Comparison of Finite Differences and WKB approximation Methods for PT symmetric complex potentials

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Abstract. We consider the one dimensional schrödinger eigenvalue problem on a finite domain (Strum-Liouville problem) for several PT-symmetric complex potentials, studied by Bender and Jones using the WKB approximation method. We make a comparison between the solutions of theses PT-symmetric complex potentials using both the finite difference method (FDM) and the WKB approximation method and show quantitative and qualitative agreement between the two methods.

1. Introduction

Recently, there has been growing interest in non-hermitian Hamiltonians having real energy spectra [1], these complex potentials extend quantum mechanics to several open fields of theoretical, experimental as well as technological physics [2]. In conventional formulation of quantum mechanics the Hamiltonian must be Hermitian $H = H^+$ (mathematical axiom) in order to ensure the reality of the energy spectrum (the eigenvalues of H). In alternative formulation the mathematical axiom of Hermiticity is replaced by the physically transparent axiom called space-time reflection symmetry (PT-symmetry). In this light, Bender and his collaborators [3] [4] and later others [5] have studied and solved non-Hermitian Hamiltonians, who leads to real eigenvalues by using numerical and analytical techniques see [9]-[10] and references there in.

The goal of this paper is to investigate a class of PT-symmetric Hamiltonian with complex potentials, for which we compare between WKB approximation and finite difference method and systematically show the qualitative and quantitative agreement between the two.

2. WKB Analysis of PT -Symmetric Sturm-Liouville problems

Most problems encountered in PT-symmetric QM cannot be solved exactly. The solution of the schrödinger eigenvalue problem exist only for an infinite domain, one must resort to approximate methods, a variety of such methods have been developed and each has its own area of applicability. One of these methods is the Wentzel-Kramers-Brillouin approximation used by Bender and Jones [6]-[7] to investigate PT-symmetric systems defined on finite domain whose

eneregy eigenvalues grow like n^2 for large n. Another future of the PT eigenvalue problem on a finite domain is the showing up of a sequence of critical points at which pairs of eigenvalues cease to be real and become complex conjugates of one another. For the potentials considered here this sequence of critical points is associated with a turning point on the imaginary axis in the complex plane. In the next section we will briefly review the WKB analysis of [6][7], where the authors focus on the complex potentials to calculate the real eigenvalues of energy and plotted as function of the coupling parameter λ.

2.1. WKB calculation of eigenvalues for "one turning point "

In their paper [6] Bender and Jones considered the one -dimensional time independent schrödinger equation :

$$-\Psi^{''}(x) + V(ix)\Psi(x) = \lambda\Psi(x), \tag{1}$$

where λ is the energy eigenvalue, and the following boundary condition $\Psi(+1) = 0$, $\Psi(-1) = 0$ are imposed. In a preparatory step, they treat both the eigenvalues λ and g (coupling parameter) as large and proportional $\lambda = a \cdot g$, thus substituting in (1)one obtains:

$$-\Psi^{''}(x) = -g \cdot Q(x) \cdot \Psi(x), \tag{2}$$

where $Q(x) = V(ix) + a$. We must notice that the asymptotic solution of (2) is controlled by a turning point (see FIG[1]) on the imaginary X axis, satisfying $V(-b) + a = 0$.
We will here summarize the methodology and skip the details of the calculation presented in [6], where we refer the interested reader.

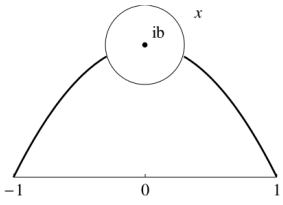

Figure 1. schematic path with end point $x = \pm 1$ of one turning point $x = ib$.

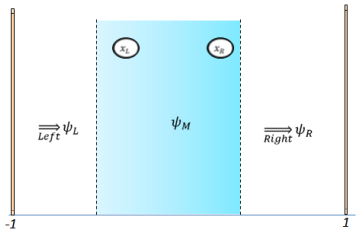

Figure 2. schematic the path of integration of WKB function for two turning point.

