Quantum Particle in a PT-symmetric Well

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ABSTRACT

In this thesis, we study the role of boundary conditions via $\mathcal{PT}$-symmetric quantum mechanics. Where $\mathcal{P}$ denotes parity operator and $\mathcal{T}$ denotes time reversal operator. We present the boundary conditions so that the $\mathcal{PT}$-symmetry remains unbroken. We give exact solvable solutions for a free particle in a box. In the first approach, we consider one dimensional Schrödinger Hamiltonian for a free particle in an infinite well. The energy equation is obtained and the results for the Eigenfunctions of the $\mathcal{PT}$-symmetry are observed completely different form the usual textbooks ones. The second approach is the solution of the Klein Gordon equation in 1+1 dimensions for the free particle in an infinite well. For both cases, the $\mathcal{PT}$-symmetric eigenfunctions are normalized and plotted. The asymptotic behavior of the eigenfunction is provided. We consider a variational principle for $\mathcal{PT}$-symmetric quantum system and examine an invertible linear operator $\hat{\eta}$ for a weak-pseudo-hermicity generators for non-Hermitian Hamiltonian.

Keywords: Hamiltonian, $\mathcal{PT}$-symmetric Quantum Mechanics, Variational Principle, Eigenvalues and Eigenfunctions.

ÖZ

Bu tezde,sınır koşullarının rolü, $\mathcal{PT}$ -simetrik kuantum mekaniği aracılığıyla incelenmiştir. $\mathcal{P}$ parite operatörü; $\mathcal{T}$ ise zaman tersinmesi operatörünü ifade etmektedir. $\mathcal{PT}$ -simetri koşulunu yerine getiren sınır koşullarını sunduk. İlk bölümde, sonsuz kuyu içindeki serbest bir parçacık için bir boyutta Hamilyoniyeni ele alınıyo $\mathcal{PT}$ -simetri özfonksiyonlarını, alışılmış ders kitaplarında gördüğümüzden tamamen farklı bir biçimde elde ederken enerji denklemini bulduk. İkinci bölümde ise sonsuz kuyu içindeki serbest parçacık için 1+1 boyutta Klein Gordon denkleminin çözümüdür. Her iki durum için de, $\mathcal{PT}$ -simetri özfonksiyonları normalize edilmiş ve çizilmiştir. Özfonksiyonun asimptotik davranışı sağlanmıştır. Son bölümde, $\mathcal{PT}$ -simetrik kuantum systemi için varyasyon prensibi dikkate alınmış ve non-hermityen Hamiltoniyen kullanarak, zayıf psödo hermityenlik üreteçleri için tersinir bir lineer operatör incelenmiştir.

Anahtar Kelimeler: Hamiltoniyen, $\mathcal{PT}$ -simetrik Kuantum Mekaniği, Varyasyon prensibi, Özdeğerler ve Özfonksiyonlar.

DEDICATION

To My Family

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INTRODUCTION

Quantum mechanics is one of the fundamental theories in physics that has not been altered many decades after the theory was first discovered and formulated. One fundamental postulate in the quantum theory is the Hermiticity of observables which is one of the necessary and sufficient conditions for the reality of expectation values [5]. Recently, studies have revealed that it is possible to formulate non-Hermitian inner products in quantum mechanics. The non-Hermitian operator provides a new field of study in quantum mechanics known as $\mathcal{PT}$-symmetry. Where $\mathcal{P}$ denotes party operator $\left(\mathcal{P}x\mathcal{P}=-x\right)$, $\mathcal{T}$ denotes time reversal $(\mathcal{T}\, i\mathcal{T}=-i)$ and $\mathcal{PT}$-symmetric potential satisfies $V^{*}\left(-r\right)=V\left(r\right)$.

This theory was first introduced by Carl M. Bender (1998). They claimed that the new $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians has characteristics similar to the Hermitian one with real energy spectrum ref. [13]. In (1999), Bender, Boettcher and Meisinger [6] proposed a generalized class of one-dimensional Hamiltonian operator which exhibits $\mathcal{PT}$-symmetry.

$$\hat{H}=-\frac{\hbar^{2}}{2m}\frac{\partial^{2}}{\partial x^{2}}+x^{2}\left(ix\right)^{\epsilon},\quad \left(\epsilon>0\right), \tag{1.1}$$

where ϵ is a real deformation parameter. Their research showed that (using numerical and semi-classical techniques) this Hamiltonian acquires some asymptotic behavior by setting the deformed parameter $\in \geq 0$, have real and positive spectra [6].

There have been several studies on non-Hermitian Hamiltonians with a real spectrum and their physical applications. Perhaps the most common is the pseudo-Hermitian and $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian used in modeling unitary quantum system [1, 2].

Moreover, works on non-Hermitian Hamiltonians with periodic boundary conditions have been analyzed [17]. Solvable $\mathcal{PT}$-symmetric potentials in 2 and 3 dimensions have also been examined [8]. In addition, surprising spectra of $\mathcal{PT}$-symmetric point interaction have been studied [20]. Completeness and orthonormality in $\mathcal{PT}$-symmetric quantum systems were also examined [12].

Mathur and Isaacson (2011) proposed new approach to study the role of non-Hermitian boundary conditions for a particle in a box. Hence, one may ask, what would happen to the physical system if the Hamiltonian remains Hermitian, but the boundary conditions are changed in such a way that the wave functions are is $\mathcal{PT}$-symmetric?

The aim of this thesis is to provide an exact solution for a $\mathcal{PT}$-symmetric quantum mechanical particle in a box using a Hermitian Hamiltonian. This method is a useful technique that can be added to known types of $\mathcal{PT}$-symmetric quantum mechanical problems [10]. Furthermore, we provide a comparison of solutions to the Klein-Gordon equation in 1+1-dimensions with Hermitian boundary and using $\mathcal{PT}$-boundary wave functions. We formulate a variational principle for $\mathcal{PT}$-symmetry;

this has studied in nonlinear waves and applications in nonlinear optics and atomic physics [19]. We consider throughout this thesis one-dimensional time-independent Schrödinger equation.

This study is structured as follows: In chapter 2; we present our one-dimensional Hermitian Hamiltonian operator for a particle in an infinite square well and introduced our $\mathcal{PT}$ -symmetric boundary condition and their dimensionless constants. We obtain the solution of the energy eigenvalues and corresponding eigenfunction based on the $\mathcal{PT}$ -symmetry.

We also present our calculations for the Klein-Gordon equation in 1+1-dimensions and we study its solution for Hermitian boundary and $\mathcal{PT}$ -symmetry boundary cases. Plots of probability densities for both the Hermitian and $\mathcal{PT}$ -symmetric boundary conditions are also presented.

In chapter 3, we give a brief review of the variational principle based on Rayleigh-Ritz principle and present the variational principle formulation for the $\mathcal{PT}$ -symmetry. In chapter 4, a contradicting example of exact solvability is introduced. An invertible linear operator η for weak-pseudo-hermicity generators for non-Hermitian Hamiltonians is used and a simple generating function potential is presented. Plots of the wavefunction, energy levels, real potential function as well as the effective potential are all presented. Finally, in chapter 5, the conclusions of the results are presented.

Chapter 2

PARTICLE IN A BOX

2.1 Boundary Conditions

In this chapter, we consider the one- dimensional Schrödinger Hamiltonian for a free particle in an infinite potential well of size L ,

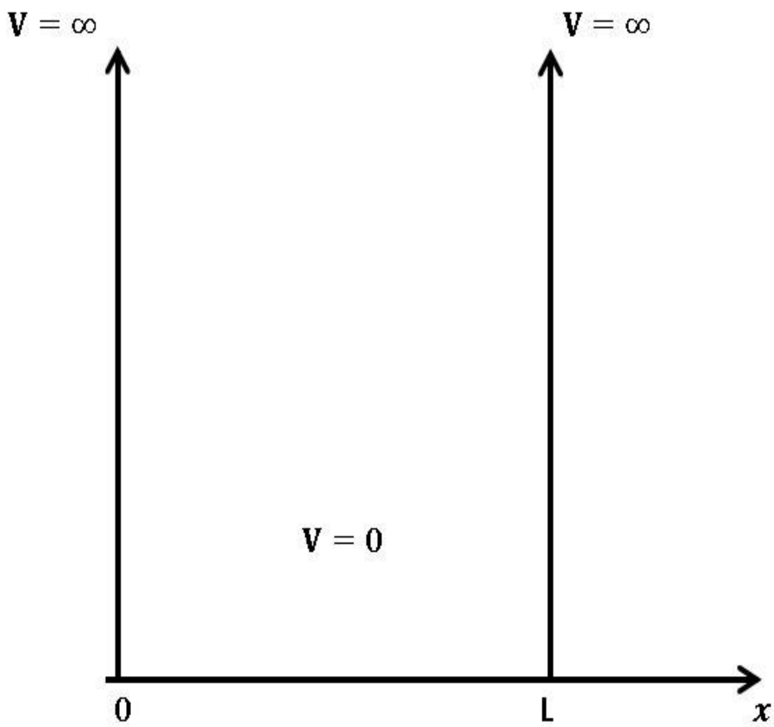

Figure 2.1 Quantum particle in a one dimensional box

Hence, the Hamiltonian operator reads

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,; \qquad 0 < x < L, \tag{2.1}$$

and with $\hbar = m = 1$ units, one gets

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2}. \tag{2.2}$$

From the time-independent Schrödinger equation, $\hat{H}\psi(x) = E\psi(x)$, we obtain

$$\frac{\partial^2}{\partial x^2}\psi(x) + q^2\psi(x) = 0, \tag{2.3}$$

where $q^2 = 2E$. Eq. (2.3) admits a solution of the form

$$\psi(x) = Ae^{iqx} + Be^{-iqx}. \tag{2.4}$$

Applying the parity operator to the eigenfunction above gives

$$\mathcal{P}\psi(x) = \psi(L-x). \tag{2.5}$$

And the time reversal operator is the anti-linear operator,

$$\mathcal{T}\psi(x) = \psi^*(x) = \psi(x), \tag{2.6}$$

where the operator's $[\mathcal{P},\mathcal{T}] = 0$, $\mathcal{P}^2 = 1$ and $\mathcal{T}^2 = 1$. The eigenfunction must satisfy the boundary conditions.

$$\psi(0) = \lambda_1\psi'(0), \quad \psi(L) = \lambda_2\psi'(L), \tag{2.7}$$

where λ_1 and λ_2 are complex numbers. The set (λ_1, λ_2) can be used to describe any boundary condition. However, the case where $\lambda_1 = \lambda_2 = 0$, will take us back to the usual boundary condition in quantum mechanical problems. We will now analyze the similarities and differences between the quantum mechanical model and its $\mathcal{PT}$-symmetric counterpart for a particle in an infinite well. In quantum mechanics, the inner product of two states is given by

$$(\phi(x), \psi(x)) = \int_0^L \phi^*(x)\,\psi(x)\,dx. \tag{2.8}$$

To ensure that the Hamiltonian is Hermitian, the constraint from the boundaries which are applied on the eigenfunctions should be taken into account. Thus, integration by parts of eq. (2.8) gives the self adjointness condition

$$\left(\phi(x), H\psi(x)\right) = \left(H\phi(x), \psi(x)\right),$$

and subsequently

$$\left[\phi^*(x)\psi'(x) - \psi^*(x)\phi'(x)\right]_0^L = 0. \qquad (2.9)$$

which is fulfilled if and only if the surface term, eq. (2.9), vanishes. If the boundary conditions eq. (2.7) on $\psi(x)$ hold, then we can also impose the boundary conditions on the adjoint $\varphi(x)$ as

$$\phi(0) = \lambda_1^*\phi'(0), \quad \phi(L) = \lambda_2^*\phi'(L). \qquad (2.10)$$

In order to fulfill the surface condition of eq.(2.9). Now, we shall formulate the $\mathcal{PT}$ symmetry case. Since $\psi(x)$ obeys the boundary conditions, we can write $\xi(x)$ which also obeys the boundary condition given by

$$\xi(x) = \mathcal{PT}\psi(x) = \psi^*(L-x). \qquad (2.11)$$

The $\mathcal{PT}$-symmetric boundary conditions of eq. (2.11), imply

$$\xi(0) = \psi^*(L), \qquad \xi(\mathrm{L}) = \psi^*(0), \qquad (2.12)$$

and hence

$$\xi'(0) = -\psi^{*\prime}(L), \qquad \xi'(L) = -\psi^{*\prime}(0). \qquad (2.13)$$

If $\psi(x)$ obeys eq. (2.7), we find that $\xi(x)$ automatically fulfills the same boundary conditions if and only if $\lambda_2 = -\lambda_1^*$. Hence, we can write $\mathcal{PT}$-symmetric boundary conditions in terms of the two parameter sets l_1 and l_2 given by

$$(l_1 + il_2, \quad -l_1 + il_2), \qquad (2.14)$$

where l_1, l_2 are real, and are analogous to the Hermitian boundary conditions correspond to (λ_1, λ_2). Furthermore, the two sets are similar, whenever $l_2 = 0$ and $\lambda_1 = -\lambda_2$, respectively. The case $l_1 = 0$ leads to maximally non-Hermitian [3].

