ABSTRACT

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THE ITERATIVE METHOD FOR QUANTUM DOUBLE-WELL AND

SYMMETRY-BREAKING POTENTIALS

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Numerical solutions of quantum mechanical problems have witnessed tremendous advances over the past years. In this thesis, we develop an iterative approach to problems of double-well potentials and their variants with parity-time-reversal symmetry- breaking perturbations. We show that the method provides an efficient scheme for obtaining accurate energies and wave functions. We discuss in this thesis potential applications to a variety of related topics such as phase transitions, symmetry breaking, and external field-induced effects.

THE ITERATIVE METHOD FOR QUANTUM DOUBLE-WELL AND

SYMMETRY-BREAKING POTENTIALS

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LIST OF ABBREVIATIONS

PT   Parity Time

DWP   Double-well Potential

EMM   Eigenvalue Moment Method

MFR   Multiscale Reference Function

CHAPTER I

INTRODUCTION

Physical systems can be classified as Hamiltonian or non-Hamiltonian. In a
Hamiltonian system, the total energy of the system is conserved within the system, and
the Hamiltonian operator is a description of the total energy (potential and kinetic) of a
system in any given configuration. For energy levels to be real, the Hamiltonian operator
must be Hermitian, meaning it is a square matrix that is self-adjoint and symmetric. The
Hermiticity of a Hamiltonian can be expressing as $H = H^{\dagger}$, where the symbol $\dagger$ denotes
the usual Dirac conjugation, the transpose, and complex conjugate.

In the past few years, it has been concluded that the necessity of Hermiticity
might be supplanted by the physical prerequisite of space-time reflection symmetry (PT
symmetry) without violating any of the fundamental physical concepts of quantum
mechanics. Theories defined by non-Hermitian PT-symmetric Hamiltonians (P denotes
parity reflection $x \rightarrow -x, p \rightarrow -p$; T denotes time reversal $x \rightarrow x, p \rightarrow -p, i \rightarrow -i$)
display strange and unexpected properties at the classical level and also at the quantum
level [1]. The requirement of Hermiticity and the properties of some non-Hermitian PT-
symmetric quantum theories were discussed in Bender [2]. Non-Hermitian Hamiltonian
potentials play a crucial role to several physical phenomena such as Higgs boson
interaction [3], quantum tunneling, and PT phase transition in higher-dimensional
quantum systems [4].

Understanding certain systems in quantum mechanics are essential for scientists to have an in-depth comprehension for future applications. In general, there are only a few analytical solutions available for solving many quantum problems. One of the Primary reason is the slow convergence of the outcomes. Therefore, it is required to resort to numerical methods. Over time, there have been a variety of studies driving toward an accurate solution to the non-Hermitian quantum problem. This has been advanced by utilizing the Hill determinant, Airy function approach, Numerov method, perturbative method, and eigenvalue moment method [5-10]. The iteration method was introduced by Tymczak et al. [11]. This approach is simple to implement, and the outcomes are adequate for numerical purposes. It does not require a careful algebraic analysis; as other methods require.

The purpose of this thesis is to present an exact and direct technique for bound state energies. Comparing this thesis results with the numerical values obtained by earlier works, our method provides exact results through the full range of parameter values. In this work, we use the iteration method for double-well potential$-Z^2x^2 + x^4$, complex double-well potential $-Z^2x^2 + x^4 + iax$, and PT-symmetry breaking for $ix^3 + iax$ Hamiltonian and $x^4 + iax$ Hamiltonian. This thesis is organized into two chapters followed by conclusions. Chapter Ⅱ recalls the iteration method for one-dimensional parity symmetric system such as the double-well potential, and for PT-symmetry Hamiltonian. Chapter Ⅲ presents results of the iteration method along with discussion that covers wave functions for the potential as well as a comparison of these results with others.

CHAPTER II

FORMULATION OF THE PROBLEM

2.1. The iterative method for parity-invariant Hamiltonian

Schrödinger Equation is the fundamental equation of physics for describing quantum mechanical behavior. The Hill determinant approach and power-series expansion [5] are efficient methodologies for solving Schrödinger equation. Studies have combined those techniques that result in the iterative method [12]. The power-series expansion can be written in terms of the wave function

$$\Psi(x) = \sum_J a_J(E) x^J R_\alpha(x). \tag{2.1}$$

The coefficient $R_\alpha(x)$ in our work is the Gaussian (symmetrical curve representing the normal distribution) reference function,

$$R_\alpha(x) = e^{-\beta x^2}, \tag{2.2}$$

where β is an adjustable parameter introduced to accelerate the rate of convergence of the iteration method.

The importance of choosing reference functions that satisfy the boundary condition was discussed in earlier work by Wijewardena et al. [13]. The reference

function (wave function) is utilized to acquire bound state energies for the studied potential. Wijewardena et al. demonstrated that it is conceivable to accomplish convergence and obtain exact eigenvalues even if the required Stokes regions are not entirely within in the range of convergence of the reference function. However, it is suggested to use a wave function that meets the Stokes and anti-Stokes regions in order to dispose of the low rate of convergence. Tymczak et al. [14] proved that the recursive structure of the Hill determinant gives the capacity to acquire the eigenvalues. The starting point for the recursion relation is the transformation of the Schrödinger equation into a secular equation. Once the recursion structure is obtained, exact eigenvalues are readily acquired.