Part1: firstly we approximate our schrödinger equation near the turning point, we start by $x = ib + y \cdot c$, where $y \ll 1$ then $Q(x) = iycV^{'}(-b)$, substitution of this in (2) gives

$$\frac{\partial^2}{\partial y^2}\Psi(y) = -igc^3V^{'}(-b)y\Psi(y), \tag{3}$$

the approximated schrödinger equation have a similar form as the standard Airy differential equation, we then convert (2) as

$$\frac{\partial^2}{\partial y^2}\Psi(y) = y\Psi(y)\,, \qquad with \qquad \begin{cases} y &= \frac{x-ib}{\gamma}e^{-i\pi/6} \\ c &= \gamma e^{i\pi/6} \\ \gamma &= g[V^{'}(-b)]^{-1/3} \end{cases} \tag{4}$$

For the sake of convenience the solution of the standard Airy differential equation is well known, where the solution of the schrödinger equation will take the following form:

$$\Psi(y) = K_1 Ai(y) + K_2 Ai(\omega y) \Leftrightarrow \Psi(y) = K_1 Ai(\frac{x-ib}{\gamma} e^{-i\pi/6}) + K_2 Ai(\omega \frac{x-ib}{\gamma} e^{-i\pi/6}) \quad (5)$$

Part2: They approximate the schrödinger equation away from the turning point on both sides using WKB function and invokes the appropriate boundary condition, it will be done as:

$$\Re[x] < 0 \Rightarrow \Psi_L(x) \sim \frac{L_1}{[Q(x)]^{\frac{1}{4}}} \exp[i \int_x^{ib} ds\sqrt{gQ(s)}] + \frac{L_2}{[Q(x)]^{\frac{1}{4}}} \exp[-i \int_x^{ib} ds\sqrt{gQ(s)}] \quad (6)$$

$$\Psi_L(-1) = 0 \Rightarrow 0 = L_1 \exp[i \int_{-1}^{ib} ds\sqrt{gQ(s)}] + L_2 \exp[-i \int_{-1}^{ib} ds\sqrt{gQ(s)}] \quad (7)$$

$$\Re[x] > 0 \Rightarrow \Psi_R(x) \sim \frac{R_1}{[Q(x)]^{\frac{1}{4}}} \exp[i \int_{ib}^{x} ds\sqrt{gQ(s)}] + \frac{R_2}{[Q(x)]^{\frac{1}{4}}} \exp[-i \int_{ib}^{x} ds\sqrt{gQ(s)}] \quad (8)$$

$$\Psi_R(1) = 0 \Rightarrow R_1 \exp[i \int_{ib}^{1} ds\sqrt{gQ(s)}] + R_2 \exp[-i \int_{ib}^{1} ds\sqrt{gQ(s)}] \quad (9)$$

At this point, we will have 6 arbitrary unknown constants. Obviously our key technical step to determine them by the asymptotic matching between the solution of Airy function near the turning point and WKB function away from the turning point, where they must be identical and can be expressed as:

$$\left\{ \begin{array}{rcl} \frac{K_1}{2\sqrt{\pi}} & = & L_2 g^{\frac{1}{4}} \gamma^{\frac{1}{2}} e^{-i\pi/6} \\ \frac{1}{2\sqrt{\pi}}(-K_1 e^{2i\pi/3} + K_2) & = & L_1 g^{\frac{1}{4}} \gamma^{\frac{1}{2}} \end{array} \right. \quad \left\{ \begin{array}{rcl} \frac{K_1}{2\sqrt{\pi}} & = & R_1 g^{\frac{1}{4}} \gamma^{\frac{1}{2}} e^{-i\pi/6} \\ \frac{K_2}{2\sqrt{\pi}} & = & R_2 g^{\frac{1}{4}} \gamma^{\frac{1}{2}} \end{array} \right. \quad (10)$$

Then it is more advantageous to combine it, when the calculation can be easily carried out to a secular equation that determines the real energy eigenvalues:

$$\sin[\int_{-1}^{1} ds\sqrt{gQ(s)}] + \frac{1}{2} \exp[i \int_{-1}^{ib} ds\sqrt{gQ(s)} - i \int_{ib}^{1} ds\sqrt{gQ(s)}] = 0 \quad (11)$$

