is no longer Hermitian?

2.2 Real energy levels

Now let us make the switch to \mathcal{PT} -symmetric Hamiltonians and start with the energy levels. One very important demand we just stated is that our \mathcal{PT} -symmetric Hamiltonian produces energy levels that are real. The trick we performed earlier does no longer work here, but there is a different approach that will work. Suppose we have a \mathcal{PT} -symmetric Hamiltonian, then we can easily prove the existence of real energy levels under one additional condition:

The eigenstates of the Hamiltonian H are simultaneously eigenstates of the \mathcal{PT} operator

Given this extra condition it can easily be proven that the energy eigenvalues of the \mathcal{PT} -symmetric states are real.

Lemma 1. *If a \mathcal{PT} -symmetric Hamiltonian H has the same eigenstates as the \mathcal{PT} operator, then the eigenvalues of that Hamiltonian are real.*

Proof. Assume H is a \mathcal{PT} -symmetric Hamiltonian that shares its eigenstates with the \mathcal{PT} operator. Let ψ be one of these eigenstates, then we have the following eigenvalue equations

$$H\psi = E\psi \quad \text{and} \quad \mathcal{PT}\psi = \lambda\psi, \quad (2.14)$$

Where λ is the eigenvalue of ψ corresponding to our \mathcal{PT} operator. Multiplying the second identity with \mathcal{PT} from the left u yields

$$(\mathcal{PT})^2\psi = \mathcal{PT}\mathcal{PT}\psi = \mathcal{PT}\lambda\psi = \lambda^*\mathcal{PT}\psi = \lambda^*\lambda\psi. \quad (2.15)$$

As mentioned before the \mathcal{PT} operator is antilinear, which is the reason why this complex conjugate of λ emerges. Now $(\mathcal{PT})^2$ must equal unity because $\mathcal{P}^2 = \mathcal{T}^2 = 1$, and so $\lambda^*\lambda = 1$ which leads to the solution $\lambda = e^{i\alpha}$, where α can be any real number. If we replace our eigenstate ψ by a new eigenstate $\psi' = e^{i\alpha/2}\psi$ we get

$$\mathcal{PT}\psi' = \mathcal{PT}e^{i\alpha/2}\psi = e^{-i\alpha/2}\mathcal{PT}\psi = e^{i\alpha/2} = \psi' \quad (2.16)$$

Let us now replace our state ψ with ψ' and the second equation of (2.15) becomes $\mathcal{PT}\psi = \psi$ (we relabeled our new state back to ψ for notational convenience). If we now multiply the first equation with \mathcal{PT} and use the commutation relation $[H, \mathcal{PT}] = 0$ the left-hand side becomes

$$\mathcal{PT}H\psi = H\mathcal{PT}\psi = H\psi = E\psi, \quad (2.17)$$

while the right-hand side becomes

$$\mathcal{PT}E\psi = E^*\mathcal{PT}\psi = E^*\psi. \quad (2.18)$$

This means either ψ is zero (trivial) or $E^* = E$ which implies real energy levels. □

Given this lemma the real problem lies in showing that the Hamiltonian and \mathcal{PT} operator share eigenstates. Unfortunately, this condition is not always satisfied, and so we distinguish two cases:

- 1 *Unbroken* or *exact* \mathcal{PT} -symmetry; all eigenstates of H are simultaneously eigenstates of PT .
- 2 *Broken* \mathcal{PT} -symmetry; not all eigenstates of H are necessarily also eigenstates of PT .

One might think that PT and H commuting would already imply that all their eigenstate are joint and that this is a trivial condition. In conventional quantum mechanics we would have had Hermitian (linear) operators X and H such that $H(X\psi) = XH\psi = XE\psi = E(X\psi)$ which would imply if

1. **E non-degenerate:** E has only one eigenvector so $X\psi$ must be a scalar multiple of ψ . That means $X\psi = \lambda\psi$.
2. **E degenerate:** There are multiple eigenvectors corresponding to E spanning a subspace. In this subspace X is still Hermitian and therefore diagonalizable which enables us to find eigenvectors of X that span the subspace corresponding with E . These eigenvectors of X are also eigenvectors of H with energy E .

In both cases we conclude that if X and H commute we have shared eigenstates. But in our \mathcal{PT} -symmetric system this no longer works because the operator PT is anti-linear¹. So we are forced to make a distinction between broken and unbroken symmetry. To give an example that illustrates this consider the Hamiltonian of (2.9) and its energy levels as seen in figure 2.2.

For $N = 2$ we have the familiar harmonic oscillator. If $N \geq 2$ then there are infinitely many real energy levels as was calculated by Bender. It is this region where the Hamiltonian shares all its eigenstates with the \mathcal{PT} operator and which we call unbroken \mathcal{PT} -symmetry. For $1 < N < 2$ this is no longer the case and we have only finitely many real energy eigenvalues together with infinitely many complex ones as was established in [2], which is broken \mathcal{PT} -symmetry. As N drops below 2 more and more real eigenvalues disappear and become pairs of complex eigenvalues. When N is almost 1 its groundstate energy starts to diverge and for

¹Note that linearity is necessary for this argument, but not sufficient. In case of degenerate states we also need to make sure we can diagonalize X , which can for instance be done by imposing Hermiticity

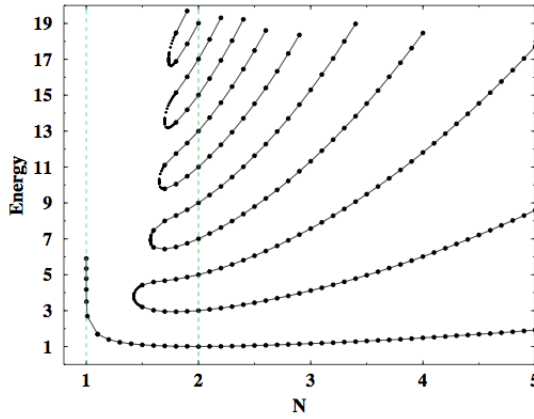


Figure 2.2: The energy levels of (2.9) as function of N calculated by Bender in [2]. For $N \geq 2$ there are infinitely many real eigenvalues, but for $N < 2$ there are only finitely many real ones together with infinitely many complex ones. *Source: [2], page 6*

$N \leq 1$ there are no more real eigenvalues. Note that the figure allows non-integer values of N to have real energies.