The one-dimensional time-independent Schrödinger equation is given by

$$\frac{d^2\Psi}{dx^2} + E\Psi(x) = V(x)\Psi(x), \tag{2.3}$$

in which E is the eigenenergy, and $V(x)$ is the potential. Tymczak et al. have confirmed that truncating the coefficient functions $a_j(E)$ in Eq. (2.1) by choosing a truncation point provide exact solutions

$$a_J(E) = 0, \tag{2.4}$$

where the value J is the number of iterations. The coefficient $a_J(E)$ is a polynomial in E. The roots of this polynomial give the exact eigenvalues. The accuracy of the eigenvalues depends on increasing the number of iterations. The polynomial coefficient for $a_j(E)$ can be expressed as in the following, which is a combination of odd and even polynomials

$$a_j(E) = b_0 + b_1 E + b_2 E^2 + \cdots = \sum_{j=0} b_j E^j. \qquad (2.5)$$

2.2. The iterative method for *PT*-symmetric Hamiltonian

We generalized the iterative method implied in Eq. (2.1) to contain the *PT*-symmetric potentials. The coefficient $a_j(E)$ linearly depends on the wave function and its derivative, $a_0 = \Psi(0)$ and $a_1 = \Psi'(0)$. Thus, we cannot compute the eigenvalues with Eq. (2.4) alone. To extend the method to solve *PT*-symmetric Hamiltonian we used an approach similar to that which was discussed for non-conserving Hamiltonian [12]. Wijewardenal et al. considered two polynomials determined from iterating the recursion relation [13].

From [13] let us consider the following two coefficients

$$a_j(E) = P_{j,0}(E)a_0 + iP_{j,1}(E)a_1,$$

$$a_{j+1}(E) = iP_{j+1,0}(E)a_0 + P_{j+1,1}(E)a_1, \qquad (2.6)$$

where $P_{(j,0),(j,1)}$ and $P_{(j+1,0),(j+1,1)}$ are polynomials in E determined by the iteration of the recursion relation. The two consecutive iteration can be written as follows

$$\vec{a_J} = P^J(E)\vec{a_0}, \qquad (2.7)$$

where

$$\vec{a_J} = \begin{bmatrix} a_J(E, a_0, a_1) \\ a_{J+1}(E, a_0, a_1) \end{bmatrix}, \ \vec{a_0} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix}, \text{ and } P^J(E) = \begin{bmatrix} P_{J,0}(E) & P_{J,1}(E) \\ P_{J+1,0}(E) & P_{J+1,1}(E) \end{bmatrix}. \qquad (2.8)$$

The solution $\vec{a_J}$ can be obtained from the matrix P^J which is acquired from the iterative

approach. To solve Eq. (2.7) we need to set the matrix $\vec{a_J} = \vec{0}$. Then we can obtain the energies by taking the determinant

$$det[P^J(E)] = 0. \tag{2.9}$$

The 2x2 matrix determinant represents an independent polynomial for a_0 and a_1. Exact eigenvalues are obtained from the converged roots of Eq. (2.9). After we obtained the eigenvalues, we could then determine the wave function from the following

$$\Psi(x) = \sum_{J=0}^{\infty} a_J(E)e^{-\beta x^2}. \tag{2.10}$$

The wave function can also be written as

$$\Psi_{even}(x) = (a_0 + a_2 x^2 + \cdots)e^{-\beta x^2},$$

$$\Psi_{odd}(x) = (a_1 x + a_3 x^3 + \cdots)e^{-\beta x^2}.$$

Numerical determination of the wave functions will be discussed further in Chapter III. We will calculate the wave functions for the ground and first excited states and sketch their figures.

2.3. Extraction of the recursion relation

Recursion relation can be straightforwardly derived after we choose the wave function. First, we find the second derivative of the wave function. Then, we plug the wave function and its second derivative into Schrödinger equation. Then, we remove the variable x by carrying out the shift for the iterative number of the equation. Therefore, we have the recursion relation which is the iterative approach to get the eigenenergies.

CHAPTER III

RESULTS AND DISCUSSION

In this Section, we demonstrate the capacity of the iterative method described in the section above. We numerically implement the iteration method by obtaining the recursion structure for double-well, complex double-well potential, and PT-symmetry breaking potentials, then obtain the eigenvalues and the eigenfunctions for each potential.

3.1.1. The iterative method for symmetric double-well

The first example we study in this thesis is the double-well potential, which is an essential problem in quantum mechanics dealing with the energy level of two adjoining states. Specifically, the ground and first excited states energies are small due to the non-degenerate nature of eigenvalues of bound states for one-dimensional potential.
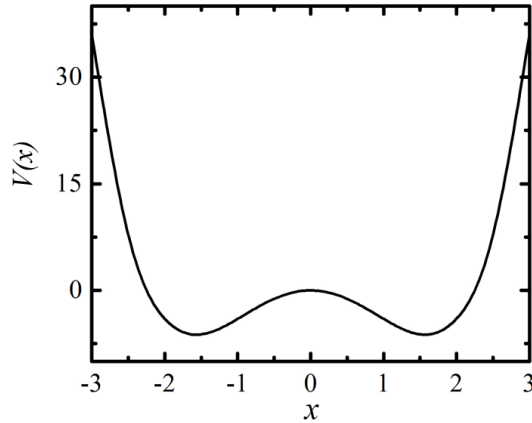
Figure 1. The potential $V(x) = -Z^2x^2 + x^4$ for $Z^2 = 5$.