2.2. WKB calculation of eigenvalues for " More than one turning point "

Let us mention here that the previous secular equation (11) fails to reproduce the expected energy eigenvalues for more than one turning point. Therefore the authors in a subsequent paper [7] readapted their treatment with some modification to the case the path of integration passes through two turning points x_L and x_R as schematized in FIG[2]. The WKB approximation of the wave function Ψ_R (8) and Ψ_L (6) are respectively the wave functions on the left region of the x_L and the right region of x_R turning points. Nevertheless, there is additional basic conditions requiring the wave function in the region between the two turning points Ψ_M to be PT-symmetric, to finally yield the new following secular equation:

$$\sin[\int_{-1}^{1} ds\sqrt{gQ(s)}] + e^{\Delta} \cos[i \int_{x_L}^{x_R} ds\sqrt{gQ(s)}] = 0\,, \qquad where \quad \Delta \equiv 2ImI_L, I_L \equiv [\int_{-1}^{x_L} ds\sqrt{gQ(s)}] \quad (12)$$

In fact this constraint can be viewed as a compact way of setting a secular equation of the WKB analysis involving the pertinent boundary condition and also for complex potential which had more then one turning point, this is what makes the method so effective.

3. Finite Difference Method

Finite difference method is a numerical method based on mathematical discretization of differential equation of boundary problems. The basic idea of FDM (Finite Difference Method) is to replace each term of the partial derivative $\frac{df(x)}{dx}$ by a finite difference approximation $\frac{\Delta f(x)}{\Delta x}$ obtained by Taylor's expansion near the point of interests and neighboring points as schematized in FIG[3].

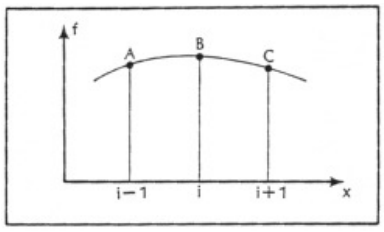

Figure 3. describe the three area of function $f(x)$ presented in finite difference scheme.

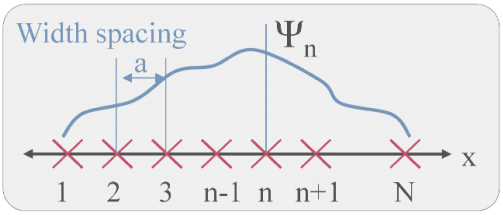

Figure 4. the describtion of the wave function in discretization space with the boundary condition.

Let us summarize the FDM to solve the time independent schrödinger equation in a close form, where we must notice that we will consider a complex PT-symmetric potential. This leads to discretize the geometric domain of the X-space into grid points x_n, $n = 1, 2.....N$ (see FIG[4]) and at each point the stationary 1D schrödinger equation can be written as:

$$H\Psi = E\Psi \Leftrightarrow H_n\Psi(x_n) = E\Psi(x_n) \Leftrightarrow -\Psi^{''}(x_n) + V(x_n)\Psi(x_n) = E\Psi(x_n). \tag{13}$$

We now have a system of N equations, producing N solutions. The next step is to approximate the second derivative of the wave function $\Psi^{''}(x)$ using finite difference scheme [8] such that:

$$\begin{cases} [\frac{d\Psi}{dx}]_{n+1} = \frac{\Psi_{n+1}-\Psi_n}{\Delta x} \\ [\frac{d\Psi}{dx}]_n = \frac{\Psi_n-\Psi_{n-1}}{\Delta x} \end{cases} \qquad [\frac{d^2\Psi}{dx^2}]_n = \frac{[\frac{d\Psi}{dx}]_{n+1} - [\frac{d\Psi}{dx}]_n}{\Delta x} = \frac{\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}}{(\Delta x)^2}. \tag{14}$$

Where $\Delta x_{n+1} = \Delta x_n = \Delta x = a.$

The system (13) becomes:

$$E\Psi_n = V(x_n)\Psi_n - t_0[\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}] \qquad t_0 \equiv \frac{1}{(\Delta x)^2}. \tag{15}$$