Interestingly enough figure 2.2 also seems to implicate real energy levels for $H = p^2 - x^4$ which corresponds with $N = 4$. One might wonder how this is possible for a potential that is not bound below. This can be explained by looking at the motion of a particle described by this Hamiltonian. You would expect the particle to run off to \pm infinity and that is to some extent correct, namely when you start on the real axis. But with a $(ix)^N$ potential we are forced to extend our particles motion to the complex plane. Why do we need to consider the complex plane? Recall that normally we have a particle trapped in a potential well and that the turning points of that potential are those points where the energy E and the potential V are equal. The particle then classically seems to oscillate between those two points. The turning points of our \mathcal{PT} -symmetric potential lie no longer necessarily on the real axis. Instead they are placed in the complex plane and so a particle obeying our $N = 4$ Hamiltonian will have a periodic trajectory, only it will lie in the complex plane as figure 2.3 shows.

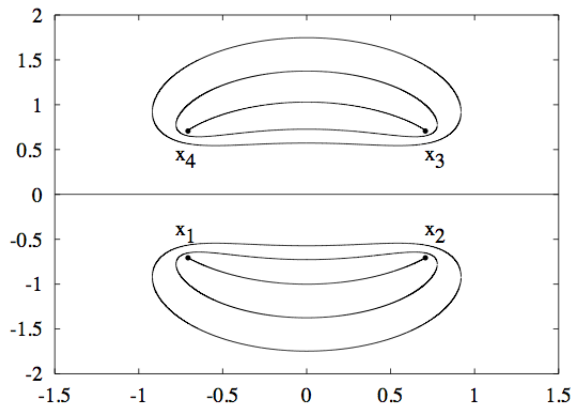


Figure 2.3: Trajectory of a particle in the complex plane described by $H = p^2 - x^4$ with $E = 1$. There are two periodic orbits that oscillate between two of the four turning points. Then there are also closed orbits possible that enclose a pair of turning points. Note that all these orbits have the same period [2]. *Source: [1], page 6*

In general it remains difficult to know beforehand if our Hamiltonian shares its eigenstates with the \mathcal{PT} operator and therefore whether we have real energies. Throughout the years many

physicists however constructed tools to prove these real energies of \mathcal{PT} -symmetric Hamiltonians. For instance in [3] Zafar Ahmed analyzed Hamiltonians of the form $H = \frac{(p+i\beta\nu(x))^2}{2m} + V(x)$ where $\nu(x)$ is an arbitrary function and was able to state under which conditions this Hamiltonian has a real spectrum while being \mathcal{PT} -symmetric. For our Hamiltonian from (2.9) it was proven in [4] by P. Dorey, C. Cunning and R. Tateo in 2001 that its energy levels for $N \geq 2$ are indeed real.

2.3 Unitary time-evolution

Lemma 2. *A Hamiltonian H that has unbroken \mathcal{PT} -symmetry will have unitary time-evolution. That is if $\psi(t)$ is a state obeying the Schrödinger equation for H , then $\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = 0$.*

Proof. Let $\psi(t) = \sum_n c_n(t)\psi_n$ where ψ_n are all eigenstates of the (unbroken) \mathcal{PT} -symmetric Hamiltonian H with energy levels E_n such that $H\psi_n = E_n\psi_n$. Unbroken \mathcal{PT} -symmetry guarantees (by lemma 1) that these energy eigenstates E_n are real. Along that Schrödinger tells us that

$$i\hbar\frac{d}{dt}\psi = H\psi,$$

Now we calculate the time evolution scaled with a term $i\hbar$ (to make the math a bit nicer):

$$i\hbar\frac{d}{dt}\langle\psi|\psi\rangle = \langle -i\hbar\frac{d}{dt}\psi|\psi\rangle + \langle\psi|i\hbar\frac{d}{dt}\psi\rangle \quad (2.19)$$

Let us work out the first term of the right-hand side:

$$\begin{aligned} \langle -i\hbar\frac{d}{dt}\psi|\psi\rangle &= \sum_n \sum_m \langle -i\hbar\frac{d}{dt}(c_n\psi_n)|c_m\psi_m\rangle = \sum_n \sum_m \langle -c_n H\psi_n|c_m\psi_m\rangle \\ &= \sum_n \sum_m E_n \langle -c_n\psi_n|c_m\psi_m\rangle = \sum_n -E_n|c_n|^2 \end{aligned} \quad (2.20)$$

In the same way we get for the second term $\sum_n E_n|c_n|^2$ and so together they eliminate each other:

$$i\hbar\frac{d}{dt}\langle\psi|\psi\rangle = \sum_n E_n|c_n|^2 - \sum_n E_n|c_n|^2 = 0 \quad (2.21)$$

This implies $\frac{d}{dt}\langle\psi|\psi\rangle = 0$, so our time-evolution is unitary. □

But what now if we have broken symmetry? Computing the time-derivative of a states norm as we just did goes more or less the same, but the difference is that our energies are no longer necessarily real. For the same eigenvalue equations with $E_n = a_n + b_n i$ the result looks like this:

$$i\hbar\frac{d}{dt}\langle\psi|\psi\rangle = \sum_n (E_n - E_n^*)|c_n|^2 = \sum_n 2b_n i|c_n|^2. \quad (2.22)$$

Again this shows that for the unbroken case we get zero because all b_n 's are zero, but with a broken symmetry our norm is no longer conserved.

2.4 WKB approximation

The last section of this chapter is concerned with actually calculating the energy eigenvalues of a \mathcal{PT} -symmetric Hamiltonian. Knowing that the energy eigenvalues of our Hamiltonian are real and positive, we now must find a way to calculate them. In this section we will find these energies for our \mathcal{PT} -symmetric Hamiltonian from (2.9). The computations are only complicated by the fact that our Hamiltonian has a complex potential. It is however possible using the well-known WKB method. This method can be very helpful in computing the energy levels of

complicated potentials. The technique uses a clever approximation in the classical region of the potential well, that is the region where $E > V$. If we assume the potential is flat in this region we would get solutions like[5]:

$$\psi(x) = Ae^{\pm ikx}, \quad (2.23)$$

where $k = \sqrt{2m(E - V)}/\hbar$. Unfortunately our 'complicated' potential $V(x)$ is not flat in this region, but if it changes very slowly compared with the particles wavelength, then we can say it is practically flat. This approximation works best if n is large such that the amplitude of the particles wave function is minimally influenced by changes in $V(x)$.

