

APPLICATION OF PSEUDO-HERMITIAN THEORY TO
THE PT-SYMMETRIC DELTA FUNCTION POTENTIAL
WITH CONTINUOUS REAL SPECTRUM

by

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ABSTRACT

PT-symmetric Hamiltonians and their relation with pseudo-Hermiticity are introduced. For a diagonalizable Hamiltonian H with a discrete spectrum, equivalence of the reality of its spectrum and its E-pseudo-Hermiticity for some positive definite operator E is shown. For such an E-pseudo-Hermitian Hamiltonian H defined on a Hilbert space HS , physical Hilbert space $HS(\text{phys})$ which is consistent with Quantum Measurement Theory is constructed and its unitary equivalence with HS is shown. Then using pseudo-Hermitian Theory the Hamiltonian H , defined on real line and having a PT-symmetric double Delta function potential with a purely imaginary coupling constant Z , is explored. The existence of a critical Z value Z_c which ensures the reality of the spectrum for those Z values whose absolute value is less than the absolute value of Z_c is shown. A biorthonormal system consisting of bounded eigenfunction solutions of H and its adjoint is then chosen to construct a metric operator E up to the first order terms in Z . The equivalent Hermitian Hamiltonian h up to the second order terms in Z is then found. The result is used to calculate the energy expectation values of some Gaussian wave packets and to examine the non-Hermiticity effect on those expectation values. Both in position and momentum spaces interaction regions, outside of which non-Hermiticity effect diminishes rapidly, are found.

ÖZ

PT-Simetrik Hamiltonlar tanıtıldı ve pseudo-Hermisyenlikle olan ilişkileri gösterildi. Kesikli spektrumu olan diyagonalleştirilebilir Hamiltonların spektrumlarının reelliği ile bu Hamiltonların herhangi bir pozitif -belirli bir E operatörü için E -pseudo-Hermisyen olmalarının eşdeğerliği gösterildi. Bir HS Hilbert uzayında tanımlanmış herhangi bir E -pseudo-Hermisyen Hamilton H için Kuantum Ölçüm Teorisi ile uyumlu fiziksel Hilbert uzayı $HS(\text{fiz})$ kuruldu ve bu uzayın HS Hilbert uzayıyla olan üniter eşdeğeliği gösterildi. Daha sonra Pseudo-Hermisyen Teori kullanılarak reel eksen üzerinde tanımlı ve potansiyel kısmı tamamiyle sanal bir Z eklenti sabitli PT-simetrik çift Delta fonksiyonundan oluşan Hamilton H incelendi. H 'in spektrumunun, mutlak değeri belli bir kritik değerden az olan bütün Z değerleri için reel olduğu gösterildi. Z 'de birinci dereceye kadar bir E metrik operatörü oluşturmak için H 'in sınırlı özdeğer fonksiyonlarından oluşan bir çiftlikey sistem seçildi. Daha sonra Z 'de ikinci dereceye kadar eşdeğer Hermisyen Hamilton h bulundu. Sonuç bazı Gaussal dalga paketlerinin beklenen enerji değerlerini hesaplamak için kullanıldı ve H 'in Hermisyen olmayan kısmının bu beklenen enerji değerleri üstündeki etkisi incelendi. Hem pozisyon hem de momentum uzaylarında, dışarısında bu etkilerin hızlıca yok olduğu etkileşim alanları bulundu.