The formalism of the symmetric double well potential, see Fig. 1, is illustrated by the

Hamiltonian

$$H = \frac{P^2}{2m} - Z^2 x^2 + x^4, \tag{3.1}$$

where Z^2 is a real constant. As we can qualitatively see from Figure 1, the double-well

potential is symmetric when $Z^2 = 5$.
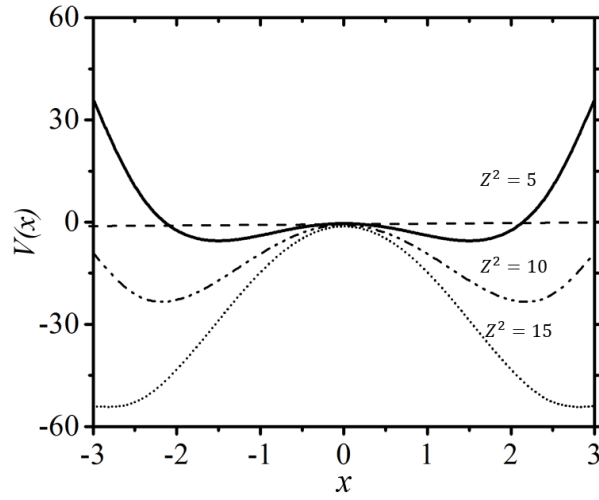
Figure 2. Divergence of the potential $V(x) = -Z^2 x^2 + x^4$, where $Z^2 = 5,10$ and 15.

Figure 2 shows the divergences of the double well potential. It is observed that the

wells depth depends on the value of the parameter Z^2 and the selected points in the x-axis.

In this case, we select points in the x-axis to be between $-3<x<3$, and notice that the value

of Z^2 need to be between the range $1<Z^2<25$ or the potential will be degenerate.

We obtain the recursion relation by rewriting Schrödinger equation Eq. (2.3) in

the following form

$$-\frac{d^2 \Psi}{dx^2} - (Z^2 x^2 - x^4)\Psi(x) = E\Psi(x), \tag{3.2}$$

where $\Psi(x) = \sum_j a_j(E)x^j e^{-\beta x^2}$, β is a positive real number. $\tag{3.3}$

The recursion relation obtained using Eq. (2.1) and Eq. (3.2) is

$$a_j(E) = \frac{[4\beta j - 6\beta - E]a_{j-2}(E) - [4\beta^2 + Z^2]a_{j-4}(E) + a_{j-6}(E)}{j(j-1)}, \quad (3.4)$$

where $[a_0 = 1, a_1 = 0]$ or $[a_0 = 0, a_1 = 1]$. Then, from the relation, Eq. (3.4) we get the

eigenvalues by finding the roots of Eq. (2.4).

3.1.2. Computing the eigenvalues for the symmetric double-well

As mentioned earlier, in order to obtain the energies, we use the straightforward

coefficient $a_j(E)$ which is a polynomial in E. In Table 1, we display the calculated

polynomials of energies that were obtained from solving the recursion relation Eq. (2.4).

Table 1. Calculated polynomials in E which are obtained by solving the relation Eq. (2.5).

j	E^0	E^1	E^2	E^3	E^4	E^5
0	1	0	0	0	0	0
1	1	0	0	0	0	0
2	1	-0.5	0	0	0	0
3	1	-0.17	0	0	0	0
4	0.42	-0.5	0.04	0	0	0
5	0.45	-0.17	0.01	0	0	0
6	0.12	-0.23	0.04	-0.0013	0	0
7	0.14	-0.07	0.01	-0.0001	0	0

It is observed that the polynomials can be written as a polynomial that combines all the odd and the even terms of Eq. (2.5). This coefficient satisfies the recursion relation that we got above in Eq. (3.4).

Table 2 displays the calculated energies for the ground and the first excited states for Eq. (3.4) which for the quartic anharmonic oscillator. The energies were obtained by our numerical method when the number of iterations is 160. The degeneracy of the two lowest states in the double-well potential is shown in the table. In figure 3, we plotted the results of the energies for the ground, first, and second excited states in DWP with parameters $\beta=3$ and $Z^2 = 1$. These energies were obtained by means of 160 iterations.

Table 2. The calculated the ground and the first excited states energies for DWP.

Z^2	Parity	E
$Z^2 = 0$	+	1.060 362 090 484 172
	-	3.799 673 029 801 485
$Z^2 = 1$	+	0.657 653 005 180 715
	-	2.834 536 202 119 293
$Z^2 = 5$	+	-3.410 142 761 239 825
	-	-3.250 675 362 289 231
$Z^2 = 10$	+	-20.633 581 690 973 539
	-	-20.633 557 834 357 433
$Z^2 = 15$	+	-50.841 454 633 550 270
	-	-50.841 474 252 254 841
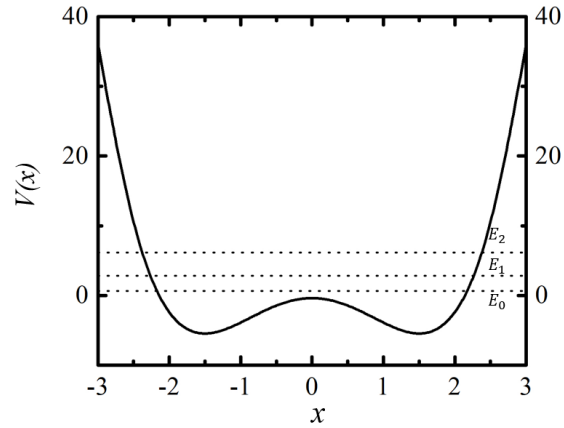
Figure 3. The symmetric double-well potential, the energies in the ground, the first and the second excited states.

3.1.3. The wave functions of double-well potential

Since the potential is symmetric, as it is shown in Figure 1, the eigenfunctions should be symmetric. Thus, the wave function would be either even or odd, leading to the condition $\Psi(0) = 0$ for odd and $\Psi'(0) = 0$ for even.