To increase the usefulness of our calculations, the approximation will be applied to a more general case of our Hamiltonian: $H = p^2 + a(ix)^N$, where a is an arbitrary constant. The approximation leads to the following statement [5]:

$$(n + \frac{1}{2})\pi = \int_{x_1}^{x_2} \sqrt{E_n + a(ix)^N} dx, \quad (2.24)$$

Where x_1 and x_2 are the two turning points beaor solutions to the equation $E - a(ix)^N = 0$. For a real potential $V(x)$ these would be the two edges of the classically allowed region, the space in which $E > V$. For this potential we will see that these two points lie in the complex plane which makes the problem a bit more difficult. Solving the equation for x gives the two possible points

$$x_1 = \left(\frac{E}{a}\right)^{\frac{1}{N}} e^{i\pi(\frac{3}{2} - \frac{1}{N})} \quad \text{and} \quad x_2 = \left(\frac{E}{a}\right)^{\frac{1}{N}} e^{i\pi(\frac{3}{2} + \frac{1}{N})}. \quad (2.25)$$

They lie on a circle with radius $(E/a)^{\frac{1}{N}}$ in the complex plane, both displaced an equal distance from the imaginary axis. The integral will be calculated over a contour going in a straight line from x_1 to the 0 and then in a straight line from 0 to x_2 to assure that it remains real. First we split the integral into two parts:

$$\int_{x_1}^{x_2} \sqrt{E_n + a(ix)^N} dx = - \int_0^{x_1} \sqrt{E_n + a(ix)^N} dx + \int_0^{x_2} \sqrt{E_n + a(ix)^N} dx. \quad (2.26)$$

Applying the substitution $x = x_1 s$ to the first term produces the following

$$- \int_0^1 \sqrt{E_n + a(ix_1 s)^N} (x_1 ds) = -x_1 \int_0^1 \sqrt{E_n + (-E_n) s^N} ds = -x_1 E_n^{\frac{1}{2}} \int_0^1 \sqrt{1 - s^N} ds. \quad (2.27)$$

In the exact same manner the second term of (2.26) can be rewritten to $x_2 E_n^{\frac{1}{2}} \int_0^1 \sqrt{1 - s^N} ds$ and adding these together results in

$$(x_2 - x_1) E_n^{\frac{1}{2}} \int_0^1 \sqrt{1 - s^N} ds. \quad (2.28)$$

Both points share as we know the same amplitude of $(E/a)^{1/N}$ but have a different phase. Writing the phase part in sine and cosine form will give $-i \cos(\pi/N) + \sin(\pi/N) - (-i) \cos(-\pi/N) - \sin(-\pi/N) = 2 \sin(\pi/N)$ and so we end up with

$$a^{\frac{1}{N}} E^{\frac{1}{2} + \frac{1}{N}} 2 \sin\left(\frac{\pi}{N}\right) \int_0^1 \sqrt{1 - s^N} ds \quad (2.29)$$

Now the problem is reduced to an integral over the real axis from 0 to 1. Despite looking so nice, it is not easily integrated, but luckily $\sqrt{1 - s^N}$ can be written as a special function:

$$\int_0^1 \sqrt{1 - s^N} ds = \int_0^1 {}_2F_1\left(-\frac{1}{2}, 1, 1, s^N\right) ds, \quad (2.30)$$

where ${}_2F_1(a, b, c, x)$ is the 'hypergeometric function'. Using Wolfram Alpha [6] the antiderivative

of this function is found to be:

$$\int {}_2F_1\left(-\frac{1}{2}, 1, 1, s^N\right) ds = \frac{sN \cdot {}_2F_1\left(\frac{1}{2}, \frac{1}{N}, 1 + \frac{1}{N}, 1\right) + 2s\sqrt{1-s^N}}{N+2} \quad (2.31)$$

Filling in the values of $s = 0$ and $s = 1$ to solve the integral leads to

$$\frac{N}{N+2} {}_2F_1\left(\frac{1}{2}, \frac{1}{N}, 1 + \frac{1}{N}, 1\right) - 0 = \frac{N}{N+2} \cdot \frac{\sqrt{\pi}\Gamma\left(1 + \frac{1}{n}\right)}{\Gamma\left(\frac{1}{2} + \frac{1}{n}\right)}. \quad (2.32)$$

Then finally using the identity $\Gamma(x+1) = x\Gamma(x)$ for the denominator yields

$$\frac{N}{N+2} \cdot \frac{N+2}{2N} \cdot \frac{\sqrt{\pi}\Gamma\left(1 + \frac{1}{n}\right)}{\Gamma\left(\frac{3}{2} + \frac{1}{n}\right)} = \frac{\sqrt{\pi}\Gamma\left(1 + \frac{1}{n}\right)}{2\Gamma\left(\frac{3}{2} + \frac{1}{n}\right)} \quad (2.33)$$

This result can be inserted into (2.29) which is the left-hand side of (2.24). Solving it for E_n gives the (approximate) energy levels:

$$E_n = a^{\frac{2}{N+2}} \left(\frac{(n+1/2)\sqrt{\pi}\Gamma(3/2+1/N)}{\sin(\pi/N)\Gamma(1+1/N)} \right)^{\frac{2N}{N+2}}. \quad (2.34)$$

If we encounter a Hamiltonian like this with a constant c in front of the p^2 term, we will always be able to scale it back to $\frac{1}{c}H = p^2 + \frac{a}{c}(ix)^N$ and solve it with (2.34). Now to check the validity of this result let us use it to compute the energies of the harmonic oscillator. For the quantum harmonic oscillator $H = \frac{1}{2}p^2 + \frac{1}{2}x^2$ we know from [5] that the energy $E_n = n + \frac{1}{2}$. So for a Hamiltonian $H = p^2 + x^2$, which corresponds to our $N = 2$ potential we expect an energy of $E_n = 2n + 1$. Filling in $N = 2$ yields

$$E_n = 1 \cdot \frac{(n+1/2)\sqrt{\pi}\Gamma(2)}{\sin(\pi/2)\Gamma(3/2)} = 2n + 1, \quad (2.35)$$

which exactly matches our expectation.

Equation 2.9 is therefore a perfect example of how \mathcal{PT} symmetric Hamiltonians work. The condition of \mathcal{PT} -symmetry itself does not meet our demands, but if we look at a specific subset of these Hamiltonians for which we have unbroken symmetry, then we do get real eigenvalues and the desired unitary time-evolution. It is also possible as we just saw to compute these energy levels and in the next chapter we will see how this result can be used for a different problem.