2.2 Eigenvalues and Eigenfunctions

In this section we solve for the energy eigenvalues and eigenfunctions for the free particle in an infinite well with the $\mathcal{PT}$-symmetric boundary conditions. In quantum mechanics problems the energy eigenvalues are consider real provided that the Hamiltonian is Hermitian. Hence, there is no guarantee that the energy eigenvalue obtained will be real for non-Hermitian problem, as well the eigenfunctions obtain will be complete. However, under certain conditions the energy spectrum of the $\mathcal{PT}$-symmetric particle in an infinite well is completely real. Moreover, the wave function can be chosen to be the same for both the Hamiltonian and the $\mathcal{PT}$-symmetric, this condition is known as Unbroken $\mathcal{PT}$-symmetry. We can write eq (2.4) in the form

$$\psi(x) = Ce^{iqx} + De^{-iqx}, \tag{2.15}$$

where q , C and D are real constants.

Thus, imposing $\mathcal{PT}$-symmetric boundary condition leads to the quantization

$$e^{i2qL} = \frac{1 - i2ql_1 - q^2(l_1^2 + l_2^2)}{1 + i2ql_1 - q^2(l_1^2 + l_2^2)}. \tag{2.16}$$

Using $\psi(0) = (l_1 + il_2)\psi'(0)$ boundary condition with

$$\psi(0) = C + D, \tag{2.17}$$

and

$$\psi'(0) = (l_1 + il_2)(iqC - iqD). \tag{2.18}$$

gives the amplitude ratio as
$$\frac{C}{D} = -\frac{1 - ql_2 + iql_1}{1 + ql_2 - iql_1}. \tag{2.19}$$

Note that the quantization condition determines the allowed values of q which leads to energy levels. Using eq. (2.15) and eq (2.19) we can obtain the $\mathcal{PT}$-symmetric eigenfunctions. Now, if we take $l_1 = 0$ imply to the non-Hermitian case, which lead the quantization condition $e^{i2qL} = 1$. This condition allowed us to obtain the exact value of q and the energy spectrum is real. However, $l_1 = 0$ refers also to the maximally non-Hermitian case. This also admits real values for q and energy. Hence, we can say the only solution to eq. (2.15) is located on the real axis of plane q only if $l_1 > 0$, and also for $l_1 < 0$, one can obtain complex solutions known as broken $\mathcal{PT}$-symmetric.

In this study, we will focus on $l_1 = 0$ maximally non-Hermitian case, to find the allowed dimensions.

Substituting $l_1 = 0$ into eq. (2.16), implies

$$e^{i2qL} = \frac{1-q^2l_2^2}{1-q^2l_2^2} = 1. \tag{2.20}$$

Hence, one finds

$$2qL = 2n\pi, \Rightarrow q_n = \frac{n\pi}{L}, \ n = 1, 2, 3.. \tag{2.21}$$

Then the energy eigenvalues from $q^2 = 2E$ will be

$$E_n = \frac{n^2\pi^2}{2L^2}. \tag{2.22}$$

Using eq. (2.19) with $l_1 = 0$ implies $\frac{C}{D} = -\frac{1-ql_2}{1+ql_2}$. Eq. (2.15), then becomes

$$\psi_n(x) = D[-\frac{1-ql_2}{1+ql_2}e^{iq_nx} + e^{-iq_nx}], \tag{2.23}$$

which can be simplified to

$$\psi_n(x) = \mathbf{N}_n[\sin(q_nx) + iq_nl_2\cos(q_nx)], \tag{2.24}$$

where $\mathbf{N}_n = \frac{-i2D}{1+q_nl_2}$, is the normalization constant.

Hence, we can observe that the eigenvalues of the maximally non Hermitian Hamiltonian case are analogous to the Hermitian quantum mechanical one. The eigenfunctions, however, are quite different. From eq. (2.24) we can write the adjoint of eigenfunctions in the form

$$\phi_n(x) = \mathbf{N}_c \left[\sin(q_n x) - i q_n l_2 \cos(q_n x)\right]. \tag{2.25}$$

Then, by bi-orthogonality, the normalization constant can be determined from the normalization condition

$$\left(\phi(x), \psi(x)\right) = \int_0^L \phi_m^*(x) \psi_n(x)\, dx = \delta_{m,n}. \tag{2.26}$$

Let us, for simplicity, $m = n,$ and $N_n^2 = N_c N_n.$

$$N_n^2 \int_0^L (\sin(q_n x) + i q_n l_2 \cos(q_n x))^2 \, dx = 1. \tag{2.27}$$

And subsequently,

$$N_n^2 [\frac{(L - q_n^2 l_2^2 L)}{2}] = 1 \quad \Rightarrow N_n^2 = \frac{2}{L} \frac{1}{(1 - q_n^2 l_2^2)}. \tag{2.28}$$

Thus, normalization constant will be

$$N_n^2 = \frac{2}{L} \frac{1}{(1 - q_n^2 l_2^2)}. \tag{2.29}$$

A symmetric way to partition eq. (2.29) is to choose the normalization constant as

$$N_n = \sqrt{\frac{2}{L(1 - q_n^2 l_2^2)}}. \tag{2.30}$$

where $N_c = -sgn(n) N_n$ and $sign(n)$ is the sign of $q_n^2 \, l_2^2 - 1.$

The eigenfunctions can be written as

$$\psi_n(x) = \mathbf{N}_n [\sin(q_n x) + i q_n l_2 \cos(q_n x)]. \tag{2.31}$$

where $N_n = \sqrt{\frac{2}{L(1 - q_n^2 l_2^2)}}.$

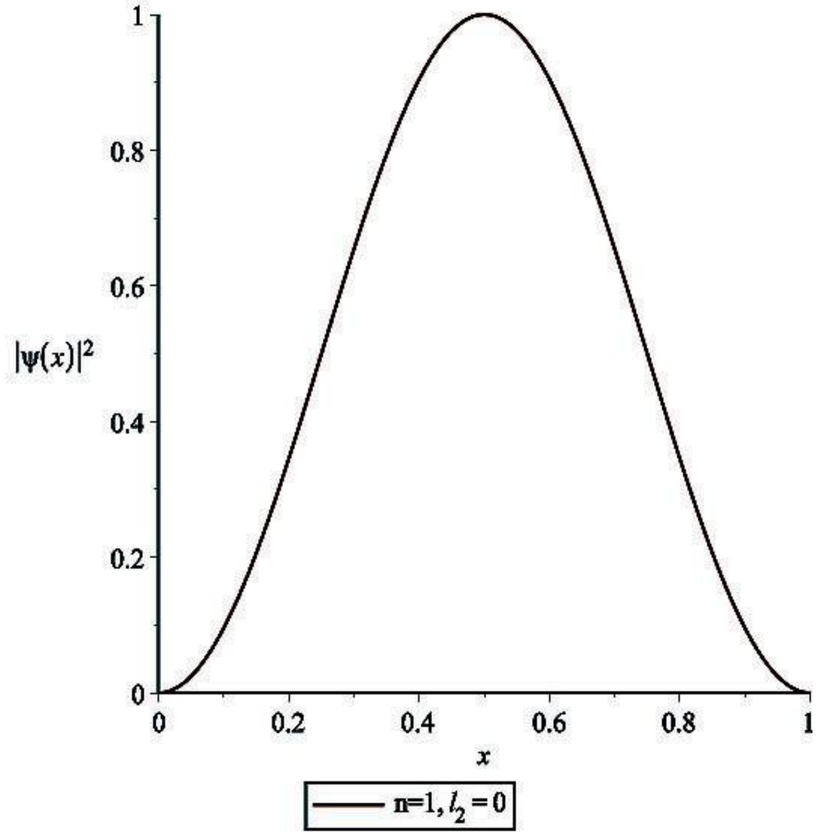

Figure 2.2: Probability density using the wavefunction in eq. (2.31).

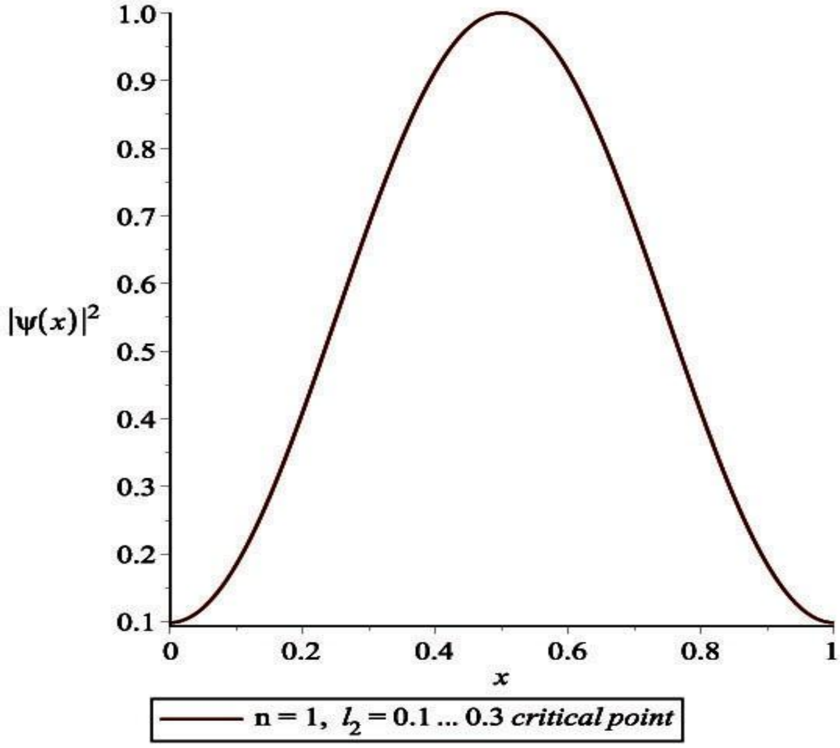

Figure 2.3: Probability density at critical point $l_2 = 0.3$.