TABLE OF CONTENTS

List of Figures	vii
Chapter 1: Preliminaries	1
1.1 Linear Algebra	1
1.2 Postulates of Quantum Mechanics	8
Chapter 2: Introduction	12
Chapter 3: Characterization of the Reality of the Spectrum	14
Chapter 4: Physical Aspects	17
Chapter 5: Calculation Methods of the Metric Operator η_+ and the Equivalent Hermitian Hamiltonian h	20
Chapter 6: \mathcal{PT}-Symmetric Delta Function Potential	22
6.1 Analysis of the Spectrum	24
6.2 Finding a Biorthonormal System	26
6.3 Construction of the Metric Operator	32
6.4 Physical Analysis	34
6.5 Energy Expectation Value of Some Gaussian Wave Packets	35
Chapter 7: Conclusion	40
Appendices	42
Appendix A: Existence of a Critical G Value G_c	42

Appendix B: Boundedness of η_{+1}	44
Bibliography	46

LIST OF FIGURES

6.1	Plots of the solutions of $Eq1$ (the full curve) and $Eq2$ (the dashed curve) on complex plane for different G values $G_1 = 0.35$, $G_2 = 0.20$, $G_3 = 0.14$ and $G_4 = 0.02$. Horizontal and vertical axes represent real and imaginary axes, respectively. In the first picture, there is no intersection points in the left half plane, so we are in the safe region. For $G = 0.20$ the full curve gets closer to the imaginary axis and there is a pair of intersection points on the imaginary axis. This gives us our critical G value. In the third picture the full curve shifts to the left a little bit more and there appears a complex conjugate pair of intersection points on the left half plane and we get our corresponding complex energy eigenvalues. In the last one we see that while the first pair keeping stay in the left half plane, now there comes a new pair of intersection points to the left half plane as well.	27
6.2	Plots of B_1 as a function of k_0 for $\sigma = 0.5$, $\sigma = 1$, $\sigma = 2$, $\sigma = 3$, $\sigma = 4$ and $\sigma = 5$ in units where $a = 1$	38
6.3	Plots of B_2 as a function of x_0 for $\sigma = 0.2$, $\sigma = 0.5$, $\sigma = 1$, $\sigma = 2$, $\sigma = 6$ and $\sigma = 10$ in units where $a = 1$	39

Chapter 1

PRELIMINARIES

1.1 Linear Algebra

Definition: (Complex Inner Product Space) A Complex Inner Product Space is a complex vector space \mathbb{V} which is endowed with a complex inner product function $\langle \cdot | \cdot \rangle : \mathbb{V} \times \mathbb{V} \longrightarrow \mathbb{C}$ satisfying the following properties:

$\forall v, w, z \in \mathbb{V}$ and $\forall a \in \mathbb{C}$

- $\langle v|v \rangle \in \mathbb{R}^+ \cup \{0\}$ (positivity)
- $\langle v|v \rangle = 0 \Leftrightarrow |v\rangle = 0$ (definiteness)
- $\langle v|(w + z)\rangle = \langle v|w\rangle + \langle v|z\rangle$ (additivity in second slot)
- $\langle v|aw\rangle = a\langle v|w\rangle$ (homogeneity in second slot)
- $\langle v|w\rangle = \langle w|v\rangle^*$ (conjugate symmetry)

where z^* means complex conjugate of z .

Definition: (Normed Vector Space) A Normed Vector Space is a complex vector space \mathbb{V} which is endowed with a norm function $\| \cdot \| : \mathbb{V} \longrightarrow \mathbb{R}$ satisfying the following properties: $\forall v, w \in \mathbb{V}$ and $\forall a \in \mathbb{C}$

- $\|av\| = |a|\|v\|$
- $\|v + w\| \leq \|v\| + \|w\|$
- $\|v\| = 0 \Leftrightarrow v = 0$

Realize that every complex inner product space \mathbb{V} becomes a normed vector space with a norm $\| \cdot \|$ defined as $\|v\| := \sqrt{\langle v|v \rangle} \forall v \in \mathbb{V}$. So when we talk about a topological property of an inner product space, we mean that the topological property exists with respect to the norm induced from its inner product.

Definition: (Complete Normed Space) A normed vector space is called a complete normed space if every Cauchy sequence in it converges, i.e., for every sequence $\{v_n\}_{n \in \mathbb{N}}$ such that $\lim_{M \rightarrow \infty} \|v_M - v_{M+n}\| = 0$ whatever n is, then $\lim_{M \rightarrow \infty} v_M = v$ for some $v \in \mathbb{V}$.