Chapter 3

Separatrix solutions of Painlevé equations

3.1 Introduction to Painlevé equations

Differential equations appear everywhere when we try to describe real-world phenomena. From thermodynamics to quantum physics, differential equations play an important part in many physical theories. They are in a nutshell simply equations that relate functions to their own derivatives. Solutions to these differential equations can sometimes easily be calculated using analytical methods, but some are too complicated to solve exactly. In that case we are left with two options: Using a computer to solve them numerically or make an attempt at solving it analytically using some clever approximation. This part of the paper will be concerned with using such an analytical approximation to find a certain set of solutions. But before defining the problem, we first must briefly discuss a few properties of differential equations.

Often solutions of differential equations will have so-called 'singularities'. These are points of the solution that are ill-defined. These singularities can for instance be poles, points where the solution goes to infinity, but there are also other types of singularities. Solving differential equations often involves integration constants popping up, and these might have influence on where these singularities are. If a singularity is indeed influenced by such an integration constant we say that is a 'movable singularity'. Lazarus Immanuel Fuchs studied first-order differential equations with non-movable singularities [7] and showed they are all of the form

$$\frac{dy}{dt} = A(t) + B(t)y + C(t)y^2. \quad (3.1)$$

After that it was Paul Painlevé that started to look at second order differential equations. He examined those equations whose only movable singularities are poles, which is now known as the Painlevé property. He managed to collect 50 canonical second-order differential equations that satisfied this property and they are of the form

$$\frac{d^2y}{dt^2} = F\left(\frac{dy}{dt}, y, t\right). \quad (3.2)$$

Of those 50 equations, 44 could be simplified to known functions and so he ended up with six non-linear second-order differential equations that we now know as the Painlevé equations. Their solutions are called the Painlevé transcendents, because these solutions are transcendental functions; i.e., functions that cannot be written in terms of elementary functions.

In this second part of the thesis Painlevé equations I, II and IV will be studied and in particular their solution curves that either go through the origin ($y(0) = 0$) or whose slope when crossing the y-axis equals zero ($y'(0) = 0$). The parameters b and c will be used to denote $y'(0)$ and $y(0)$ respectively which will describe two distinct initial value problems for each of the three Painlevé equations:

$$\text{Painlevé I, II or IV}^1 \text{ with } y(0) = 0 \text{ and } y'(0) = b \quad (3.3)$$

$$\text{Painlevé I, II or IV with } y(0) = c \text{ and } y'(0) = 0 \quad (3.4)$$

When looking at these solutions sudden changes in their behaviour will be observed when the parameter crosses certain values. For parameters b and c these 'critical values' are called eigenvalues and will be denoted by b_n and c_n . Their corresponding solutions will be unstable separatrices; raising or lowering the parameter with an infinitesimal amount causes drastic changes in the solution curve and draws completely different graphs. Finding these eigenvalues will be the goal of this chapter and doing so will be possible in two different ways. One option is using a computer to numerically compute the solutions curves for several values of b (or c), plot them and try to narrow down the possible eigenvalues. One can however also find these values using an analytical procedure. Along the way certain approximations will be required, but the result is very accurate and even more compelling is the fact that our method will involve \mathcal{PT} -symmetric Hamiltonians. This second method was applied by Carl M. Bender in [8] to the first and second Painlevé equation and here we will try to do the same. Next to that the fourth Painlevé equation will also be tackled using this approach.

Using some basic calculus and a clever approximation the differential equations will be reduced to a (possibly \mathcal{PT} -symmetric) Hamiltonian of which the energy levels can be related to $y(0)$ and $y'(0)$. Using (2.34) these energy levels can then be computed and will enable us to find b_n or c_n . Bender also numerically established the asymptotic behaviour of these eigenvalues as n goes to infinity in [8]. This behaviour looks like

$$b_n \sim B \cdot n^x \quad \text{for } n \rightarrow \infty, \quad (3.5)$$

where x is a rational number. For all eigenvalues we strive to calculate these coefficients B , find the exponent x and check with Bender if they match his numerical result. We will also compare some numerically calculated eigenvalues with the ones that our analytical method predicts to get a feeling of how good this approximation really works.

3.2 Painlevé I

3.2.1 Behaviour of the solutions

Let us start by stating the first Painlevé equation and its initial conditions:

$$y''(t) = 6y(t)^2 + t \quad \text{where } y(0) = c \text{ and } y'(0) = b. \quad (3.6)$$

First note that there are two so-called 'asymptotic behaviours' that we can spot. These are the curves $-\sqrt{-t/6}$ and $+\sqrt{-t/6}$ as proposed in [9] that are only defined for $t \in (-\infty, 0]$. Before plotting the solutions we can show that former is a stable curve and the latter an unstable curve, that is they attract and repel the solutions respectively. To see this we examine points near these curves. If at some point $t < 0$ in time we are just slightly above the curve $\sqrt{-t/6}$, let us say a distance δ , then we assume $y = \sqrt{-t/6} + \delta$ and calculate y'' :

$$y'' = 6(\sqrt{-t/6} + \delta)^2 + t = 12\delta\sqrt{-t/6} + 6\delta^2 \approx 12\delta\sqrt{-t/6}. \quad (3.7)$$

If we assume $\delta \ll 1$ then we can drop the squared term. This shows us that if we are just above the curve ($\delta > 0$) the solution is pushed upward and when we are just beneath the curve ($\delta < 0$) then the solution is pushed downward. Therefore the $\sqrt{-t/6}$ repels solutions and with an equally simple trick one can show that the other asymptote $-\sqrt{-t/6}$ attracts solutions. Because the domain of these two curves is restricted to negative values of t we will examine solutions as $t \rightarrow -\infty$.