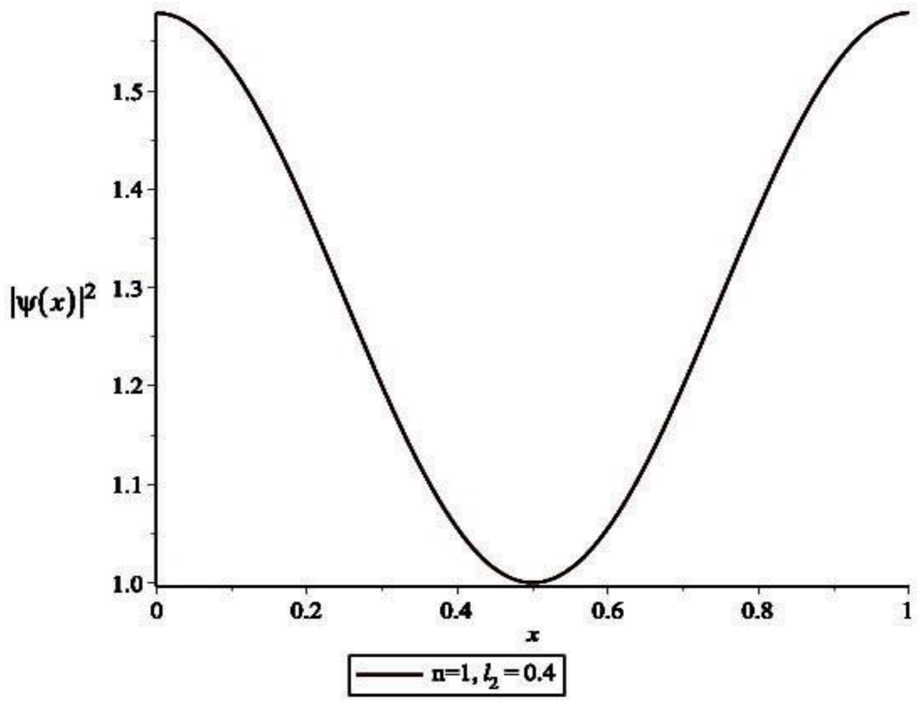

Figure 2.4: Probability density beyond critical point $l_2 > 0.3$.

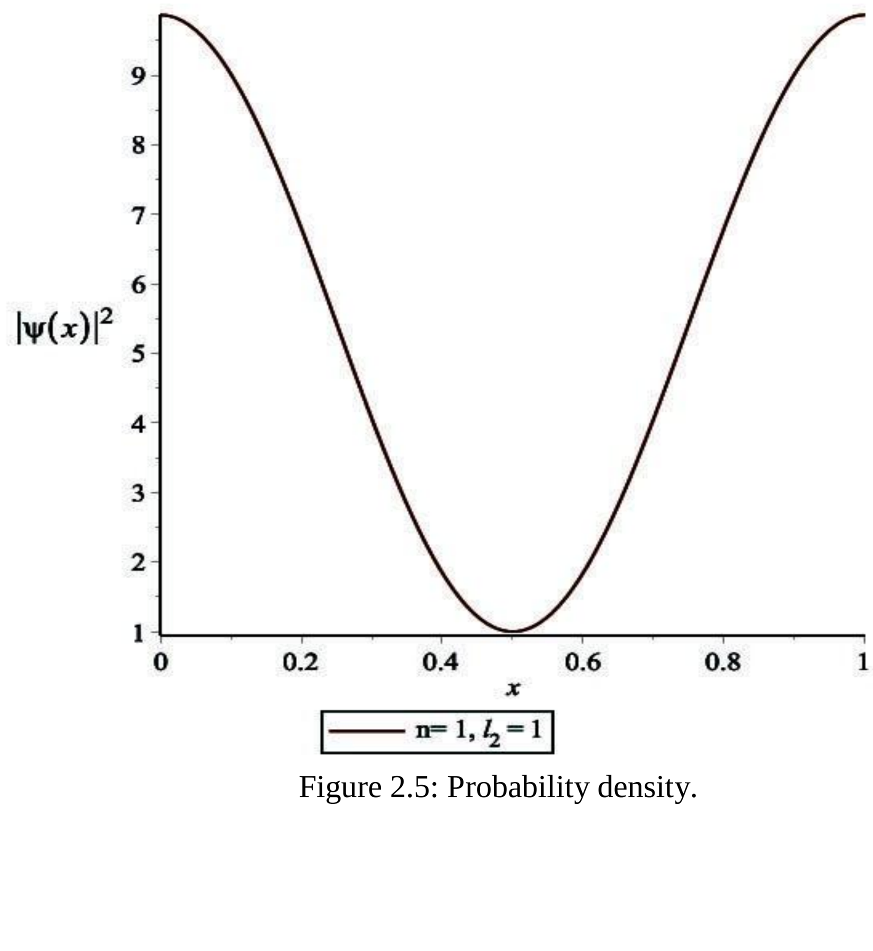

Figure 2.5: Probability density.

2.3 Inner Products

Referring to the $\mathcal{PT}$ -symmetric boundary conditions, we may introduce a $\mathcal{PT}$ scalar product which is self-adjoint. Prior to the work in ref. [2] the Self-adjointness of the $\mathcal{PT}$ inner product is a condition that the wavefunction of a $\mathcal{PT}$ -symmetric quantum Hamiltonian must satisfy. Hence, from $\mathcal{PT}$ -symmetric self adjointness we can observe that upon the PT scalar product the eigenstates are orthonormal for an infinite well. The orthogonality is disparate from the bi-orthogonality utilized in finding the normalization constants above.

For a finite dimensional arrangement, the Eigenstate can be embodied as a column of complex numbers given by $\psi(x)$ and the inner product given in eq. (2.8), can be composed as $\left(\phi(x),\psi(x)\right)=\phi^{\dagger}(x)\,\psi(x)$. However, the $\mathcal{PT}$ inner product can be written as

$$\left(\phi(x),\psi(x)\right)_{\mathcal{PT}}=\left(\mathcal{PT}\phi(x)\right)^{\mathcal{PT}}\ \psi(x)=\int_0^L\phi^*(L-x)\,\psi(x)\,dx. \tag{2.32}$$

We may observe that eq. (2.32) ought to be different from the common inner product eq. (2.8). This result shows that the $\mathcal{PT}$ -symmetric inner product suffers from a defect which may not be a positive definite. Eq. (2.32) has the commutation property $\left(\phi(x),H\,\psi(x)\right)_{\mathcal{PT}}=\left(\ H\,\phi(x)\,,\psi(x)\right)_{\mathcal{PT}}$.

Hence, the $\mathcal{PT}$ -symmetry equality can certainly hold provided the surface term vanishes,

$$\left[\phi^*(L-x)\psi'(x)+\phi^{*\prime}(L-x)\,\psi(x)\right]_0^L, \tag{2.33}$$

and provided both $\psi\left(x\right)$ as well as $\phi(x)$ satisfy the boundary conditions.

2.4 Klein-Gordon Particle in One Dimensional Box

In this section, we will find the solution for the Klein-Gordon equation in 1 + 1 dimensions for a free particle in an infinite square well using the $\mathcal{PT}$ -symmetric boundary condition.

We start with the Klein Gordon equation

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}-\frac{\partial^2\psi}{\partial x^2}+m_0^2c^2\psi=0, \tag{2.34}$$

where

$$\psi(x,t)=R(x)e^{-\frac{iEt}{\hbar}}. \tag{2.35}$$

Hence, with $\hbar=1$, one finds

$$\frac{d^2R}{dx^2}+q^2R=0, \tag{2.36}$$

Where
$$q^2=\frac{E^2}{c^2}-m_0^2c^2. \tag{2.37}$$

Using eq.(2.37), one can find the energy equation given by

$$E=\pm c\sqrt{q^2+m_0^2c^2}=\pm\left|E_q\right| \tag{2.38}$$

Eq. (2.36) admits a solution given by

$$R(x)=Ae^{iqx}+Be^{-iqx}. \tag{2.39}$$

Substituting eq. (2.39) into eq. (2.35), we obtain

$$\psi(x,t)=A\,e^{i(qx-Et)}+\ B\,e^{-i(qx+Et)}, \tag{2.40}$$

which can be simplified to

$$\psi(x,t)=A\cos(qx)e^{-iEt}+\ B\sin(qx)\,e^{-iEt}. \tag{2.41}$$

Now, we will use Eq. (2.41) to study the boundary conditions in related to a particle in a box and the corresponding $\mathcal{PT}$ symmetric case.

2.5 Case I; Hermitian Boundary Condition

Boundary conditions: At $x = 0, \quad R(0) = 0.$

$$A\cos(0) + B\sin(0) = 0, \; A = 0. \tag{2.42}$$

Hence, one finds

$$\psi(x,t) = B \; \sin(qx). \tag{2.43}$$

At $x = L, \quad R(L) = 0,$ imply

$$B \; \sin(qL) = 0, \tag{2.44}$$

and subsequently

$$qL = n\pi, \quad q = \frac{n\pi}{L}, \quad n = 1, 2, 3... \tag{2.45}$$

Finally, the wave function can be written as

$$\psi_n(x,t) = B\sin\left(\frac{n\;\pi}{L}x\right)e^{-iEt}, \tag{2.46}$$

where *B* is the normalization constant.

To find B, we use the normalization condition

$$\langle\psi\,|\,\psi\rangle = \int_v \rho dx = constant, \tag{2.47}$$

where ρ is the charge density ,

$$\rho = \frac{i}{2\;m\;c^2}\left(\psi^* \;\frac{\partial\psi}{\partial t} - \;\psi\;\frac{\partial\psi^*}{\partial t}\right). \tag{2.48}$$

Hence

$$\rho(\pm) = \;\pm\frac{e|E_q|}{m\;c^2}\,\psi_\pm^*(x,t)\psi_\pm(x,t). \tag{2.49}$$

Therefore, the eigenfunction and it adjoint can be written as

$$\psi_n(x,t) = B\,e^{-i(qx-Et)}, \quad \psi_n^*(x,t) = Be^{i(qx-Et)}. \tag{2.50}$$

Substituting eq. (2.50) and eq. (2.49) into eq. (2.47), we get

$$\int_0^L \frac{\pm e\left|E_q\right| \; B^2}{m\, c^2} dx = \ \pm e, \tag{2.51}$$

which simplifies to obtain

$$B = \ \pm \sqrt{\frac{m\, c^2}{\left|E_q\right| \; L}}. \tag{2.52}$$

Finally, the general solution becomes

$$\psi_n(x,t) = \pm \sqrt{\frac{m\, c^2}{\left|E_q\right| \; L}} \; \sin\left(\frac{n\ \pi}{L} x\right) e^{-iEt}. \tag{2.53}$$

2.6 Case II; $\mathcal{PT}$ -Symmetry

The $\mathcal{PT}$ symmetry boundary condition is governed by

$$\psi\left(0\right) = \left(l_1 + il_2\right)\psi'(0). \tag{2.54}$$

and subsequently

$$\psi\left(x\right) = Ae^{i(qx-Et)} + Be^{-i(qx+Et)}, \ \Rightarrow \psi\left(0\right) = Ae^{-iEt} + Be^{-iEt}. \tag{2.55}$$

Hence

$$\psi'\left(x\right) = iqAe^{i(qx-Et)} - iqBe^{-i(qx+Et)}, \quad \Rightarrow \psi'\left(0\right) = iqAe^{-iEt} - iqBe^{-iEt}. \tag{2.56}$$