(a)

(b)
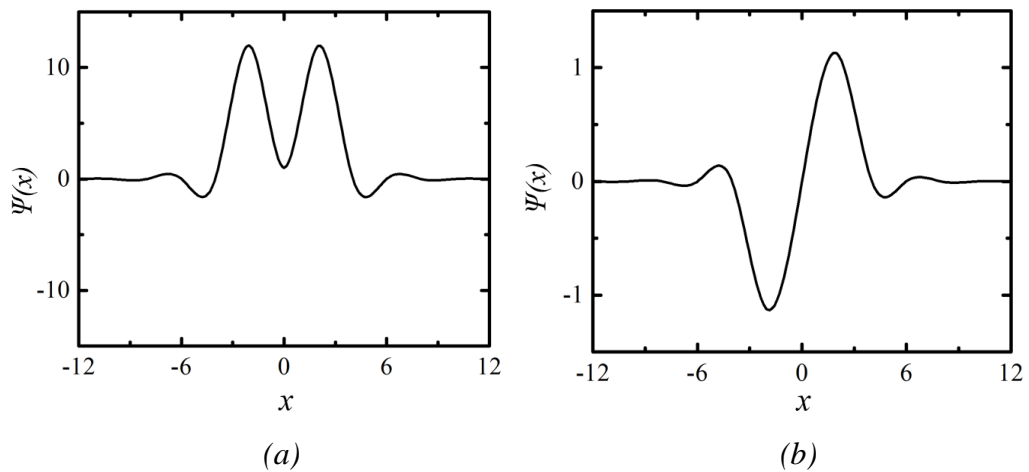
Figure 4. The ground-state of the even (a) and odd(b) wave functions for the anharmonic oscillator, $Z^2 = 5$.

(a)   *(b)*
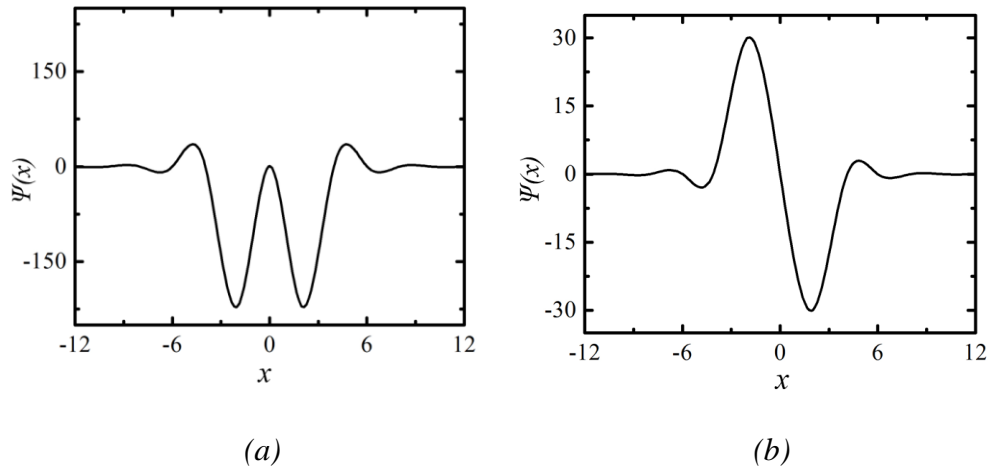
Figure 5. The first excited-state of even (a) and odd (b) wave functions for the anharmonic oscillator, $Z^2 = 5$.

Plots of the initial eigenfunctions of the double-well potential appear in Figures 4 and 5. The figures show the ground- and the first excited states wave functions obtained using the iteration method for $Z^2 = 5$, and in the range of $-3 \leq x \geq 3$, where we observe even function Ψ_0 and odd function Ψ_1.

3.2.1. The iterative method for *PT*-symmetry breaking double-well potential

The example presented here shows results for the eigenvalues and the

eigenfunctions for the *PT*-symmetry breaking for asymmetric double-well potential, (see

Figure 6). The potential can be expressed as in the following Hamiltonian,

$$H = \frac{P^2}{2m} - Z^2 x^2 + x^4 + iax. \qquad (3.5)$$
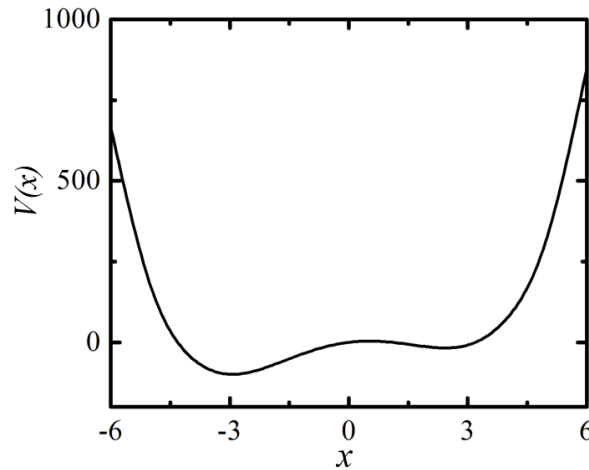
Figure 6. The *PT*-symmetry breaking asymmetric double-well potential.

The obtained recursion relation for this potential is giving by

$$a_j(E) = \frac{[4\beta j - 6\beta - E]a_{j-2}(E) - [4\beta^2 + Z^2]a_{j-4}(E) + a_{j-6}(E) + iga_{j-3}(E)}{j(j-1)}, \qquad (3.6)$$

where g is the constant a.

3.2.2. Computation the eigenvalues of *PT*-symmetry breaking asymmetric double-well

The eigenenergies can be solved simply by our numerical approach for Eq. (3.6).

In Table 3, we generate the convergence for the ground state for selected values of a, Z^2

and where $\beta = 3$. The value of β is arbitrary which influenced the speed of convergence.

To verify the accuracy of our result, let us compare the present result for the *PT*-

symmetry breaking for asymmetric double-well potential with the result of $V(x) = x^4 +$

iax potential when $Z^2 = 0$. We observed that we got the same results that confirms the

validity of our result. In addition, in Table 3 we found that the energies are decreasing as

the value of Z^2 is increased, which is the same as what happened with the potential

$V(x) = -Z^2 x^2 + x^4$, (see Table 2).