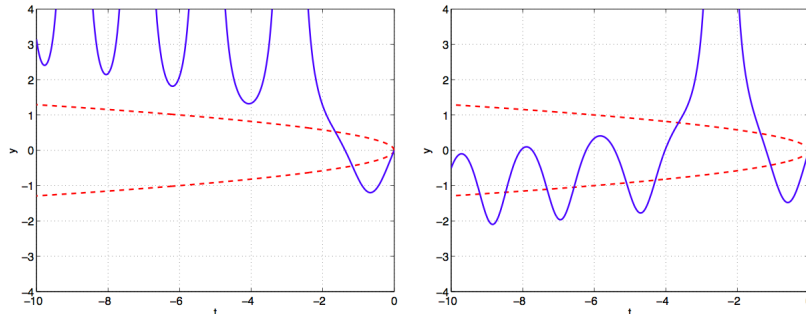


Figure 3.1: Solutions to Painlevé I with $y(0) = 0$ and $y'(0) = b$. On the **left** the solution with $b = 2.5040$ and on the **right** the solution with $b = 3.504$. *Source: [8]*

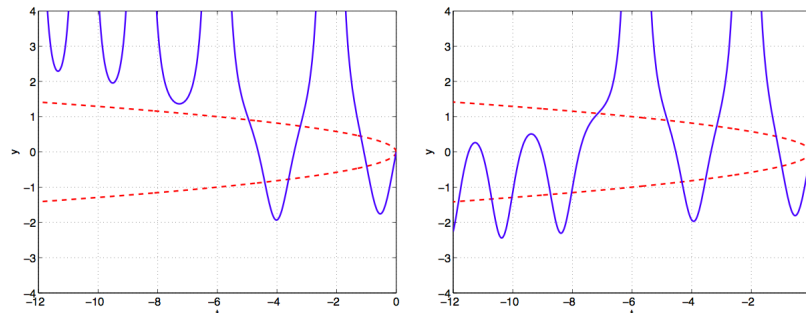


Figure 3.2: Solutions to Painlevé I with $y(0) = 0$ and $y'(0) = b$. On the **left** the solution with $b = 4.583$ and on the **right** the solution with $b = 4.783$. *Source: [8]*

When we look at the (numerically found) solutions that start at the origin with variable slope $y'(0) = b$ we observe extreme changes when the parameter b passes certain values. Figure 3.1 shows two of those solutions. When b equals 2.5040 the solution shows an endless sequence of poles. Every time it comes down the unstable curve $\sqrt{-t/6}$ seems to push our solution away. If we increase the parameter b we eventually cross the (found by Bender) critical value of 3.004 and observe completely different behaviour: After hitting a pole it comes down and starts to oscillate around the stable curve $-\sqrt{-t/6}$ while slowly decaying to it. Increasing b further will eventually make the curve jump back to an endless sequence of poles (see the left panel of figure 3.2), which it will continue to do until we once more pass a critical value for b (leading to the right panel of figure 3.2). Figures 3.1 and 3.2 show these types of behaviour and challenge us to find these critical values.

Before doing so we also want to examine solutions with $y(0) = c$ and a flat slope $y'(0) = 0$. These solutions seem to show very similar behaviour like we saw in figures 3.1 and 3.2. For these too we are interested in when exactly these solutions so abruptly change.

3.2.2 Calculating the eigenvalues

We start with rewriting the first Painlevé equation by multiplying both sides with $y'(t)$ and then integrating the whole thing from 0 to x which looks like

$$\int_0^x y'(t)y''(t)dt = 6 \int_0^x y(t)^2 y'(t)dt + \int_0^x ty'(t)dt. \quad (3.8)$$

The left-hand side is easily recognized as a known derivative of $\frac{1}{2}y'(t)^2$ which saves us from doing the integral. A similar trick can be done for the first term on the right-hand side yielding

$$\frac{1}{2}y'(t)^2|_0^x = 2y(t)^3|_0^x + \int_0^x ty'(t)dt. \quad (3.9)$$

The remaining term that still has an integral sign in front of it will be called $I(x)$ and after reordering we have

$$\frac{1}{2}y'(x)^2 - 2y(x)^3 = \frac{1}{2}y'(0)^2 - 2y(0)^3 + I(x). \quad (3.10)$$

This is the place where our approximation comes in. As argued in [8] the $I(x)$ term becomes very small compared to the left-hand side when we look for higher eigenvalues, or equivalently as $n \rightarrow \infty$. This only seems to apply when $y(x)$ is one of the solutions that corresponds to an eigenvalue. Now we can treat $y(x)$ as a one-dimensional variable of a Hamiltonian system where we set $m = 1$ and $\hbar = 1$ which looks like

$$H = \frac{1}{2}(y')^2 - 2y^3 = E_n, \quad (3.11)$$

with spectrum $E_n = \frac{1}{2}y'(0)^2 - 2y(0)^3$. The initial conditions imply that either $y(0)$ or $y'(0)$ was fixed, which means that if one calculates the energy levels of this Hamiltonian the other quantity can easily be computed. To do so the potential is rotated into the complex plane² (multiplied by $-i$) and after renaming some variables the following \mathcal{PT} -symmetric Hamiltonian emerges:

$$H = \frac{1}{2}p^2 + 2ix^3. \quad (3.12)$$

This is the 'cubic' ($N = 3$) \mathcal{PT} -symmetric Hamiltonian that is part of the class of Hamiltonians in (2.9). It is a very fortunate result because the energy levels have been proven to be real (for $N \geq 2$) and can even be calculated using our WKB calculation in (2.34). A small adjustment must be made, because the momentum term carries a factor $\frac{1}{2}$. This is solved by defining a new Hamiltonian $H' = 2H = p^2 + 4ix^3$ which is solved for $a = 4$ and $N = 3$ in (2.34)

$$E'_n = 4^{\frac{2}{5}} \left(\frac{(n+1/2)\sqrt{\pi}\Gamma(11/6)}{\frac{1}{2}\sqrt{3}\Gamma(4/3)} \right)^{6/5} \approx 4.3771 \cdot (n + \frac{1}{2})^{6/5}. \quad (3.13)$$

Our energy level $E'_n = 2E_n = y'(0)^2 - 4y(0)^3$ can now be used to find the eigenvalues b_n for a fixed $c = 0$ and eigenvalues c_n for a fixed $b = 0$. Rewriting this equality gives for $y(0) = 0$ and a variable slope

$$b_n = y'(0) = \sqrt{E'_n} \sim 2.092 \cdot n^{3/5} \quad \text{for } n \rightarrow \infty. \quad (3.14)$$

The " $+\frac{1}{2}$ " term is omitted because in the case of n becoming really large its contribution is insignificant. For a flat slope ($b = 0$) but a variable c we get

$$c_n = y(0) = \left(-\frac{1}{4}E'_n\right)^{1/3} \sim -1.030 \cdot n^{2/5} \quad \text{for } n \rightarrow \infty \quad (3.15)$$