Thus, substituting eq. (2.56) and eq. (2.55) into eq. (2.54), we get

$$Ae^{-iEt} + Be^{-iEt} = \left(l_1 + il_2\right)\left(iqAe^{-iEt} - iqBe^{-iEt}\right), \tag{2.57}$$

which can be simplified to

$$A + B = \left(il_1 q - il_2 q\right) A + \left(-iql_1 + l_2 q\right) B. \tag{2.58}$$

And collecting like terms we have

$$A\left(1 - il_1 q - il_2 q\right) = -\left(1 + iql_1 - l_2 q\right) B. \tag{2.59}$$

Finally, from eq. (2.59) we obtain the amplitude ratio as

$$\frac{A}{B} = -\frac{(1+iql_1 - l_2 q)}{(1-il_1 q + il_2 q)}. \tag{2.60}$$

From quantization equation

$$e^{i2qL} = \frac{1-i2ql_1 - q^2\left(l_1^2 + l_2^2\right)}{1+i2ql_1 - q^2\left(l_1^2 + l_2^2\right)}.$$

Since we consider $l_1 = 0,$ then one can write the quantization in the form

$$e^{i2qL} = \frac{1-q^2 l_2^2}{1-q^2 l_2^2} = 1. \tag{2.61}$$

And subsequently

$$2qL = 2n\pi, \quad \Rightarrow q = \frac{n\pi}{L}, \; n = 1,2,3.. \tag{2.62}$$

Therefore, the energy equation can be obtain from the two equations of wave number q that is given by

$$q = \frac{n\pi}{L}, \qquad q = \sqrt{\frac{E^2}{c^2} - m_0^2 c^2}. \tag{2.63}$$

Hence, equating the wave number eq. (2.63) and solving for energy we obtain

$$E_n^2 = \frac{n^2\pi^2}{L^2} c^2 + m_0^2 c^4. \tag{2.64}$$

However, to solve for the eigenfunction we substituted $l_1 = 0$ into eq.(2.60) and using eq. (2.40) we get

$$\psi_n(x,t) = B\left[\frac{A}{B} e^{iq_n x} + e^{-iq_n x}\right] e^{-iEt}. \tag{2.65}$$

Substituting the amplitude ratio into eq. (2.65), we have

$$\psi_n(x,t) = B\left[-\frac{(1-l_2 q)}{(1+l_2 q)} e^{iqx} + e^{-iqx}\right] e^{-iEt}. \tag{2.66}$$

This can be written as

$$\psi_n(x,t) = B[-\frac{(1-ql_2)}{(1+ql_2)}(\cos(q_n x)+\sin(q_n x))+\cos(q_n x)-\sin(q_n x)]e^{-iEt}. \quad (2.67)$$

Expanding the bracket and collecting like terms

$$\psi_n(x,t) = B[-i\sin(q_n x)(1+\frac{1-q_n l_2}{1+q_n l_2})+\cos(q_n x)(1-\frac{1-q_n l_2}{1+q_n l_2})]e^{-iEt}, \quad (2.68)$$

which can be simplified to

$$\psi_n(x,t) = B[-i\sin(q_n x)(\frac{2}{1+q_n l_2})+\cos(q_n x)(\frac{2q_n l_2}{1+q_n l_2})]\, e^{-iEt}. \quad (2.69)$$

And finally,

$$\psi_n(x,t) = \frac{-2i}{(1+q_n l_2)}\, B[\sin(q_n x)+iq_n l_2 \cos(q_n x)]\, e^{-iEt}, \quad (2.70)$$

where B is the normalization constant.

To find B, using normalization condition

$$\langle \psi \,|\, \psi \rangle = \int_v \rho dx, \quad (2.71)$$

Where ρ is the charge density,

$$\rho = \frac{i}{2\, m\, c^2}\left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}\right), \quad (2.72)$$

in which the eigenfunction $\psi_n(x,t)$ is given by

$$\psi_n(x,t) = \frac{-2i}{(1+q_n l_2)}\, B\left[\sin(q_n x)+iq_n l_2 \cos(q_n x)\right]e^{-iEt}, \quad (2.73)$$

and subsequently

$$\psi_n^*(x,t) = \frac{2i}{(1+q_n l_2)}\, B[\sin(q_n x)-iq_n l_2 \cos(q_n x)]e^{iEt}. \quad (2.74)$$

Hence

$$\frac{\partial}{\partial t}\psi_n(x,t) = \frac{-2E}{(1+q_n l_2)}\, B[\sin(q_n x)+iq_n l_2 \cos(q_n x)]e^{-iEt}, \quad (2.75)$$

which implies

$$\frac{\partial}{\partial t}\psi_n^*(x,t)=\frac{2E}{(1+q_nl_2)}B[\sin(q_nx)-iq_nl_2\cos(q_nx)]e^{iEt}. \qquad (2.76)$$

Note that

$$\{\sin(q_nx)-iq_nl_2\cos(q_nx)\}\{\sin(q_nx)+iq_nl_2\cos(q_nx)\}=\left(\sin^2(q_nx)+q_n^2l_2^2\cos^2(q_nx)\right).$$

Thus, substituting eq. (2.76), eq. (2.75), eq. (2.74), eq. (2.73) and eq. (2.72) into eq. (2.71), we get

$$\frac{i}{2\,m\,c^2}\int_0^L -\frac{4iE}{(1+q_nl_2)^2}B^2\left(\sin^2(q_nx)+q_n^2l_2^2\cos^2(q_nx)\right)dx$$

$$-\frac{i}{2\,m\,c^2}\int_0^L\frac{4iE}{(1+q_nl_2)^2}B^2\left(\sin^2(q_nx)+q_n^2l_2^2\cos^2(q_nx)\right)dx=\pm 1. \qquad (2.78)$$

Simplifying eq. (2.78), we obtain

$$\frac{B^2}{m\,c^2}\int_0^L\frac{4E}{(1+q_nl_2)^2}\left(\sin^2(q_nx)+q_n^2l_2^2\cos^2(q_nx)\right)dx=\pm 1. \qquad (2.79)$$

Using the relation $\sin^2(\theta)=\frac{1}{2}\left[1-\cos(2\theta)\right],$ then eq. (2.79) becomes

$$\frac{4\,B^2E}{m\,c^2(1+q_nl_2)^2}\int_0^L\frac{1}{2}\{(1-\cos(2q_nx))+q_n^2l_2^2(1+\cos(2q_nx)\}dx=\pm 1. \qquad (2.80)$$

Integrating eq. (2.80) simplifies to

$$\frac{4B^2E}{m\,c^2(1+q_nl_2)^2}\left[\frac{(L-q_n^2l_2^2L)}{2}\right]=\ \pm 1. \qquad (2.81)$$

Hence, the normalization constant can be written as

$$B=\pm\sqrt{\frac{m\,c^2(1+q_nl_2)^2}{4E(1-q_n^2l_2^2)L}}. \qquad (2.82)$$

Finally, the general wave function eq. (2.70), becomes

$$\psi_n(x,t)=\pm\sqrt{\frac{m\,c^2(1+q_nl_2)^2}{4\,E(1-q_n^2l_2^2)L}}\,\frac{-2i}{(1+q_nl_2)}[\sin(q_nx)+iq_nl_2\cos(q_nx)]e^{-iEt}, \qquad (2.83)$$

which can be simplified to

$$\psi_n(x,t) = \pm\sqrt{\frac{m\,c^2}{4E(1-q_n^2 l_2^2)L}}(-2i)\left[\sin(q_n x) + i q_n l_2 \cos(q_n x)\right]e^{-iEt}. \qquad (2.84)$$

Hence,

$$\psi_n(x,t) = \mp i\sqrt{\frac{m\,c^2}{E(1-q_n^2 l_2^2)L}}\left[\sin(q_n x) + i q_n l_2 \cos(q_n x)\right]e^{-iEt}. \qquad (2.85)$$

In summary, the usual particle in a box Klein-Gordon equation eigenfunction and energy equations are eq. (2.38) and eq. (2.64), while the case of $\mathcal{PT}$ symmetry are given by eq. (2.53) and eq. (2.85). However, we could observe the energy equations are identical while the eigenfunction differs due to the $\mathcal{PT}$ symmetry boundary conditions.

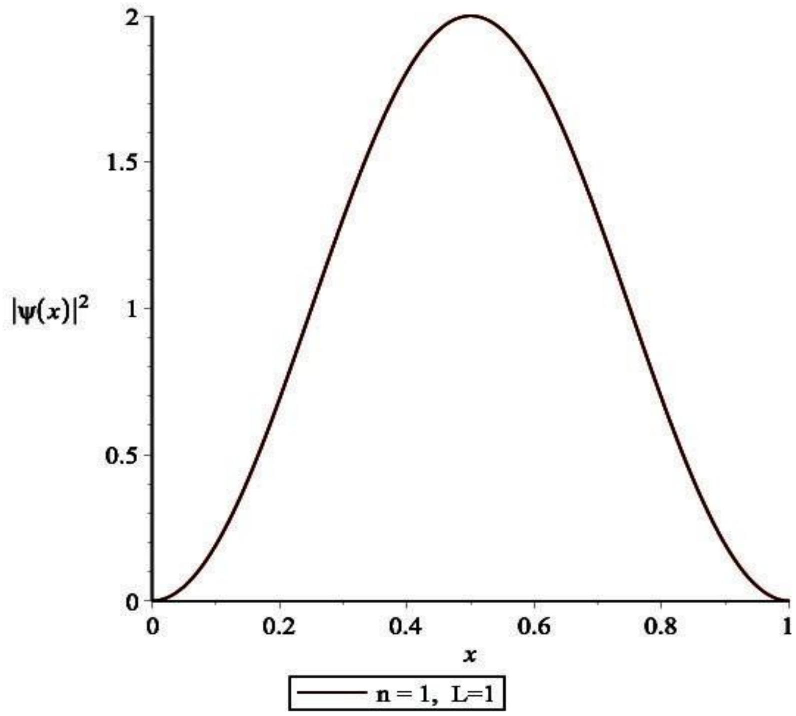

Figure 2.6: Probability density for the wavefunction in eq. (2.53) for infinite square well with Hermitian case boundary conditions.

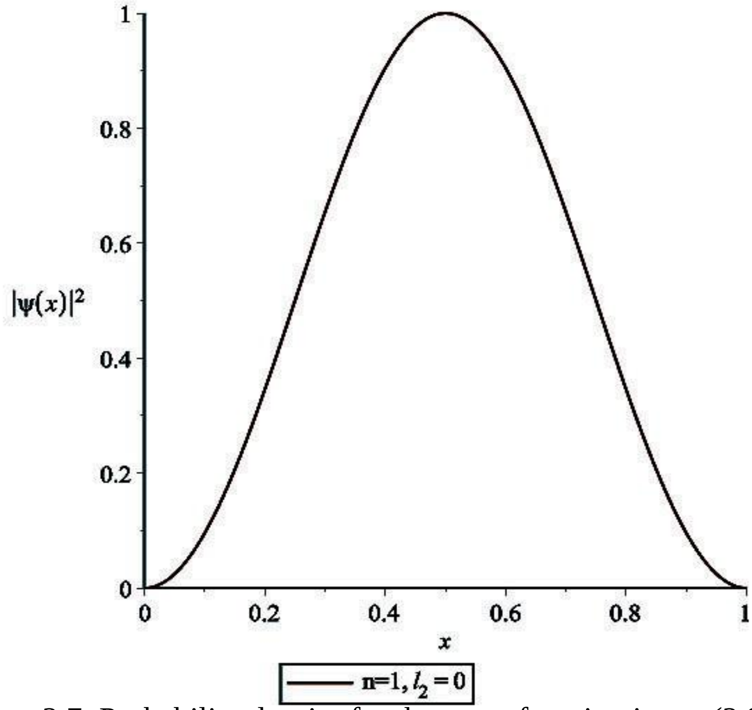

Figure 2.7: Probability density for the wave function in eq. (2.85) square well with $\mathcal{PT}$ -symmetry boundary conditions.