Table 3. Calculated energies of the $-Z^2 x^2 + x^4 + iax$ when $\beta = 3, I = 100$.

Z^2	a	Ground state energy
0	0	1.060 362 090 484 182 899
	1/2	1.093 466 139 188 256 564
	1	1.194 489 941 700 681 387
1	0	0.657 653 005 180 715 123
	1/2	0.709 766 641 840 917 137
	1	0.874 018 501 170 905 018
10	0	-0.746 861 430 490 580 877
	1/2	-0.608 541 702 234 180 966
	1	-0.329 658 719 536 922 472
15	0	-10.986 879 892 897 338
	1/2	-11.061 490 126 645 762 828
	1	-2.319 216 019 191 387 423

Table 4, below, shows the rate of convergence when the number of iterations

changes. It is apparent that the convergence is increased if we increased the number of

iteration. This iteration method gives accurate results for the eigenvalues; the

convergence is apparent in 27 digits when the number of iterations was around 500 and

800.

Table 4. The eigenvalues for PT-symmetry breaking DWP for different value for I

Iteration	Ground state energy
20	0.873
80	0.874 018 497
100	0.874 018 501 105
160	0.874 018 501 170 905
240	0.874 018 501 170 905 018
400	0.874 018 501 170 905 018 521 306
500	0.874 018 501 170 905 018 521 306 261
800	0.874 018 501 170 905 018 521 306 261 741 242 634 813 750 935 387

3.2.3. The wave functions of the PT-symmetry breaking asymmetric double-well

Once we obtained the eigenvalues for the potential $V(x) = -Z^2 x^2 + x^4 + iax$

using the Gaussian function by the iteration approach, the wave functions are calculated

using (2.10). In Figure 7 and 8 we show the calculated wave functions for the ground and

first excited states. In both figures, (a) and (b) represent the real and the imaginary parts

of the ground and first excited states.

$$PT\ \Psi^0(x) = -\Psi^0(x)$$

$$PT\ \Psi^1(x) = -\Psi^1(x)$$
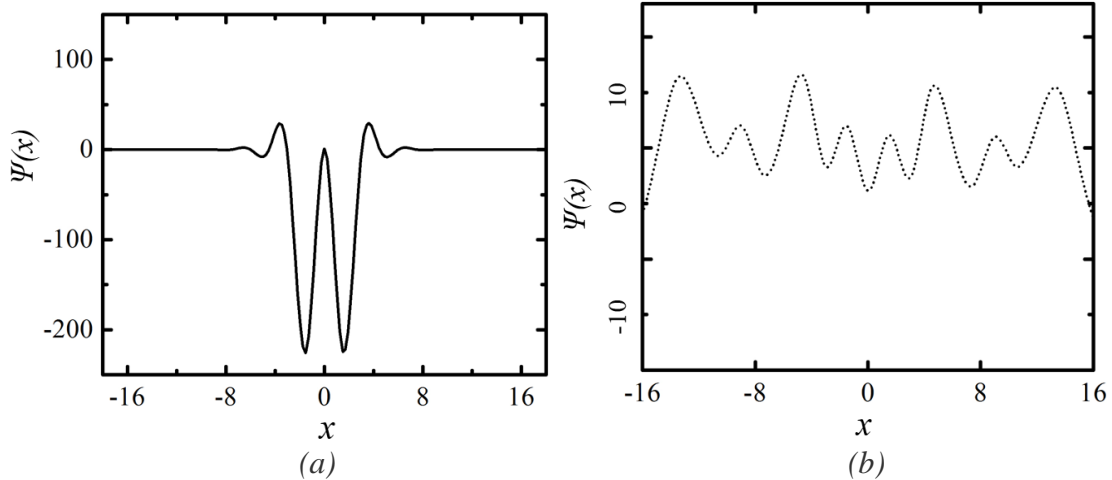
Figure 7. The real and the imaginary parts of the ground state wave function for $-Z^2x^2 + x^4 + iax$; *(a)* the real and *(b)* the imaginary.
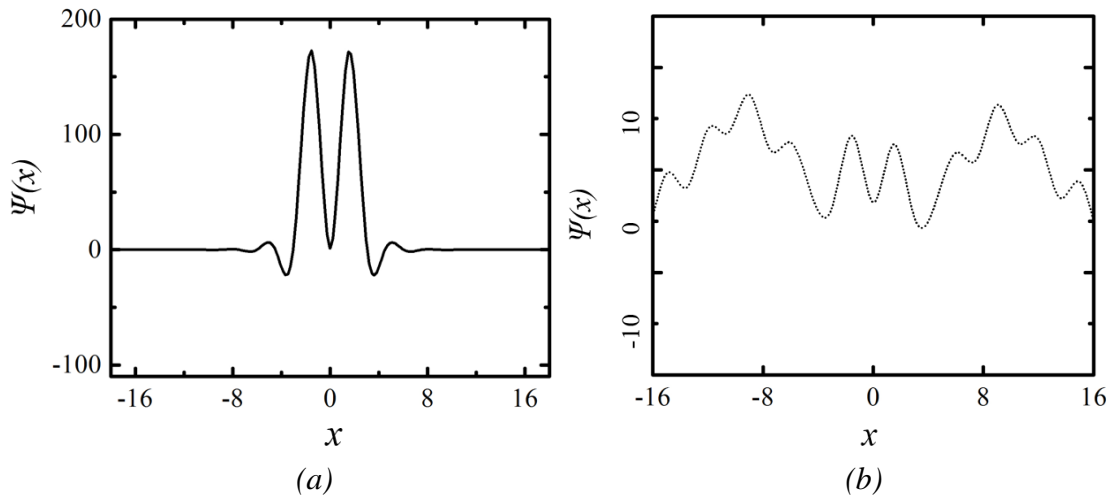
Figure 8. The real and the imaginary parts of the first excited state wave function for $-Z^2x^2 + x^4 + iax$; *(a)* the real and *(b)* the imaginary.