²Doing this leaves E_n unchanged, see [8] and [10]

3.3 Painlevé II

3.3.1 Behaviour of the solutions

The second Painlevé equation is best known in the form³ of

$$y''(t) = 2y(t)^3 + ty(t) \quad \text{where } y(0) = c \text{ and } y'(0) = b. \quad (3.16)$$

For this equation we again plot solutions for $t \rightarrow -\infty$ and we can already spot a few curves that describe asymptotic behaviour. We can see that the t -axis is a stable asymptote and the curves $\pm\sqrt{-t/2}$ form unstable asymptotes. This was done in the same way as with Painlevé I, looking at solution in a δ -neighbourhood around these curves. Now plotting the solutions and tweaking the parameter b produces interesting graphs seen in figures 3.3 and 3.4. Again passing a certain eigenvalue will drastically change the behaviour of the solution. They seem to switch between covering endless poles to stable oscillations around the t -axis and back again which also confirms our assertion that the t -axis is a stable asymptote and the curves $\pm\sqrt{-t/2}$ are unstable.

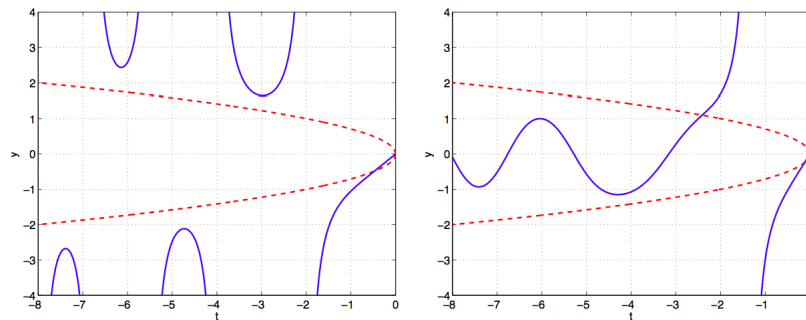


Figure 3.3: Solutions to Painlevé II with $y(0) = 0$ and $y'(0) = b$. On the **left** the solution with $b = 1.029$ and on the **right** the solution with $b = 2.029$. *Source: [8]*

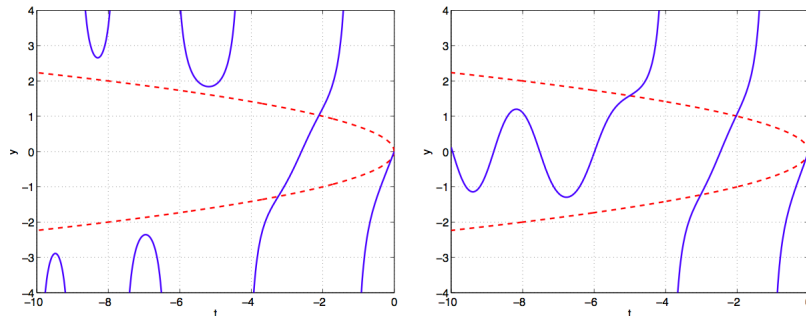


Figure 3.4: Solutions to Painlevé II with $y(0) = 0$ and $y'(0) = b$. On the **left** the solution with $b = 2.601$ and on the **right** the solution with $b = 2.801$. *Source: [8]*

³Wikipedia and other sources also add an arbitrary constant α at the end of the equation

3.3.2 Calculating the eigenvalues

Deriving the Hamiltonian that corresponds to the second Painlevé equation goes in a similar way as we did for the first painlevé equation. Multiply both sides with $y'(t)$ and integrate from 0 to x and we will get

$$\frac{1}{2}y'(t)^2 \Big|_0^x = \frac{1}{2}y(t)^4 \Big|_0^x + \int_0^x ty(t)y'(t)dt. \quad (3.17)$$

Evaluating the functions at $t = 0$ and $t = x$ and after some reordering leads to

$$\frac{1}{2}y'(x)^2 - \frac{1}{2}y(x)^4 = \frac{1}{2}y'(0)^2 - \frac{1}{2}y(0)^4 + I(x) \quad (3.18)$$

where $I(x) = \int_0^x ty(t)y'(t)dt$. Here again as stated in [8] the $I(x)$ term vanishes just like with the derivation for Painlevé I. The left-hand side then is our new \mathcal{PT} -symmetric Hamiltonian H and the right-hand side (without $I(x)$) is the corresponding energy level. After multiplication by two and rewriting it in a more familiar notation we have

$$H = p^2 - x^4, \quad (3.19)$$

where $E_n = y'(0)^2 - y(0)^4$. We immediately recognize the \mathcal{PT} -symmetric Hamiltonian (2.9) with $N = 4$ and that is why we multiplied it by two, so we can use our WKB result (2.34) for this problem. With parameters $N = 4$ and $a = 1$ the energy levels are computed:

$$E_n = \left(\frac{(n + 1/2)\sqrt{\pi}\Gamma(7/4)}{\frac{1}{2}\sqrt{2}\Gamma(5/4)} \right)^{4/3} \approx 3.4686 \cdot (n + \frac{1}{2})^{4/3}. \quad (3.20)$$

For fixed $c = 0$ the eigenvalues $b_n = \sqrt{E_n}$ are now easily calculated:

$$b_n \sim 1.8624 \cdot n^{2/3} \quad \text{for } n \rightarrow \infty. \quad (3.21)$$

When we fix the slope at $y'(0) = 0$ we get a negative energy $E_n = -c_n^4$. This problem is resolved in a similar way as we did for Painlevé I: we rotate the potential over the complex plane to get the new Hamiltonian

$$H = p^2 + x^4. \quad (3.22)$$

This Hamiltonian no longer belongs to our family of Hamiltonians described in (2.9) but is a regular Hermitian one. However we can still compute its eigenvalues using (2.34) only with a slight modification. Somewhere along the derivations that lead to this equation a "sin(π/N)" term popped up due to the complex integration. With our Hermitian Hamiltonian we now no longer need to integrate over the complex plane (but along the real axis) and so this term disappears in (2.34). The resulting energy now is

$$E_n = \left(\frac{(n + 1/2)\sqrt{\pi}\Gamma(7/4)}{\Gamma(5/4)} \right)^{4/3} \approx 2.1851 \cdot (n + \frac{1}{2})^{4/3}, \quad (3.23)$$

and taking the one-fourth power of this energy delivers the desired relation for c_n

$$c_n \sim 1.2158 \cdot n^{1/3} \quad \text{for } n \rightarrow \infty. \quad (3.24)$$