After using an appropriate FD scheme to approximate the schrödinger equation, we must impose the boundary condition (see FIG[4]) as a consequence of the consideration of finite domain $\Psi(x_1) = \Psi(x_N) = 0$. In fact the system of equations (15) can be easily written in matrix notation, where we must represent the wave functions in vector and the Hamiltonian in matrix forms who includes the potential as:

$$E \cdot \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \\ \vdots \\ \Psi_N \end{bmatrix} = \begin{bmatrix} 2t_0 + V(x_1) & -t_0 & 0 & 0 & 0 & 0 \\ -t_0 & 2t_0 + V(x_2) & -t_0 & 0 & 0 & 0 \\ 0 & -t_0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \ddots & \ddots & -t_0 \\ 0 & 0 & 0 & 0 & -t_0 & 2t_0 + V(x_N) \end{bmatrix} \cdot \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \\ \vdots \\ \Psi_N \end{bmatrix} \tag{16}$$

4. Numerical Results and Discussion

We give numerical results showing the agreement between both methods. In order to make a comparison between the FDM and the WKB approximation for non-hermetian Hamiltonians we choose a class of complex PT-symmetric potentials studied by Bender and Jones [6]-[7]. For the FDM we have developed a code for solving the eigenvalue problem of the Hamiltonian (16) with boundary condition similar to those considered using WKB analysis [6]-[7]. We have taken into account additional considerations, as variation of the dimension of our Hamiltonian matrix, which also connect to the number of the grid points as well as the width of spacing distance between them (see FIG[4]).

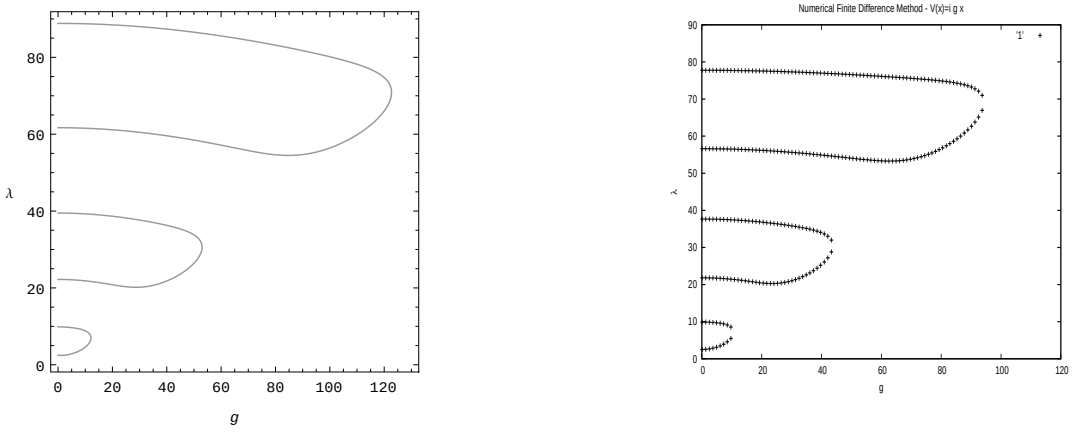

Figure 5. Real energy levels for WKB analysis(Right) and FD method(Left) of $V(x) = igx$.

We start our comparison between the two methods for potentials which have one turning point $V(x) = igx$, the results are represented in FIG[5], where we do find that FD method reproduces the one obtained from WKB analysis. The same result is obtained for the sinusoidal potential $V(x) = ig\sin(2x)$, shown in FIG[6].