The real part of the ground and first excited states wave functions are odd, and the imaginary part for both states (ground and first excited states) are odd. Thus, *PT*-symmetry is broken since the eigenfunctions of a non-Hermitian Hamiltonian are not the eigenfunctions of the *PT* operator.

3.3.1 The iterative method for $ix^3 + iax$ potential

The Schrödinger equation for the complex cubic oscillator takes the form

$$-\frac{d^2\Psi}{dx^2} + (ix^3 + iax)\Psi(x) = E\Psi(x),\tag{3.7}$$

where $\Psi(x)$ is a Gaussian function Eq. (7). Moreover, a is a real number.

The recursion relation obtained using Eq. (2.1) and Eq. (3.7) is

$$a_j(E) = \frac{[4\beta j - 6\beta - E]a_{j-2}(E) - [4\beta^2]a_{j-4}(E) + ia_{j-5}(E) + iga_{j-3}(E)}{j(j-1)}\tag{3.8}$$

where g is the constant a.

3.3.2. The eigenvalues for PT-symmetry breaking $ix^3 + iax$

The main interest in studying PT-symmetry breaking potentials is focused on proving the reality and the analyticity of the spectrum. We obtain the eigenvalues by using the recursion relation above, Eq. (3.8). Table 5 represents the rate of convergence for the ground and first excited states energies when we use the iteration method. We obtain converging lower bounds to the real and the imaginary parts of the spectrum. To illustrate, we have only considered the ground and first excited states energies for PT-symmetry breaking potential for different numbers of iteration in Table 6. We compare our result with EMM and MFR results. Table 6 is an examination of our results using the

iteration method with others [5,7]. Our results make a clear comparison between the present results and others.

Table 5. The ground and the first excited states energies for $ix^3 + iax$.

I	Ground state	First-excited state
20	1.894	6.576
50	1.856 102	5.149 956
100	1.856 110 766 050	5.150 168 955 811
200	1.856 110 766 056 684 162	5.150 168 955 614 649 670
400	1.856 110 766 056 684 162 135	5.150 168 955 614 650 048 905
800	1.856 110 766 056 684 162 135 435 661	5.150 168 955 614 650 048 905 575 658

Table 6. The calculated ground energies of $ix^3 + iax$ potential.

g	Ground state energy	Refs. [7]	Refs. [5]
0	1.1562670681075082420	1.1562673	1.15626695
1	1.8561107115851683097	1.8561128	1.85611065
2	2.7467401183563921144	2.7467434	2.74673952
3	3.7985546301426592457	3.7985559	3.79855387

3.3.3. The wave functions for $ix^3 + iax$

We considered the wave functions for the ground and first excited states and sketched them in Figures 9 and 10. Figure (a) represent the real parts of the ground and first excited states. Figure (b) represent the imaginary parts of both states. The real and imaginary parts of the wave functions are even and odd for the ground and first excited states.

(a)   *(b)*
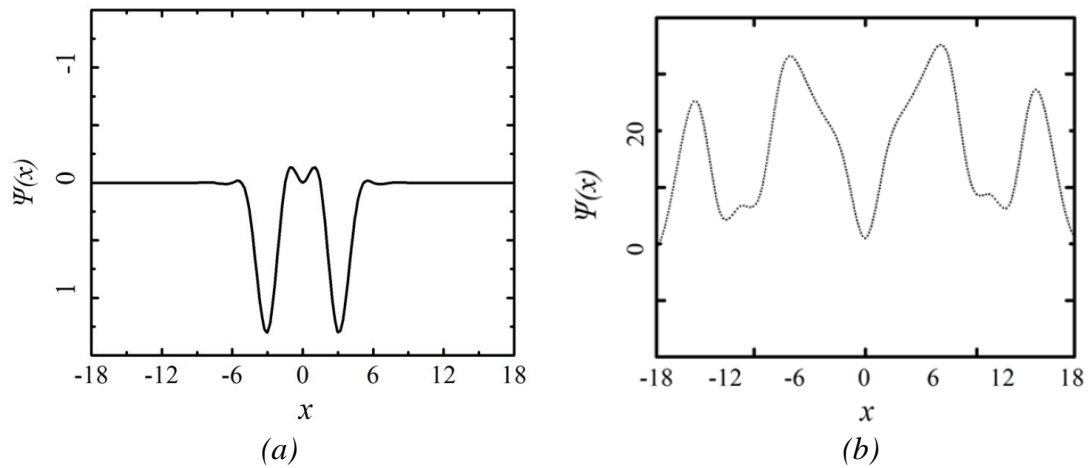
Figure 9. (a) the real and (b) the imaginary ground state wave function for $ix^3 + iax$.

(a)   *(b)*

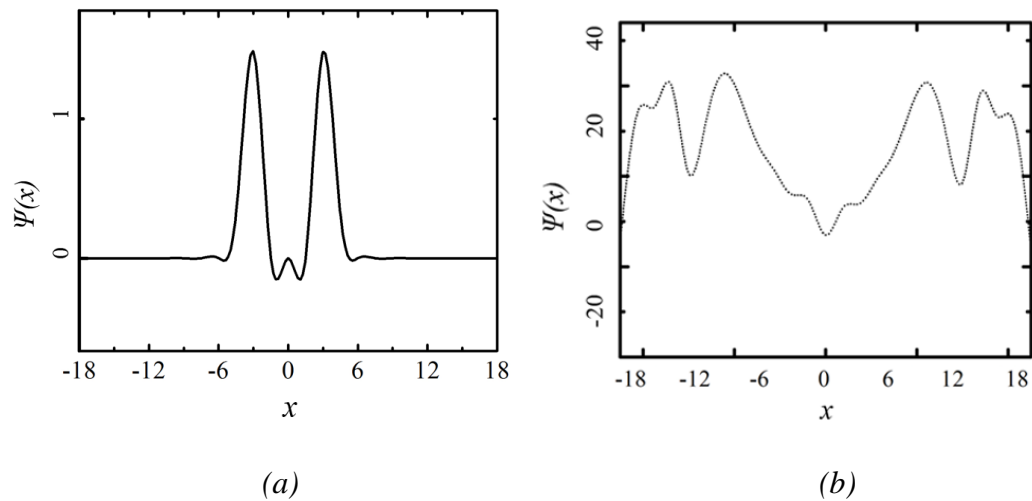Figure 10. (a) the real and (b) the imaginary first-excited state wave function for $ix^3 + iax$.