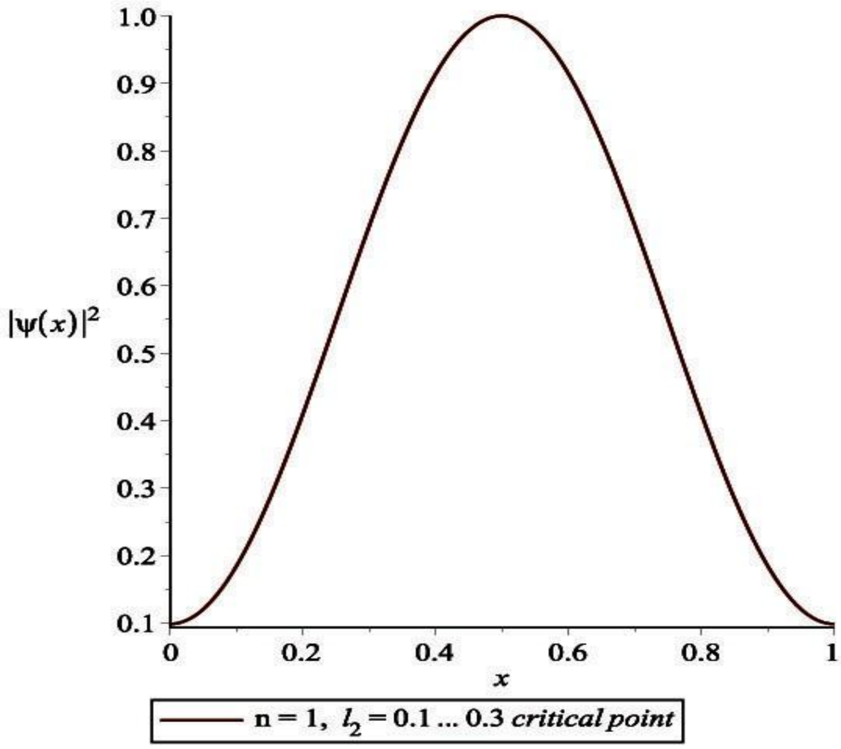

Figure 2.8: Probability density for the wave function in eq. (2.85) up to critical limits 0.3 for an infinite square well with $\mathcal{PT}$ -symmetry boundary conditions.

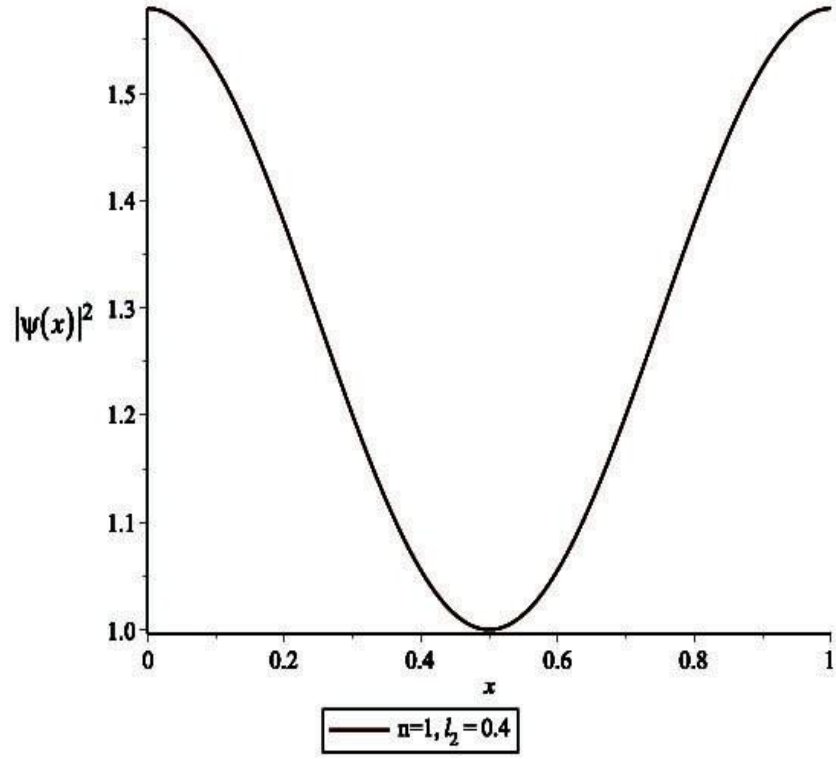

Figure 2.9: Probability density for the wave function in eq. (2.85) beyond critical limits an infinite square well with $\mathcal{PT}$ symmetry boundary conditions.

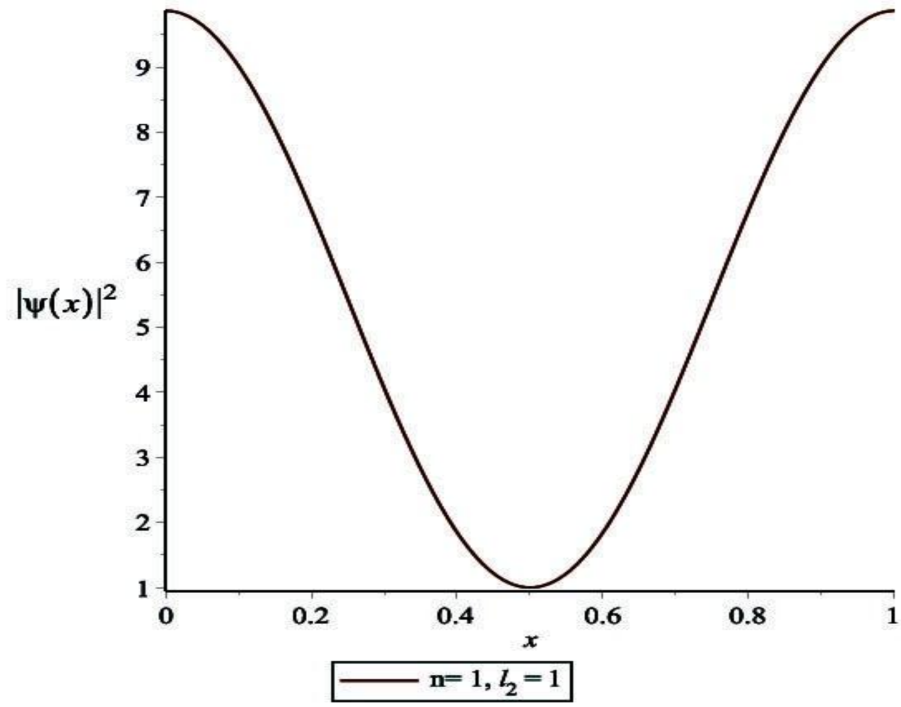

Figure 2.10: Probability density for the wave function in eq. (2.85) beyond critical point.

Chapter 3

VARIATIONAL PRINCIPLE FOR $\mathcal{PT}$ QUANTUM MECHANICS

3.1 Introduction

In this chapter, we will concentrate on the variational principle to study the $\mathcal{PT}$ -symmetric quantum Mechanics. The variational principle applies to another method used to obtain the Schrödinger equation. It an alternative theorem for finding a state or dynamics of a physical system, by noting it minimum or extrema point. For instance, it improves an approximation technique to find the ground-state energy or the presence of bound states for arbitrarily weak binding potentials in a single or in quantum many body problems. It is possible to apply a variational principle to study the $\mathcal{PT}$ quantum mechanics, but only for the cases where the Hamiltonians fulfill the following requirements; $\mathcal{PT}$ -symmetry, Unbroken $\mathcal{PT}$ -symmetry and $\mathcal{PT}$ self-adjointness. Hence, we consider a finite dimensional Hilbert space in which the state function $\psi(x)$ can be represented as a N -component column vector with components $\psi_i(x)$. The Hamiltonian is then a $n \times n$ matrix with element H_{ij} . Let consider a function $\mathbf{R}$ known as Rayleigh function defined as

$$\mathbf{R} = \psi^\dagger(x) H \psi(x), \tag{3.1}$$

where $\mathbf{R}$ is real for Hermitian H .

Proof: Let us define $H\psi(x) = E\psi(x), \quad H^\dagger\psi(x) = E^*\psi(x),$

hence

$\langle\psi(x) | H | \psi(x)\rangle = E\langle\psi(x) | \psi(x)\rangle$, $\Rightarrow \langle\psi(x) | H^\dagger | \psi(x)\rangle = E^*\langle\psi(x) | \psi(x)\rangle.$

Subtracting, the relations we have

$$(E - E^*)\langle \psi(x) | \psi(x) \rangle = 0,$$

Since $\langle \psi(x) | \psi(x) \rangle \neq 0,$ then one finds $E = E^*$, hence this implies $\mathbf{R}$ is real.

Thus, the eigenstates of the Hamiltonian are the states that extremize the Rayleigh Functional subject to normalization condition constraints according to variational principle. From the method of Lagrange multiplier, we must therefore extremize

$$R = \psi^\dagger(x) H \, \psi(x) - \lambda(\psi^\dagger(x)\psi(x) - 1). \qquad (3.2)$$

Taking $\frac{\partial R}{\partial \psi^\dagger} = 0$, then eq. (3.2) gives the Schrödinger equation.

$$H\psi(x) = \lambda \psi(x).$$

Also $\frac{\partial R}{\partial \psi} = 0,$ gives the conjugate part of Schrödinger equation as stated below.

$$\psi^\dagger(x) H = \lambda \psi^\dagger(x), \qquad \Rightarrow H^\dagger \psi(x) = \lambda^* \psi(x).$$

This shows that Hermitian equation H is equivalent, since $H^\dagger = H$ and λ is real.

3.2 Variational Principle of $\mathcal{PT}$ Symmetric Case

We consider the parity and time reversal operators

$$\mathcal{P}\psi(x) = Q\psi(x) \ , \ \mathcal{T}\psi(x) = \psi^*(x),$$

where Q is diagonal matrix with all diagonal entries equal to ± 1. In Hilbert space of $2n$ dimensional case is given by

$$Q = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad (3.3)$$

where I denotes $n \times n$ identity matrix. The $\mathcal{PT}$ inner product, then can be written as

$$\langle \phi(x) | \psi(x) \rangle_{\mathcal{PT}} = (\mathcal{PT}\phi(x))^{\mathcal{PT}} \psi(x) = \phi^\dagger(x) Q \psi(x).$$

Thus, the condition that $\mathcal{PT}$ and the Hamiltonian should commute, implies

$$HQ = QH^*.$$

This imposes the form

$$H = \begin{pmatrix} a & ib \\ ic & d \end{pmatrix}, \tag{3.4}$$

where a,b,c,d are real $n \times n$ matrices.

Proof: $\quad [\mathcal{PT}, H] = 0 \;, \; HQ = QH^\dagger$

Hence

$$[\mathcal{PT}, H]\psi(x) = -\frac{1}{2}[\mathcal{PT}\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x^2}\mathcal{PT}]\psi(x) = -\frac{1}{2}\,[\mathcal{PT}\frac{\partial^2}{\partial x^2} - \mathcal{PT}\frac{\partial^2}{\partial x^2}]\psi(x) = 0.$$

And subsequently

$$HQ = \begin{pmatrix} a & ib \\ ic & d \end{pmatrix}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \begin{pmatrix} a & -ib \\ ic & -d \end{pmatrix}.$$

Hence, we have

$$QH^\dagger = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} a & ib \\ ic & d \end{pmatrix} = \begin{pmatrix} a & -ib \\ ic & -d \end{pmatrix}.$$

This implies $HQ = QH^\dagger$ or equivalently $c = b^\dagger$ in H.