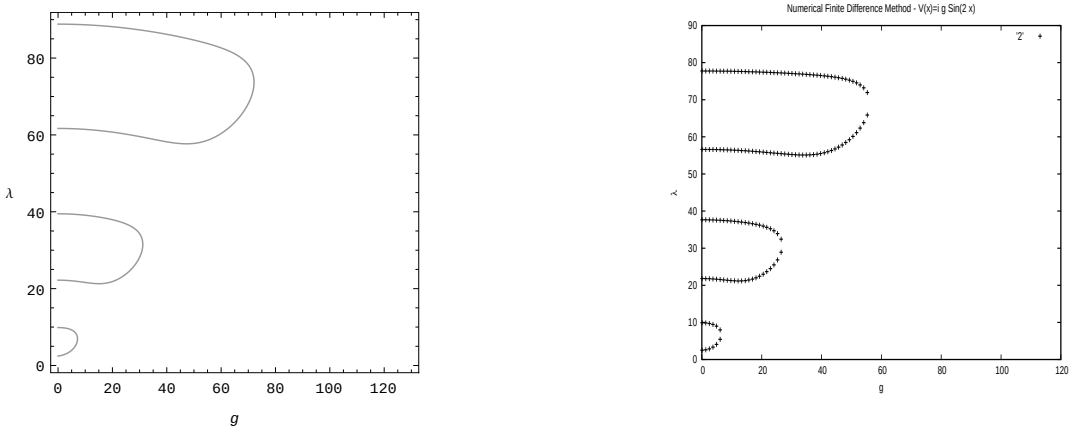

Figure 6. Real energy levels for WKB analysis (Right) and FD method (Left) of $V(x) = ig\sin(2x)$.

Briefly, we must note that in WKB analysis the energy eigenvalues λ and the coupling parameter g was treated as large and proportional, in contrary the range of validity of FD method is for small values of both (λ, g) nevertheless we note the excellent agreement between the two results.
We end this paper by showing numerical results for potentials having more than one turning point using the potential $V(x) = igx^3$ as an example. In FIG[7] one sees that FD method approximately reproduces the structure of the eigenvalues obtained by the WKB analysis. This is a consequence of truncation errors involved in the numerical computations due to the fact that in FD representation of derivatives with Taylor's series expansion the higher order terms are neglected. In other words it means that the truncation error identifies the difference between the exact solution of a differential equation and its finite difference solution.

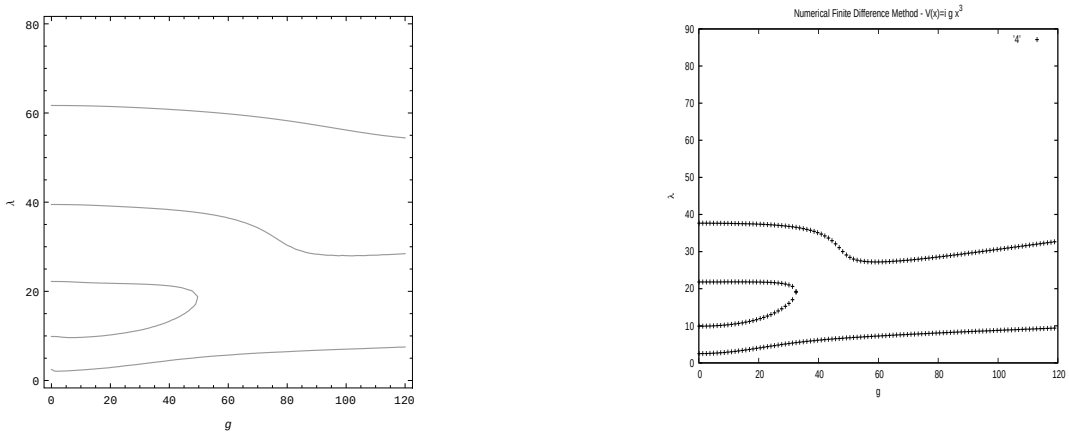

Figure 7. Real energy levels for WKB analysis (Right) and FD method (Left) of $V(x) = igx^3$.

5. Conclusion

Summarizing the results presented in this paper: The FD method can effectively offer an easy way to solve the one-dimensional schrödinger complex PT-symmetric eigenvalues problem.
The developed methodology of FDM provides a significant advantage over conventional analytical method like WKB analysis. Further study may include the high-order terms of Taylor's series expansion to obtain more accuracy (diminish the truncation error) especially for the complex potentials (having more then one turning points). Which will be the subject of future investigations.

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