3.4.1. The iterative method for complex quartic oscillator $x^4 + iax$

In this example, we examine the PT-symmetry breaking potential $x^4 + iax$ which leads the Schrödinger equation to the form

$$-\frac{d^2\Psi}{dx^2} + (x^4 + iax)\Psi(x) = E\Psi(x), \qquad (3.9)$$

where $\Psi(x)$ is a Gaussian Function Eq. (2.2) and a is a real number.

For the quartic oscillator, the obtained recursion equation takes the form

$$a_j(E) = \frac{[4Bj - 6B - E]a_{j-2}(E) - [4B^2]a_{j-4}(E) + a_{j-6}(E) + iga_{j-3}(E)}{j(j-1)} \qquad (3.10)$$

where g is the constant a.

3.4.2. Computing the eigenvalues for PT-symmetry breaking $x^4 + iax$

Some previous works [8,14,15] developed techniques to study the PT-symmetry breaking Hamiltonian. Within the framework of the iterative approach mentioned in the Chapter Ⅱ, the complex quartic oscillator eigenenergies are calculated by using Eq. (3.10). We calculated the energies for the ground and first excited states. In Table 7, we display the energies for the $x^4 + iax$ using the Gaussian function by the iteration method. The comparsion of our calculated eigenvalues with the results from reference [8] is presented in Table 8. We compare the present results for the ground state eigenvalues with the EMM [8] results by adjusting the value of a. This comparsion exhibits the accuracy of our strategy. It is observed that the obtained eigevalues are in excellent agreement with the EMM [8] results.

Table 7. Calculated energies for $x^4 + iax$, $\beta=1$, a=1/2.

I	Ground state	First-excited state
50	1.094 981	3.819 790
100	1.093 466 139	3.803 502 880
150	1.093 466 139 188	3.803 502 880 349
200	1.093 466 139 188 256 564	3.803 502 880 349 278 336
300	1.093 466 139 188 256 564 273	3.803 502 880 349 278 334 945
500	1.093 466 139 188 256 564 273 285	3.803 502 880 349 278 334 945 227
800	1.093 466 139 188 256 564 273 285 106 131	3.803 502 880 349 278 334 945 227 882 965

Table 8. Comparison of the eigenvalues for $x^4 + iax$ with those of EMM.

a	Ground state energy	Refs. [8]
0	1.060 362 090 491	1.060 362 090 481
0.5	1.093 466 139 192	1.093 466 139 185
1	1.194 489 941 700	1.194 489 941 696
2	1.630 730 794 298	1.630 730 794 288
3	2.622 699 057 180	2.622 699 057 103

3.4.3. The wave function for $x^4 + iax$ potential

Similar to the complex cubic oscillator, the real part of the wavefunction is even, and the imaginary part is odd. In Figure 11 and 12, we have plotted the wave functions for the real and the imaginary parts of the ground and the first excited states. These plots were generated with the values of x between $-8 \leq x \leq 8$.

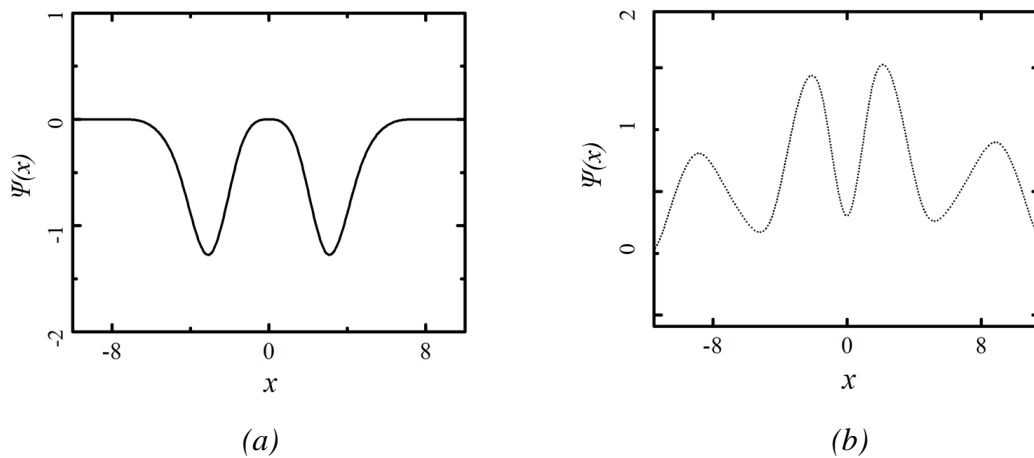(a)   (b)

Figure 11. The real and the imaginary parts of the ground state wave function for $x^4 + iax$; *(a)* the real and *(b)* the imaginary parts.