3.4 Painlevé IV

3.4.1 Behaviour of solutions

Now we arrive at the fourth Painlevé equation:

$$y(t)y''(t) = \frac{1}{2}y'(t)^2 + 2t^2y(t)^2 + 4ty(t)^3 + \frac{3}{2}y(t)^4 \quad \text{where } y(0) = c \text{ and } y'(0) = b. \quad (3.25)$$

In figure 3.5 and 3.6 we see solutions of this equation for the initial conditions $y(0) = 1$ and $y'(0) = b$. The reason for picking $y(0) = 1$ instead of 0 as we did previously is because the math will fail us at some point later if we take $y(0) = 0$. In [11] Bender supplies us with the answer for the case $y(0) = 1$, so we pick the same value in order to later check our result with his. The solutions show two unstable asymptotes that seem to repel solutions and one stable line that attracts them. We once more have these behavioural changes for particular values of b when the solution suddenly succeeds to cross the the upper asymptote. This looks more or less the same for the case $y(0) = c$ and $y'(0) = 0$.

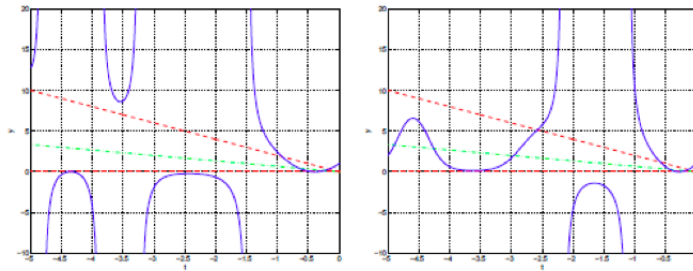


Figure 3.5: Solutions of Painlevé IV with $y(0) = 1$ and $y'(0) = b$: values of b are unknown but the **left** panel shows the first mode of behaviour and the **right** panel the second mode of behaviour. *Source: [11]*

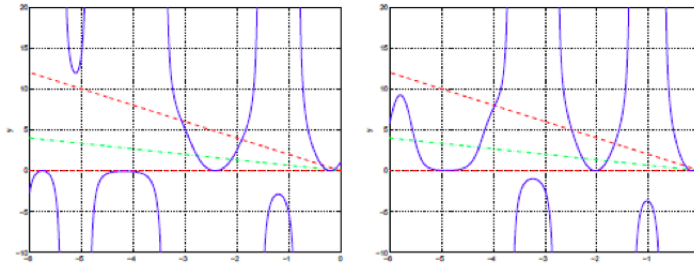


Figure 3.6: Solutions of Painlevé IV with $y(0) = 1$ and $y'(0) = b$: values of b are unknown but the **left** panel shows the third mode of behaviour and the **right** panel the fourth mode of behaviour. *Source: [11]*

3.4.2 Calculating the eigenvalues

Finding the Hamiltonian of the fourth Painlevé equation is a bit trickier as we will see. The fourth equation starts on the left-hand side with a $y(t)y''(t)$ term. So first we simplify the equation by dividing by $y(t)$ which looks like

$$y''(t) = \frac{y'(t)^2}{2y(t)} + 2t^2y(t) + 4ty(t)^2 + \frac{3}{2}y(t)^3. \quad (3.26)$$

Clearly our method of multiplying by $y'(t)$ and integrating from 0 to x creates an undesirable first term on the right-hand side. To circumvent this problem we use a substitution $y = u^2$. Some simple derivatives and quantities are calculated

$$\begin{aligned} y' &= 2uu' & y'' &= 2(u')^2 + 2uu'' \\ (y')^2 &= 4u^2(u')^2 & \frac{(y')^2}{2y} &= 2(u')^2, \end{aligned} \quad (3.27)$$

and plugging these into (3.26) gives us

$$2(u')^2 + 2uu'' = 2(u')^2 + 2tu^2 + 4tu^4 + \frac{3}{2}u^6. \quad (3.28)$$

There are two terms that eliminate each other and after dividing both sides by $2u$ we are left with a more useful equation

$$u'' = t^2u + 2tu^3 + \frac{3}{4}u^5. \quad (3.29)$$

Here we finally can follow our regular procedure of multiplication by u' and then integration from 0 to x which leads to

$$\frac{1}{2}(u')^2 \Big|_0^x = \frac{1}{8}u^6 \Big|_0^x + I(x), \quad (3.30)$$

where $I(x) = \int_0^x t^2uu'dt + \int_0^x 2tu^3u'dt$. Once more the $I(x)$ term will vanish for $n \rightarrow \infty$ because of similar reasons as before. Evaluating these functions at $t = 0$ and $t = x$, multiplying by two and reordering gives our final Hamiltonian

$$H = p^2 + \frac{1}{4}x^6, \quad (3.31)$$

with energy levels $E_n = u'(0)^2 + \frac{1}{4}u(0)^6$. From our substitution we can derive that $u = y^{\frac{1}{2}}$ and that $u' = \frac{(y')^2}{4y}$ so the energy levels in terms of $y(0)$ and $y'(0)$ are $E_n = \frac{y'(0)^2}{4y(0)} + \frac{y(0)^3}{4}$. This shows exactly the reason why we examine solutions passing $y(0) = 1$ instead of the origin. That is because for the origin the energy levels E_n blow up to infinity which would render this method useless.