Thus, we choose to introduce $\mathcal{PT}$ counter part of the Rayleigh functional which is given by

$$W = \langle \psi(x) \,|\, H\psi(x) \rangle_{PT} = \psi^\dagger(x) Q \psi(x). \tag{3.5}$$

The functional W is real and can be shown by choosing the state function

$$\psi(x) = \begin{pmatrix} \xi \\ \eta \end{pmatrix}. \tag{3.6}$$

Substituting eq. (3.6) and $Q = QH$ into eq. (3.6), imply

$$W = \begin{pmatrix} \xi^\dagger \\ \eta^\dagger \end{pmatrix}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} a & ib \\ ic & d \end{pmatrix}\begin{pmatrix} \xi \\ \eta \end{pmatrix}, \tag{3.7}$$

which can be simplified to

$$W = \begin{pmatrix} \xi^\dagger \\ \eta^\dagger \end{pmatrix} \begin{pmatrix} a & -ib \\ ic & -d \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}. \tag{3.8}$$

After expanding and simplification of eq. (3.8) we obtain

$$W = \xi^\dagger a\xi - \eta^\dagger d\eta + i\xi^\dagger b\eta - i\eta^\dagger b^\dagger \xi.$$

This shows that W is real since the first two terms are real while last terms are sum of conjugate sets. Variational principle for $\mathcal{PT}$-symmetric quantum mechanics enforces that we must extremize W subject to the constraint:

$$\langle \psi(x) | \psi(x) \rangle_{PT} = 1,\ \langle \psi(x) | \psi(x) \rangle_{PT} = 0,\ \langle \psi(x) | \psi(x) \rangle_{PT} = -1.$$

According to the method of Lagrange multiplier we must look for states $\psi(x)$ that extremize eq. (3.2).

$$\tilde{R} = \psi^\dagger(x) H\psi(x) - \lambda(\psi^\dagger(x)\psi(x) - 1). \tag{3.9}$$

and subsequently we can write

$$\tilde{R}_W = \psi^\dagger(x) QH\psi(x) - \lambda(\psi^\dagger(x) Q\psi(x) - 1). \tag{3.10}$$

Thus, imposing $\dfrac{\partial \tilde{R}_W}{\partial \psi^\dagger(x)} = 0$, yields the eigenvalue problem

$$QH\psi(x) = \lambda Q\psi(x) \quad \Rightarrow H\psi(x) = \lambda\psi(x). \tag{3.11}$$

Equation (3.10) gives the desired result, but imposing $\dfrac{\partial \tilde{R}_W}{\partial \psi(x)} = 0,$ leads to

$$\psi(x)^\dagger QH = \lambda\psi(x)^\dagger Q \quad \Rightarrow H^\dagger\psi(x) = \lambda^*\psi(x). \tag{3.12}$$

We extremize *W*,

$$W = -\frac{1}{2}\int_0^L \psi^*(L-x)\, \frac{\partial^2}{\partial x^2}\psi(x)\, dx. \tag{3.13}$$

Subject to the constraints $\int_0^L \psi^*(L-x)\psi(x)dx = -1, 0 \text{ or } 1.$

Taking variations with respect to $\psi^*(x)$ leads instantly to Schrödinger equation

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi(x)=\lambda\psi(x). \tag{3.14}$$

Also in terms of $\psi(x)$ leads to

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi^*(x)=\lambda^*\psi^*(x). \tag{3.15}$$

Provided the surface term vanishes.

$$\Big[\psi^*(L-x)\delta\psi'(x)+\psi^{*\prime}(L-x)\,\delta\psi(x)\Big]_0^L. \tag{3.16}$$

Typically, the vanishing of the surface term eq. (3.16) actually ensured the required variation of $\delta\psi(x)$ to satisfy the same $\mathcal{PT}$-symmetric boundary conditions for the eigenstates. Therefore, these show the fundamental role of the variational principle of the quantum mechanics $\mathcal{PT}$-symmetric boundary conditions for the particle inside a box.

Chapter 4

η −WEAK-PSEUDO-HERMICITY GENERATORS AND EXACT SOLVABILITY

Recently, non-Hermitian $\mathcal{PT}$-symmetric quantum mechanics has been an active field of study in quantum mechanics. It was shown that it is possible to use Hamiltonian that is Hermitian, and obtained an exact solvable solution that satisfies conditions known as unbroken $\mathcal{PT}$-symmetry, and which Hamiltonian $\hat{H}$ has real energy eigenvalues by applying certain boundary conditions [6]. However, a pseudo-Hermitian Hamiltonian can also be formulated to satisfied same condition without violating the $\mathcal{PT}$-symmetry condition. Thus, we may provide a counterpart example to the η-weak-pseudo-Hermicity generators which equally works well for systems of non-Hermitian Hamiltonian but results to a complex energy eigenvalues that contradict with ref. [18].

Let us define an invertible linear operator $\hat{\eta}$ which is Hermitian and it obey the canonical equation governed by

$$\hat{\eta} = \hat{O}^{\dagger}\,\hat{O} \tag{4.1}$$

where $\hat{O}$ and $\hat{O}^{\dagger}$ are linear operator known as intertwining operators given by

$$\hat{O} = \frac{\partial}{\partial x} + M(x) + iN(x)\,, \quad \hat{O}^{\dagger} = -\frac{\partial}{\partial x} + M(x) - iN(x) \tag{4.2}$$

in which *M(x)* and *N(x)* are real valued functions.

For the purpose of our study we will consider non-Hermitian Schrödinger Hamiltonian operator in dimensions given by

$$\hat{H} = -\frac{\partial^2}{\partial x^2} + V_{eff}(x) \tag{4.3}$$

where $\hbar = 2m = 1,$ and $V_{eff}(x)$ known as the effective potential written as

$$V_{eff}(x) = V(x) + iW(x) \tag{4.4}$$

Accordingly, the Hamiltonian operator in eq. (4.3) is said to be pseudo-Hermitian if it satisfies the relation

$$\hat{H}^{\dagger} = \hat{\eta}\hat{H}\hat{\eta}^{-1} \tag{4.5}$$

and hence one may obtain a real energy spectrum. Moreover, the two intertwining operators as well as the invertible, Hermitian operator η satisfies an intertwining relation

$$\hat{\eta}\hat{H} = \hat{H}^{\dagger}\hat{\eta}. \tag{4.6}$$

Substituting eq. (4.2) into eq. (4.1) imply

$$\hat{\eta} = \left(\frac{\partial}{\partial x} + M(x) + iN(x)\right)\left(-\frac{\partial}{\partial x} + M(x) - iN(x)\right) \tag{4.7}$$

expanding eq. (4.7) and simplifying we get

$$\hat{\eta} = -\frac{\partial^2}{\partial x^2} - 2iN(x)\frac{\partial}{\partial x} + M^2(x) + N^2(x) - M'(x) - iN'(x). \tag{4.8}$$

Evaluating the intertwining relation eq. (4.6) by substituting eq. (4.3) and eq. (4.8) and after an explicit calculation one finds

$$W(x) = -2N'(x), \tag{4.9}$$

and subsequently

$$M^2(x) - M'(x) = \frac{2N(x)N''(x) - N'^2(x) + \alpha}{4N^2(x)}, \tag{4.10}$$

which implies

$$V\left(x\right)=\frac{2N\left(x\right)N''\left(x\right)-N'^{2}\left(x\right)+\alpha}{4N^{2}\left(x\right)}-N^{2}\left(x\right)+\beta. \tag{4.11}$$

in which α and β are real constants.

From eq. (4.9), we obtain

$$N\left(x\right)=-\frac{1}{2}\int W\left(x\right)dx. \tag{4.12}$$

Subsequently from eq. (4.9), we get

$$N'\left(x\right)=-\frac{1}{2}W\left(x\right),\qquad N''\left(x\right)=-\frac{1}{2}W'\left(x\right). \tag{4.13}$$

Substituting eq. (4.13) into eq. (4.10), we have

$$M^{2}\left(x\right)-M'\left(x\right)=\frac{1}{2}\frac{N''\left(x\right)}{N\left(x\right)}-\frac{N'^{2}\left(x\right)}{4N^{2}\left(x\right)}+\frac{\alpha}{4N^{2}(x)}, \tag{4.14}$$

and in terms of *W(x)* potential function gives

$$M^{2}(x)-M'(x)=\frac{1}{2}\left(-\frac{1}{2}\int W(x)dx\right)^{-1}\left(-\frac{1}{2}W'\right)-\frac{1}{4}W^{2}\left[4\left(\frac{1}{2}\int W(x)dx\right)^{2}\right]^{-1}$$

$$+\frac{\alpha}{4}\left[\frac{1}{2}\int W(x)dx\right]^{-2}, \tag{4.15}$$

after simplification eq. (4.15) becomes

$$M^{2}\left(x\right)-M'\left(x\right)=\frac{W'\left(x\right)}{2}\left[\int W\left(x\right)dx\right]^{-1}-\frac{W^{2}\left(x\right)}{4}\left[\int W\left(x\right)dx\right]^{-2}+\alpha\left[\int W\left(x\right)dx\right]^{-2}. \tag{4.16}$$

Also substituting eq. (4.13) into eq. (4.11) and solving for $V\left(x\right)$ we obtain

$$V\left(x\right)=\frac{W'\left(x\right)}{2}\left[\int W\left(x\right)dx\right]^{-1}-\frac{W^{2}\left(x\right)}{4}\left[\int W\left(x\right)dx\right]^{-2}+\alpha\left[\int W\left(x\right)dx\right]^{-2}$$

$$-\frac{1}{4}\left[\int W\left(x\right)dx\right]^{2}+\beta. \tag{4.17}$$

Finally, we will compute the $V_{eff}(x)$ real part potential *V(x)* of the Hamiltonian equation provided by the eq. (4.4) as similar ref. [18]. However, eq. (4.17) will be used to determine the real potential function *V(x)*, using the imaginary part of the effective potential, *W(x)* as a generating function and with some adjustable values of integration constant α and β that would yield an exact solution to the Hamiltonian operator.