Definition: (Hilbert Space) A complete inner product space is called a Hilbert space.

When we represent vectors in a Hilbert space, instead of using letters, we generally use the Dirac notation in which vectors ψ are represented by ket's $|\psi\rangle$ and the corresponding dual vectors are represented by bra's $\langle\psi|$.

Definition: (Orthonormal Basis) A countable subset $\mathcal{U} := \{|u_n\rangle \in \mathcal{H} \mid n \in \mathbb{N}\}$ of an Hilbert space \mathcal{H} is called an orthonormal basis if it satisfies the following properties:

- $\langle u_n | u_m \rangle = \delta_{nm} \forall |u_n\rangle, |u_m\rangle \in \mathcal{U}$ where δ_{nm} is the Kronecker Delta function which is defined as $\delta_{nm} = 0$ for $n \neq m$, and $\delta_{nm} = 1$ for $n = m$. (orthonormality)¹
- $\forall |\psi\rangle \in \mathcal{H}, |\psi\rangle = \lim_{m \rightarrow \infty} \sum_1^m a_n |u_n\rangle$ for some sequence $\{a_n\}_{n \in \mathbb{N}}$ in \mathbb{C} . (completeness)

The Completeness property allows for a representation of every element $\psi \in \mathcal{H}$ in the orthonormal basis as

$$|\psi\rangle = \sum_n^{\infty} a_n |u_n\rangle. \quad (1.1)$$

¹Note that orthogonality principle implies the linear independence of the elements of \mathcal{U}

Applying orthonormality principle to the completeness we have $a_n = \langle u_n | \psi \rangle$, $\forall n \in \mathbb{N}$. Together with (1.1) this means we can represent any ψ as follows

$$|\psi\rangle = \sum_n^{\infty} |u_n\rangle \langle u_n | \psi \rangle. \quad (1.2)$$

We should note that it may not be possible to represent elements of an arbitrary Hilbert Space in such a way because an arbitrary Hilbert Space does not have to admit such an orthonormal basis. So classification of such Hilbert Spaces which have such an orthonormal basis is necessary.

Definition: (Separable Hilbert Space) A Hilbert space \mathcal{H} is called a separable Hilbert space if it has an orthonormal basis.²

For a finite dimensional Hilbert space an orthonormal basis always exists, so all finite dimensional Hilbert spaces are separable. Therefore when we say separable Hilbert space we mean infinite dimensional ones. In quantum mechanics one usually deals with separable Hilbert spaces. Therefore we will use the term “Hilbert space” to mean “a separable Hilbert space”, unless otherwise is clear from the context.

A Hilbert space with immediate application in quantum mechanics is the space of square integrable functions, $L^2(\mathbb{R}) := \{f : \mathbb{R} \mapsto \mathbb{C} \mid \int_{\mathbb{R}} |f(x)|^2 dx < \infty\}$, with the inner product $\langle f | g \rangle := \int_{\mathbb{R}} f^*(x)g(x)dx$.

Definition: (Linear Operator) A linear operator is a function $T : \mathbb{A} \mapsto \mathbb{B}$ from a vector space \mathbb{A} to a vector space \mathbb{B} with the following properties:

- $\text{Domain}(T)$ is a subspace of \mathbb{A} .
- $T(|v\rangle + |w\rangle) = T|v\rangle + T|w\rangle \quad \forall |v\rangle, |w\rangle \in \mathbb{A}$.
- $T(a|v\rangle) = aT|v\rangle \quad \forall |v\rangle \in \mathbb{A} \text{ and } \forall a \in \mathbb{C}$.

²This definition is mathematically consistent i.e., a separable Hilbert space is separable in topological sense, and a Hilbert space which is a separable topological space is a separable Hilbert space.