Computing the energy levels in (2.34) with parameters $N = 6$ and $a = \frac{1}{4}$ yields

$$E_n = \left(\frac{1}{4}\right)^{2/8} \cdot \left(\frac{(n + \frac{1}{2})\sqrt{\pi}\Gamma(10/6)}{\frac{1}{2}\Gamma(7/6)}\right)^{3/2} \approx 4.5302 \cdot \left(n + \frac{1}{2}\right)^{3/2}. \quad (3.32)$$

Now if we fix $y(0) = 1$ and look for eigenvalues b_n we will write out energy equation to $b_n = \sqrt{4E_n - 1}$. As we are interested in the asymptotic behaviour of the eigenvalues b_n as $n \rightarrow \infty$ we can drop the -1 term under the square root (and the $+\frac{1}{2}$ term in (3.32) as before) and we get

$$b_n \approx \sqrt{4E_n} \sim 4.2568 \cdot n^{3/4} \quad \text{for } n \rightarrow \infty. \quad (3.33)$$

What remains are the eigenvalues c_n , the initial conditions for the separatrix solutions having a flat slope when crossing the y -axis. Our equation for the energy levels is rewritten using $y'(0) = 0$ to $c_n = (4E_n)^{1/3}$ which results in

$$c_n \sim 2.6266 \cdot n^{1/2} \quad \text{for } n \rightarrow \infty. \quad (3.34)$$

3.5 Discussion of the results

Our goal was to find the coefficients B and the rational numbers x in (3.5) that predicted the eigenvalues for large n . Although there are no exact answers to compare them with, Bender did find them numerically to a very high accuracy for Painlevé I and II in [8] and for Painlevé IV in [11]. He collected a number of eigenvalues that he had found and then applied Richardson extrapolation to discover the asymptotic behaviour. This algorithm spat out relations like (3.5) with the following coefficients:

	Eigenvalue	Our result	Bender	Error
Painlevé I	b_n	2.0924674	2.09214674	$\pm 10^{-8}$
	c_n	1.0304844	-1.0304844	$\pm 10^{-7}$
Painlevé II	b_n	1.8624128	1.8624128	$\pm 2 \cdot 10^{-7}$
	c_n	1.21581166	1.21581165	$\pm 10^{-8}$
Painlevé IV	b_n	4.256843	4.256843	$\pm 10^{-6}$
	c_n	2.626587	2.626587	$\pm 10^{-6}$

Table 3.1: All the coefficients that were calculated using our WKB method, only now in more digits compared to Benders numerical result. Last column is the Error in Benders results.

As is very clear, the WKB method seems to be very accurate. Looking at the results one can say with certainty that the assumptions that were made are valid for $n \rightarrow \infty$ as the result is surprisingly good. They approximation is right for most cases until the last digit of Benders values. Only for Painlevé II eigenvalues c_n do we spot a small deviation. The Richardson extrapolation that Bender applied also gave the exponent x that described the relation between the eigenvalues and n . If we compare the results of our method with these in [8] and [11] we find exactly the same exponents.

So the method seems to find the coefficients of our eigenvalue relation very well, but how accurate is this relation itself? We know that as $n \rightarrow \infty$ the eigenvalues get arbitrarily close to the ones our relation predicts, but we also want to know how quickly they converge. Computing the eigenvalues with equation (3.14) and comparing them with the by Bender numerically found eigenvalues from [8] we get table 3.2.

	Bender	Method	Relative error
b_1	1.852	2.092	0.130
b_2	3.004	3.171	0.056
b_3	3.905	4.044	0.036
b_4	4.683	4.806	0.026
b_5	5.383	5.495	0.021
...
b_{10}	8.245	8.328	0.010
b_{11}	8.738	8.819	0.009

Table 3.2: The numerically found critical values of Bender compared with the ones equation (3.14) predicts and the relative error.

The eigenvalues converge quite well to our asymptote as the table shows. b_3 already has a relative error under 5% and once you pass b_{10} we are under 1%. Unfortunately Bender does not supply more eigenvalues of the other Painlevé equations, but if this kind of convergence is normal we can be very content.

Chapter 4

Conclusion

In this thesis we reviewed some properties of Hermitian Hamiltonians and attempted to see if the condition of \mathcal{PT} -symmetry lead to the same features. In conclusion we must say that this is not the case: we require an additional condition to ensure a real spectrum and a conserved norm. With this condition however we do have these properties and using the WKB approximation it is possible to compute the spectrum. We also examined special solutions of Painlevé equations I, II and IV. The method links our Painlevé equations to Hamiltonians of which we then calculate the energies using our WKB result. The resulting eigenvalue relations are very precise and give good predictions.

We have seen that \mathcal{PT} -symmetric Hamiltonians under certain circumstances do satisfy the two conditions we imposed and it challenges us to find more classes of Hamiltonians that might be useful. As it happens \mathcal{PT} -symmetry is just of the many symmetries one can construct. The proofs we gave for these unbroken symmetries can be extended to other anti-linear operators A for which $A^2 = I$.

Interestingly enough when addressing the time-evolution Bender has a different approach [2]. He creates a operator \mathcal{C} that together with \mathcal{PT} forms a new 'CPT' innerproduct in which we do have unitary time-evolution. The theory seems to solve the problems non-Hermiticity gives but is however slightly more complicated (see [12] and [13] for a mathematical background).

The Painlevé equations were a nice example of how these \mathcal{PT} -symmetric Hamiltonians can be applied in a different field. The method works very well and so there must be many more differential equations that can be analysed using this procedure. Maybe the other three Painlevé equations can also be examined in a similar way or as Bender suggested in [8] one can learn more about the Thomas-Fermi equation.

Bibliography

- [1] Stefan Boettcher Carl M. Bender and Peter N. Meisinger. *PT-Symmetric Quantum Mechanics*. 1998.
- [2] Carl M. Bender. *Introduction to PT-symmetric Quantum Theory*. 2008.
- [3] Z. Ahmed. *Pseudo-Hermiticity of Hamiltonians under gauge-like transformation: real spectrum of non-Hermitian Hamiltonians*. 2002.
- [4] C. Cuning P. Dorey and R. Tateo. *Spectral equivalences, Bethe Ansatz equations, and reality properties in PT-symmetric quantum mechanics*. 2001.
- [5] David J. Griffiths. *Introduction to Quantum Mechanics*.
- [6] www.wolframalpha.com.
- [7] L.I. Fuchs. *Über Differentialgleichungen, deren Integrale feste Verzweigungspunkte besitzen*. 1884.
- [8] Carl M. Bender and Javad Komijani. *Painlevé Transcendents and PT-symmetric Hamiltonians*. 2015.
- [9] Andreas Fring Carl M. Bender and Javad Komijani. *Nonlinear eigenvalue problems*. 2014.
- [10] W.P. Reinhardt. *Complex coordinates in the theory of atomic and molecular structure and dynamics*. 1982.
- [11] <http://www.rug.nl/research/vsi/events/groenewold/bender.pdf>.
- [12] Ali Mostafazadeh. *Exact PT-Symmetry Is Equivalent to Hermiticity*. 2003.
- [13] Ali Mostafazadeh. *Pseudo-Hermiticity and Generalized PT- and CPT-Symmetries*. 2002.