4.1 A Contradicting Example

Let us start with a simple generating function given by

$$W(x) = -\frac{1}{2}\frac{k}{x^2}. \tag{4.18}$$

Substituting eq. (4.18) into eq. (4.17) one finds

$$V(x) = \frac{3}{4x^2} + \frac{4\alpha x^2}{k^2} - \frac{1}{16}\frac{k^2}{x^2} + \beta, \tag{4.19}$$

thus, we choose the arbitrary constant $\alpha = \frac{1}{4}$, β=0, we get

$$V(x) = \frac{3}{4x^2} + \frac{x^2}{k^2} - \frac{k^2}{16x^2}. \tag{4.20}$$

Hence, Hamiltonian operator

$$\hat{H} = -\frac{\partial^2}{\partial x^2} + V(x) + iW(x),$$

implies

$$\hat{H} = -\frac{\partial^2}{\partial x^2} + \left(\frac{3}{4x^2} + \frac{x^2}{k^2} - \frac{k^2}{16x^2} - \frac{ik}{2x^2}\right), \tag{4.21}$$

which can be simplified to

$$\hat{H} = -\frac{\partial^2}{\partial x^2} + \left(\frac{3}{4} - \frac{k^2}{16} - \frac{ik}{2}\right)\frac{1}{x^2} + \frac{x^2}{k^2}. \tag{4.22}$$

For simplicity we will consider a new substitution, *l* so that

$$l\left(l+1\right)=\frac{3}{4}-\frac{k^2}{16}-\frac{ik}{2},\quad \omega^2=\frac{1}{\mathrm{k}^2}. \tag{4.23}$$

Then, substituting eq. (4.23) into eq. (4.22), we obtain

$$\hat{H}=-\frac{\partial^2}{\partial x^2}+\frac{l\left(l+1\right)}{x^2}+\omega^2x^2. \tag{4.24}$$

Accordingly, Schrodinger equation $\hat{H}\psi(x)=E\psi\left(x\right)$, imply

$$-\frac{\partial^2\psi\left(x\right)}{\partial x^2}+\left(\frac{l\left(l+1\right)}{x^2}+\omega^2x^2\right)\psi\left(x\right)=E\psi\left(x\right). \tag{4.25}$$

Now, if we choose *E=2E*, eq. (1.25) yields

$$\frac{1}{2}\frac{\partial^2\psi\left(x\right)}{\partial x^2}-\left(\frac{l\left(l+1\right)}{2x^2}+\frac{\omega^2x^2}{2}\right)\psi\left(x\right)=-E\psi\left(x\right). \tag{4.26}$$

We can observe that eq. (4.26) is one dimensions analogy of the 3-D harmonic oscillator which can be solved in spherical coordinates. Since the potential is only radial dependent, the angular part of the solution is a spherical harmonic. However, Let us define a variable

$$z=\gamma x. \tag{4.27}$$

So that

$$\frac{\partial}{\partial x}=\frac{\partial z}{\partial x}\frac{\partial}{\partial z}=\gamma\frac{\partial}{\partial z}, \tag{4.28}$$

and

$$\frac{\partial^2}{\partial r^2}=\left(\frac{\partial z}{\partial r}\right)^2\frac{\partial^2}{\partial z^2}+\frac{\partial^2 z}{\partial r^2}\frac{\partial}{\partial z}=\gamma^2\frac{\partial^2}{\partial z^2}. \tag{4.29}$$

Then eq. (4.26) becomes

$$\frac{\partial^2\psi\left(z\right)}{\partial z^2}+\left(\frac{2E}{\gamma^2}-\frac{l\left(l+1\right)}{z^2}-\frac{\omega^2z^2}{\gamma^4}\right)\psi\left(z\right)=0. \tag{4.30}$$

We now introduce another new substitution

$$q = \frac{2E}{\gamma^2} \ , \ \gamma = \sqrt{\omega}, \tag{4.31}$$

and subsequently

$$q = \frac{2E}{\omega}, \tag{4.32}$$

which upon substituting eq. (4.31) into eq. (4.30) we get

$$\frac{\partial^2 \psi(z)}{\partial z^2} + \left(q - \frac{l(l+1)}{z^2} - z^2 \right) \psi(z) = 0 \tag{4.33}$$

From eq. (4.33) if we consider $(z \to \infty)$ for large *z*. Then eq. (4.33) can be written in more convenient form as

$$\frac{\partial^2 \psi(z)}{\partial z^2} - z^2 \psi(z) = 0. \tag{4.34}$$

Eq. (4.34) admits a solution in the form

$$\psi(z) = Ae^{-\frac{z^2}{2}} + Be^{\frac{z^2}{2}}, \tag{4.35}$$

where A and B are constants. Since at infinity $B = 0,$ then

$$\psi(z) = Ae^{-\frac{z^2}{2}}. \tag{4.36}$$

And subsequently for $(z \to 0)$ small *z*, eq. (4.33), implies

$$\frac{\partial^2 \psi(z)}{\partial z^2} - \frac{l(l+1)}{z^2} \psi(z) = 0. \tag{4.37}$$

Hence, eq. (4.37) also admits a solution given by

$$\psi(z) = Cz^{l+1} + Dz^{-l}, \tag{4.38}$$

where *C* and *D* are constants. Also $D = 0.$ In order not to obtain infinite at $z = 0.$ Thus, we have

$$\psi(z) = Cz^{l+1}. \tag{4.39}$$

Furthermore, proposing a solution to eq. (4.33) of the type

$$\psi(z) = z^{l+1} e^{-\frac{z^2}{2}} F(z). \tag{4.40}$$

Differentiating eq. (4.40), we obtain

$$\psi'(z) = \left(\left[(l+1) - z^2 \right] F(z) + zF'(z) \ \right) z^l e^{-\frac{z^2}{2}}, \tag{4.41}$$

and hence

$$\psi''(z) = lz^{l-1} e^{\frac{z^2}{2}} \left[\left(l+1-z^2 \right) F(z) + zF'(z) \right] - z^{l+1} e^{\frac{z^2}{2}} \left(\left(l+1-z^2 \right) F(z) + zF'(z) \right)$$

$$+ z^l e^{\frac{z^2}{2}} \left[(-2z) F(z) + \left(l+1-z^2 \right) F'(z) + zF'(x) \right]. \tag{4.42}$$

Substituting eq. (4.42) and eq. (4.40) into eq. (4.33), we have

$$\begin{aligned} zF''(z) + \left(l - z^2 + l + 1 - z^2 \right) F'(z) \ + \left(\ l(l+1) z^{-1} - zl \right) F(z) & \\ + \left(-z \left(l+1-z^2 \right) - 2z + qz - l(l+1) z^{-1} - z^3 \right) F(z) = 0, & \end{aligned} \tag{4.43}$$

simplifying further gives

$$zF''(z) + 2\left(l+1-z^2 \right) F'(z) + (q - 2l - 3) zF(z) = 0. \tag{4.44}$$

Let define a new variable

$$\xi = z^2, \tag{4.45}$$

and using the transformation

$$\frac{\partial}{\partial z} = \frac{\partial \xi}{\partial z} \frac{\partial}{\partial \xi} = 2\xi^{\frac{1}{2}} \frac{\partial}{\partial \xi}, \tag{4.46}$$

in which

$$\frac{\partial^2}{\partial z^2} = 4\xi \frac{\partial^2}{\partial \xi^2} + 2\frac{\partial}{\partial \xi}. \tag{4.47}$$

Thus, upon substituting eq. (4.45), eq. (4.46) and eq. (4.47) into the differential equation (4.44) it follows that

$$4\xi^{\frac{3}{2}} F''(\xi) + \left[4(l+1-\xi) + 2 \right] \xi^{\frac{1}{2}} F'(\xi) + (q - 2l - 3) \xi^{\frac{1}{2}} F(\xi) = 0. \tag{4.48}$$

Hence, dividing through eq. (4.48) by $4\xi^{\frac{1}{2}}$ simplifies to

$$\xi F''(\xi)+\left(l+\frac{3}{2}-\xi\right)F'(\xi)+\frac{(q-2l-3)}{4}F(\xi)=0. \tag{4.49}$$

We may observe that the above differential equation (4.49) is well known as Confluent Hyper-geometric equation given in general form as

$$\xi F''(\xi)+(c-\xi)F'(\xi)-aF(\xi)=0. \tag{4.50}$$

However, we may find it exact solutions by power series method. Comparing our differential equation (4.50) with the Confluent Hyper-geometric equation for simplicity we choose to define

$$Q=l+\frac{3}{2},\ b=-\frac{(q-2l-3)}{4}, \tag{4.51}$$

then the differential equation (4.49) becomes

$$\xi F''(\xi)+(Q-\xi)F'(\xi)-bF(\xi)=0. \tag{4.52}$$

We now proceed by proposing a solution of the form

$$F(\xi)=\sum_{r=0}^{\infty}c_r\xi^{n+r}, \tag{4.53}$$

accordingly, differentiating eq. (4.54) 1st and 2nd , we get

$$F'(\xi)=\sum_{r=0}^{\infty}(n+r)c_r\xi^{n+r-1}\ ,\ F''(\xi)=\sum_{\mathrm{r}=0}^{\infty}\mathrm{c_r}\,(n+r)(n+r-1)\,\xi^{\mathrm{n+r\text{-}2}}. \tag{4.54}$$

Putting eq. (4.54) and eq. (4.53) into the differential equation (4.52) yields

$$\sum_{r=0}^{\infty}c_r\,(n+r)(n+r-1)\xi^{n+r-1}+\sum_{r=0}^{\infty}Q(n+r)c_n\xi^{n+r-1}-\sum_{r=0}^{\infty}(n+r)c_r\xi^{n+r}-\sum_{r=0}^{\infty}bc_r\xi^{n+r}=0. \tag{4.55}$$

Collecting like terms of eq. (1.56) we have

$$\sum_{r=0}^{\infty}c_r\,(n+r)\big[(n+r-1)+Q\big]\xi^{n+r-1}-\sum_{r=0}^{\infty}\big[(n+r)+b\big]c_r\xi^{n+r}=0. \tag{4.56}$$

Putting $r=r+1$ in the 1st summation terms, gives

$$\sum_{r=-1}^{\infty} c_{r+1}\left(n+r+1\right)\left[n+r+Q\right]\xi^{n+r} - \sum_{r=0}^{\infty}\left[\left(n+r\right)+b\right]c_r\xi^{n+r} = 0. \qquad (4.57)$$

Expanding the 1st summation, implies

$$c_0 n\left[n-1+Q\right]\xi^{n-1} + \sum_{r=0}^{\infty}\left\{c_{r+1}\left(n+r+1\right)\left[n+r+Q\right] - \left[\left(n+r\right)+b\right]c_r\right\}\xi^{n+r} = 0. \; (4.58)$$

From eq.(4.58) if $c_0 \neq 0,$ then we may find an indicial equation of the form

$$n\left[n-1+Q\right]=0, \qquad (4.59)$$

whose roots implies

$$n=0, \qquad n=1-Q. \qquad (4.60)$$

Hence from eq (4.58) we deduce the recurrence relation is given by

$$c_{r+1} = \frac{\left[n+r+b\right]c_r}{\left(n+r+1\right)\left[n+r+Q\right]}, \qquad (4.61)$$

We now proceed by substitution of the indicial solution $n=0$ into the recurrence relation simplifies to

$$c_{r+1} = \frac{\left[r+b\right]c_r}{\left(r+1\right)(r+Q)}. \qquad (4.62)$$

And after an explicit calculation it follows that eq.(4.62) satisfied a solution in the form

$$F_1\left(\xi\right) = 1 + \frac{b}{Q}z + \frac{b(b+1)}{Q(Q+1)}\frac{z^n}{2!} + \ldots = {}_1F_1(b,Q,\xi), \qquad (4.63)$$

where $Q \neq 0,$ and subsequently $n=1-Q,$ we have

$$c_{r+1} = \frac{\left[r+1-Q+b\right]}{\left(r+2-Q\right)\left(r+1\right)}c_r, \qquad (4.64)$$

this satisfy also to

$$F_2\left(\xi\right) = 1 + \frac{(b-Q+1)}{(2-Q)}z + \frac{(b-Q+1)(b-Q+2)}{(2-Q)(3-Q)}\frac{z^n}{2!} + \ldots, \qquad (4.65)$$

yielding the second solution as

$$F_2(\xi) = {}_1F_1(b-Q+1, 2-Q, \xi). \tag{4.66}$$

Hence, for $c \neq 0, \pm 1, \pm 2, \pm 3,$ the complete two independent solutions to the differential equation (4.52) becomes

$$F(\xi) = A\,{}_1F_1(b, Q, \xi) + Bz^{1-Q}\,{}_1F_1(b-Q+1, 2-Q, \xi), \tag{4.67}$$

where A and B are constants.