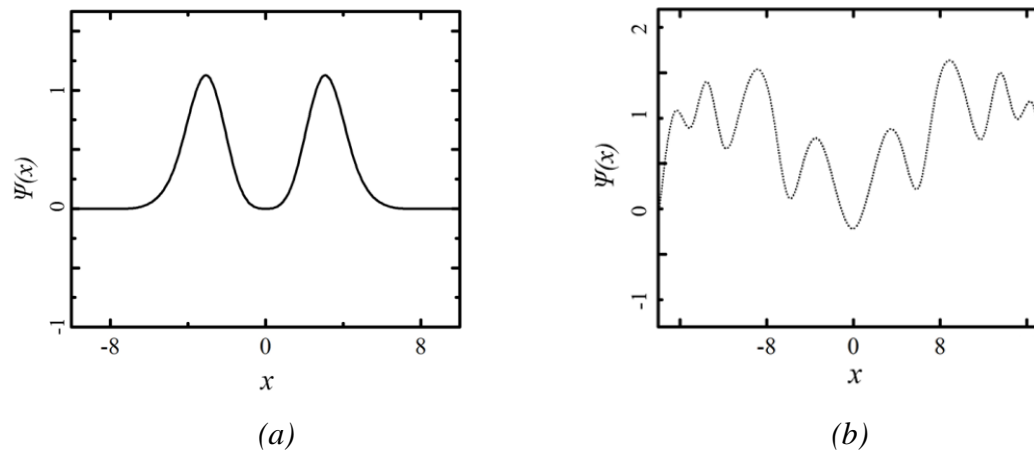(a)   (b)

Figure 12. The real and the imaginary parts of the first-excited state wave function for $x^4 + iax$; *(a)* the real and *(b)* the imaginary parts.

CHAPTER IV

CONCLUSION

To summarize, we have described in detail the use of an iterative approach to the double-well potentials. As such, for a deep well potential, the energy difference between the two levels are small for deep well potentials. This condition requires an efficient calculation method to handle the accuracy and convergence.

In addition, we considered perturbations of *PT*-symmetric Hamiltonians. We considered a particular way to truncate the power series expansion. By using the iteration method, we were able to produce the converging bounds for the complex energies. We confirmed the general results which derived by other methods. Using readily accessible algebraic programming software, we obtained tight, lower bounds to the real and imaginary parts of the discrete state range.

In this thesis, we presented a precise and simple approach for implementation in the study of various potentials energies. We proved that an iteration method is an accurate approach to numerically extract the eigenvalues. Our results conclude that the iterative method is very easy to implement for calculating double-well potential and *PT*-symmetric potentials.

APPENDIX A

The Mathematica code for $-Z^2x^2 + x^4 + iax$

The code below is formed to find the eigenvalues for the potential $-Z^2x^2 + x^4 + iax$.

```
ClearAll ["Global`*"]

n=100;(*Number of iterations*) B=3;(*Value of Beta*) g=1; (*Value of g*)   Z=0;

(*Value of Z)T=Table[Subscript[m,i,j],{i,n},{j,1}];(*Creating a column matrix to store

iterated polynomials*)

For[i=2,i<n+1,i++,For[j=1,j<2,j++,T[[i,j]]=0]]

Q=T;P=T;omg=T;A=T;Q=T;R=T;S=T;K=T;F=T;

For[i=1,i<n+1,i++,omg[[i,1]]=(4*B*(i-1)-6*B-X)]; A[[1,1]]=1;A[[2,1]]=1;

For[i=3,i<n+1,i++,(*This loop iterates the recursion relation*)

(P[[i,1]]=Expand[((omg[[i,1]]*A[[i-2,1]]))];

If[i>4,Q[[i,1]]=Expand[(-Z-4*B*B)*A[[i-4,1]]]];

If[i>6,R[[i,1]]=Expand[A[[i-6,1]]]];

If[i>3,S[[i,1]]=Expand[I*g*A[[i-3,1]]]];

A[[i,1]]=Expand[((P[[i,1]]+Q[[i,1]]+R[[i,1]]+S[[i,1]]))/((i-2)*(i-1))];)]

pa=Expand[A[[n,1]]];pb=Expand[A[[n-1,1]]];

ZZ=Expand[Re[pa]*Re[pb]+Im[pa]*Im[pb]];

FindRoot[ZZ==0,{X,1},WorkingPrecision->20
```

APPENDIX B

The Mathematica code for $x^4 + iax$

The code is formed to calculate the eigenvalues for the potential $x^4 + iax$.

```
ClearAll["Global`*"]

n=100;(*Number of iterations*)  B=1;(*Value of Beta*)   g=3; (*Value of g*)

T=Table[Subscript[m,i,j],{i,n},{j,1}];(*Creating a column matrix to store iterated

polynomials*)

For[i=2,i<n+1,i++,For[j=1,j<2,j++,T[[i,j]]=0]]

Q=T;P=T;omg=T;A=T;Q=T;R=T;S=T;

For[i=1,i<n+1,i++,omg[[i,1]]=(4*B*(i-1)-6*B-X)]; A[[1,1]]=1;A[[2,1]]=1;

For[i=3,i<n+1,i++,(*This loop iterates the recursion relation*)

(P[[i,1]]=Expand[((omg[[i,1]]*A[[i-2,1]]))];

If[i>4,Q[[i,1]]=Expand[(-4*B*B)*A[[i-4,1]]]];

If[i>6,R[[i,1]]=Expand[A[[i-6,1]]]];

If[i>3,S[[i,1]]=Expand[I*g*A[[i-3,1]]]];

A[[i,1]]=Expand[((P[[i,1]]+Q[[i,1]]+R[[i,1]]+S[[i,1]]))/((i-2)*(i-1))];)]

pa=Expand[A[[n,1]]];pb=Expand[A[[n-1,1]]];

ZZ=Expand[Re[pa]*Re[pb]+Im[pa]*Im[pb]];

 FindRoot[ZZ==0,{X,1},WorkingPrecision->20]
```

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