Definition: (Anti-linear Operator) An Anti-linear operator is a function $A : \mathbb{A} \mapsto \mathbb{B}$ from a vector space \mathbb{A} to a vector space \mathbb{B} with the following properties:

- $\text{Domain}(A)$ is a subspace of \mathbb{A} .
- $A(|v\rangle + |w\rangle) = A|v\rangle + A|w\rangle \quad \forall |v\rangle, |w\rangle \in \mathbb{A}$.
- $A(a|v\rangle) = a^*A|v\rangle \quad \forall |v\rangle \in \mathbb{A} \text{ and } \forall a \in \mathbb{C}$.

Since a vast majority of operators used in physics are linear, we shall occasionally use the term “operator” to mean a linear operator.

A trivial linear operator is the identity operator $I : \mathcal{V} \mapsto \mathcal{V}$ on a given vector space \mathcal{V} which maps every vector $\psi \in \mathcal{V}$ to itself, i.e., $I\psi = \psi$. In addition if the vector space \mathcal{V} is a separable Hilbert space then we can represent I with respect to a given orthonormal basis $\mathcal{U} := \{|u_n\rangle \in \mathcal{V} \mid n \in \mathbb{N}\}$. Actually, since for an arbitrary vector $|\psi\rangle \in \mathcal{V}$ there exists a basis representation of $|\psi\rangle$ given as (1.2), the basis representation of I is given by

$$I = \sum_n^{\infty} |u_n\rangle\langle u_n|. \quad (1.3)$$

for the given orthonormal basis \mathcal{U} . In general, for an arbitrary operator $K : \mathcal{V} \mapsto \mathcal{V}$ we have

$$K = \sum_{m,n}^{\infty} K_{mn}^{\mathcal{U}} |u_m\rangle\langle u_n| \quad (1.4)$$

where $K_{mn}^{\mathcal{U}} := \langle u_m | K | u_n \rangle$. More generally for a complete, linearly independent and countable but not necessarily orthonormal set $\tilde{\mathcal{U}} = \{|\tilde{u}_n\rangle \in \mathcal{V} \mid n \in \mathbb{N}\}$ of \mathbb{V} , it is possible to characterize a linear operator K with a (finite or infinite) square matrix $\tilde{K}^{\tilde{\mathcal{U}}}$ with entries $\tilde{K}_{mn}^{\tilde{\mathcal{U}}}$ defined by the following identity:

$$K|\tilde{u}_n\rangle = \sum_m^{\infty} \tilde{K}_{mn}^{\tilde{\mathcal{U}}} |\tilde{u}_m\rangle. \quad (1.5)$$

Here the entries $\tilde{K}_{mn}^{\tilde{\mathcal{U}}}$ are called the matrix elements of K with respect to the basis $\tilde{\mathcal{U}}$. In addition if $\tilde{\mathcal{U}}$ is an orthonormal basis, i.e., its elements satisfy orthonormality

as well, then applying to both sides of (1.4) an element $|u_k\rangle$ and comparing the result with (1.5), we see that

$$K_{mn}^{\tilde{\mathcal{U}}} = \tilde{K}_{mn}^{\tilde{\mathcal{U}}}. \quad (1.6)$$

If we have an orthonormal basis \mathcal{U} we will call the numbers $K_{mn}^{\mathcal{U}}$ matrix elements of K with respect to the orthonormal basis \mathcal{U} .

Definition: (Eigenvalue, Eigenvector) For an operator $T : \mathbb{V} \mapsto \mathbb{V}$ on a complex vector space \mathbb{V} if there is a nonzero vector $|v\rangle$, and a number $v \in \mathbb{C}$ such that $T|v\rangle = v|v\rangle$, then $|v\rangle$ is called an eigenvector of T with the corresponding eigenvalue v .

If there are linearly independent eigenvectors which correspond to the same eigenvalue v , then v is called degenerate and the number of linearly independent eigenvectors is called the geometric multiplicity or the degree of degeneracy of the eigenvalue. In this case the subspace which is spanned by eigenvectors of v is called the degeneracy subspace of v .