Accordingly, we may deduce the wave function eq. (4.40) in the form

$$\psi(z) = z^{l+1} e^{-\frac{Z^2}{2}} F(z), \tag{4.68}$$

in which

$$F(z) = A\,{}_1F_1(b, Q, z^2) + Bz^{1-Q}\,{}_1F_1(b-Q+1, 2-Q, z^2), \tag{4.69}$$

and

$$z = \gamma x, \qquad Q = l + \frac{3}{2}, \; b = -\frac{(q-2l-3)}{4}. \tag{4.70}$$

Finally, the general solution becomes

$$\psi(x) = (\gamma x)^{l+1} e^{-\frac{(\gamma x)^2}{2}} F(\gamma x). \tag{4.71}$$

Where

$$F(\gamma x) = A\,{}_1F_1(b, Q, \gamma^2 x^2) + B(\gamma x)^{1-Q}\,{}_1F_1(b-Q+1, 2-Q, \gamma^2 x^2), \tag{4.72}$$

in which

$$Q = l + \frac{3}{2}, \; b = -\frac{(q-2l-3)}{4}. \tag{4.73}$$

We shall now consider $b = -n_r$, as $x \to \infty$ for the wave function to be well behaved in order to deduce the energy equation. Hence, it follows that the relation

$$b = -\frac{(q-2l-3)}{4} = -n_r. \qquad n_r = 0, 1, 2.... \tag{4.74}$$

Therefore,

$$q = 2l + 3 + 4n_r, \tag{4.75}$$

hence from eq. (4.32) it follows that $q = \dfrac{2E}{\omega}$ upon substituting into eq. (4.74) and solving for E_n. We may obtain the energy eigenvalues given by

$$E_{n_r} = \left(2n_r + l + \frac{3}{2}\right)\omega. \tag{4.76}$$

And since $E = 2E$, then energy eigenvalues becomes

$$E_{n_r} = \left(4n_r + 2l + 3\right)\omega, \tag{4.77}$$

where $\omega^2 = \dfrac{1}{k^2}$ and $l = -(\dfrac{3}{4} - \dfrac{ik}{4})$ or $l = (\dfrac{1}{2} - \dfrac{ik}{4})$.

Thus, for simplicity we choose to work with $l = (\dfrac{1}{2} - \dfrac{ik}{4})$, and finally the complex energy eigenvalues becomes

$$E_{n_r} = \left(4n_r + 4 - \frac{ik}{2}\right)\omega, \tag{4.78}$$

where $\omega^2 = \dfrac{1}{k^2}$.

However, the complete wave function would be given by

$$\psi\left(x\right) = A\left(\gamma x\right)^{l+1} e^{-\frac{(\beta x)^2}{2}} {}_1F_1(b, Q, \gamma^2 x^2), \tag{4.79}$$

where A is normalization constant. $Q = l + \dfrac{3}{2}$, and $b = -\dfrac{\left(q - 2l - 3\right)}{4}$.

To find the normalization constant using the condition $\int_o^\infty \left|\psi(x)\right|^2 dx = 1$. We choose for simplicity $b = 0$, thus

$$ {}_1F_1(0, Q, \gamma^2 x^2) = 1, \tag{4.80}$$

and subsequently

$$\psi(x) = A(\gamma x)^{l+1} e^{-\frac{(\gamma x)^2}{2}}, \tag{4.81}$$

upon substitution in the normalization condition gives

$$A^2 \int_o^\infty (\gamma x)^{2(l+1)} e^{-(\gamma x)^2} dx = 1. \tag{4.82}$$

Comparing eq. (4.82) with the standard integral given by

$$\int_o^\infty x^{2n} e^{-x^2} dx = \frac{1}{2}\Gamma(n+\frac{1}{2}), \tag{4.83}$$

we have

$$A = \frac{\sqrt{2}}{\left[\Gamma(l+\frac{3}{2})\right]^{\frac{1}{2}}} \tag{4.84}$$

hence the complete general wave function is given by

$$\psi_n(x) = \frac{\sqrt{2}}{\left[\Gamma(l+\frac{3}{2})\right]^{\frac{1}{2}}} \frac{(\gamma x)^{l+1}}{n!} e^{-\frac{(\gamma x)^2}{2}} {}_1F_1(b, Q, \gamma^2 x^2), \tag{4.85}$$

where

$$Q = l + \frac{3}{2},\ b = -\frac{(q-2l-3)}{4} \text{ and } l = (\frac{1}{2} - \frac{ik}{4}). \tag{4.86}$$

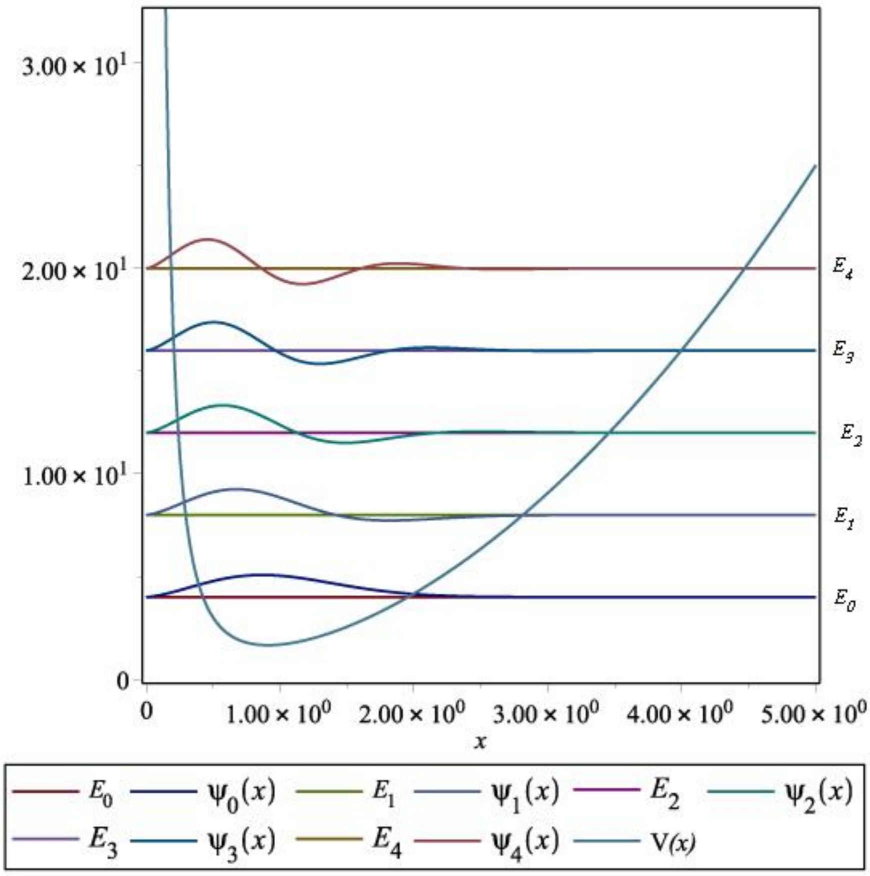

Figure 2.11: Plots of wave function, Energy levels and Potential, $l = 1$.

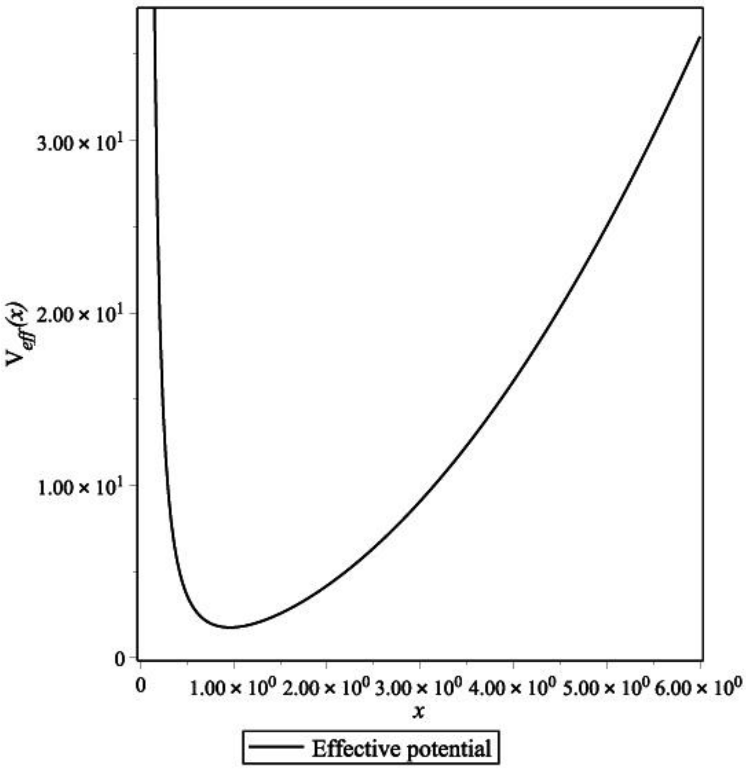

Figure 2.12: Effect potential graph, $l = 1$.

Chapter 5

CONCLUSION

In this thesis report, we study the role of boundary conditions in $\mathcal{PT}$-symmetric quantum mechanics problem. We show that for $\mathcal{PT}$-symmetric quantum particle inside an infinite well, the permitted boundary condition can be written as $(l_1 + il_2,\ -l_1 + il_2)$ where l_1 and l_2 donates real numbers, an analogy to the boundary conditions given by (λ_1, λ_2), where λ_1 and λ_2 are real numbers. However, the case where $\lambda_1 = -\lambda_2$ and $l_2 = 0$, respectively the boundary conditions result to the Hamiltonian that is Hermitian and that satisfy both parity operator as well as time reversal operator. However, in this report, we are interested only in non-Hermitian Hamiltonian but that can satisfy the $\mathcal{PT}$-symmetry problem. Thus, the case $l_1 > 0$, we find not only does the actual Hamiltonian commute with $\mathcal{PT}$ operator, but also a stronger result, known as unbroken $\mathcal{PT}$ is obtained. Basically, one can find simultaneous eigenfunctions of the Hamiltonian and $\mathcal{PT}$-symmetry as well as energy eigenvalues of the Hamiltonian that are necessarily real. In addition we find that the Hamiltonian for a particle inside an infinite well with $\mathcal{PT}$-symmetric boundary conditions is self adjoint under the $\mathcal{PT}$ inner product. This shows that the $\mathcal{PT}$-symmetric quantum particle inside an infinite well fulfills all the three requirements of $\mathcal{PT}$-symmetry quantum problem. We study the Klein Gordon equation with the same boundary conditions and comparison of the results are given for the two cases. The variational principle for the $\mathcal{PT}$-symmetric quantum mechanics that is similar to the usual text book Rayleigh-Ritz principle was studied. Moreover, we have shown that the energy eigenvalues of the maximally non Hermitian box are analogous to the energy eigenvalues of usual quantum mechanical problem, while the eigenfunctions are completely different. Lastly, we showed that $\mathcal{PT}$-symmetric quantum mechanics Hamiltonian could possibly be solved without the necessity of having an imaginary potential that makes the Hamiltonian equation non Hermitian. We also provide a contradicting solution for the η weak-pseudo-hermicity generators of non-Hermitian Hamiltonian which results to a complex energy eigenvalues. Finally, we conclude by identifying some problems for further research. A non Hermitian case $l_1 = 0$ and we limit our research to the case of free particle $V(r) = 0$.

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