Note that if K has an orthonormal eigenbasis, i.e., eigenvectors $|k_n\rangle$ of K with eigenvalues k_n forms an orthonormal basis of \mathcal{V} , then the basis representation of K with respect to its eigenbasis becomes

$$K = \sum_n^{\infty} k_n |k_n\rangle \langle k_n|. \quad (1.7)$$

The latter is called the spectral representation of K . Note that in this case the matrix representation of K is a diagonal matrix with diagonal entries k_n .

Definition: (Adjoint of an Operator, Unitary, Hermitian Operators)

Let \mathbb{V}_1 and \mathbb{V}_2 be two inner product spaces with the inner products $\langle \cdot | \cdot \rangle_1$, and $\langle \cdot | \cdot \rangle_2$, respectively, and let $T : \mathbb{V}_1 \mapsto \mathbb{V}_2$ be a linear operator between these two spaces with a dense domain. Then the unique operator $T^\dagger : \mathbb{V}_2 \mapsto \mathbb{V}_1$ satisfying $\langle \psi_2 | T\psi_1 \rangle_2 = \langle T^\dagger \psi_2 | \psi_1 \rangle_1$, $\forall \psi_1 \in \mathbb{V}_1$, $\forall \psi_2 \in \mathbb{V}_2$ is called the adjoint of the operator T .

If $T^\dagger T = I_1$ where I_1 is the identity operator of the first space then T is called a unitary operator.

In the case where $\mathbb{V}_1 = \mathbb{V}_2$, and $\langle \cdot | \cdot \rangle_1 = \langle \cdot | \cdot \rangle_2$ if $T^\dagger = T$ then T is called self-adjoint or Hermitian.

One of the most important properties of a Hermitian operator $L : \mathcal{V} \mapsto \mathcal{V}$ defined on a Hilbert Space \mathcal{V} is that its eigenvalues are real and the eigenvectors which correspond to different eigenvalues are orthogonal [8]. It is also possible to choose a set of orthogonal eigenvectors in each degeneracy subspace, which spans it. So if eigenvectors of L satisfy the completeness property as well then it is possible to form an orthonormal basis of \mathcal{V} consisting of the eigenvectors of L .

Now let us examine a case in which there is a complex vector space which is endowed with two different inner products. So assume that we have an operator $H : \mathbb{V} \mapsto \mathbb{V}$ on a vector space \mathbb{V} , and let $\mathcal{H}_1 := (\mathbb{V}, \langle \cdot | \cdot \rangle_1)$ and $\mathcal{H}_2 := (\mathbb{V}, \langle \cdot | \cdot \rangle_2)$ are two Hilbert Spaces which are identical to \mathbb{V} as a vector space but endowed with different inner products $\langle \cdot | \cdot \rangle_1$ and $\langle \cdot | \cdot \rangle_2$ as Hilbert Spaces. Realize that it is possible that while H is Hermitian with respect to one of the Hilbert Spaces, it may not be Hermitian with respect to the other one. This also shows that Hermiticity of H can only be a sufficient (not necessary) condition for H to have all its eigenvalues real since for an operator, having real eigenvalues is just an algebraic property which only concerns \mathbb{V} as a complex vector space.

Now assume that \mathcal{H}_1 and \mathcal{H}_2 are separable as well and take a countable subset $\mathcal{U} := \{|u_n\rangle\}_{n \in \mathbb{N}} \in \mathbb{V}$ such that $\{|u_n\rangle\}_{n \in \mathbb{N}}$ is an orthonormal basis of \mathcal{H}_1 . Also assume that H is Hermitian with respect to \mathcal{H}_1 . In this case matrix elements $H_{mn}^{(1)}$ should satisfy the property

$$H_{mn}^{(1)} = \langle u_m | H | u_n \rangle_1 = \langle u_n | H^\dagger | u_m \rangle_1^* = \langle u_n | H | u_m \rangle_1^* = H_{nm}^{(1)*}. \quad (1.8)$$

So matrix representation \tilde{H} of H will be a self adjoint matrix which means it is equal to its own transpose conjugate. However note that the numbers $H_{mn}^{(2)} := \langle u_m | H | u_n \rangle_2$ do not have to satisfy such a property because H does not have to be Hermitian

with respect to \mathcal{H}_2 . In this case realize that $H_{mn}^{(2)}$'s do not correspond to the matrix elements of H with respect to the basis \mathcal{U} since \mathcal{U} is not an orthonormal basis for \mathcal{H}_2 .

Definition: (Positive Definite Operator) A bounded Hermitian operator $M : \mathcal{H} \mapsto \mathcal{H}$ on a Hilbert Space \mathcal{H} is called a positive definite operator if it satisfies $\langle \psi | M | \psi \rangle > 0, \forall$ nonzero $|\psi\rangle \in \mathcal{H}$.

Here bounded means that there exists a positive constant c such that $\forall \psi \in \mathcal{H}, \|M\psi\| \leq c\|\psi\|$.

Using a positive definite operator M , and the inner product $\langle \cdot | \cdot \rangle$ of the Hilbert space \mathcal{H} on which positive definiteness of M is defined, it is possible to generate another inner product function $\langle \cdot | \cdot \rangle_M$. Actually if we define $\langle \cdot | \cdot \rangle_M := \langle \cdot | M | \cdot \rangle$, it is easy to see that $\langle \cdot | \cdot \rangle_M$ is really an inner product. Positivity and definiteness of $\langle \cdot | \cdot \rangle_M$ are satisfied by definition and linearity of M . Linearity of M also implies additivity and homogeneity, and conjugate symmetry holds since M is Hermitian. It is also important to mention that M has a unique positive-definite square root and logarithm [8], i.e., there exist unique positive-definite operators μ and ν such that M can be written in either form:

$$M = \mu^2, \tag{1.9}$$

$$M = e^\nu. \tag{1.10}$$

Definition: (Ray) A ray in a complex vector space \mathbb{V} is an equivalence class of the equivalence relation \sim defined as $\forall u, v \in \mathbb{V} \quad u \sim v$ if $\exists a \in \mathbb{C} \setminus \{0\}$ such that $u = av$.

Any two elements of a given ray differ from each other only by a scalar multiplication. Note that the set which consists only of the zero element of the corresponding vector space is also a ray which we call the zero-ray. All other rays are called non-zero-rays. We will only deal with non-zero rays and drop the qualification “non-zero” hereafter.

1.2 Postulates of Quantum Mechanics

Postulate 1: Every state of a particle is uniquely represented by a ray Δ in a Hilbert space \mathcal{H} [9].

The elements of Δ are called state vectors. In practice, instead of the ray Δ , physicists choose a representative state vector $|\psi\rangle$ in Δ to describe the state of the particle. However we should note that the choice of the representative is arbitrary and any other element $|\tilde{\psi}\rangle$ of Δ can be equivalently chosen to describe the physical state of the particle. In other words multiplication of our initial state vector $|\psi\rangle$ by a nonzero scalar does not change the physical state it describes.

Postulate 2: The independent variables x and p of classical mechanics are represented by Hermitian operators X and P with the following matrix elements in the eigenbasis of X [9]:

$$\langle x|X|x'\rangle = x\delta(x-x') \quad \langle x|P|x'\rangle = -i\hbar\delta'(x-x'). \quad (1.11)$$

The operators corresponding to dependent variables $\omega(x, p)$ are given by complete Hermitian operators

$$\Omega(X, P) = \omega(x \rightarrow X, p \rightarrow P). \quad (1.12)$$

Here $\delta(x)$ is the Dirac delta function and complete operator means its eigenvectors form a complete basis.

Note that the eigenbasis of X cannot be an orthonormal basis for any Hilbert Space because it is uncountable. However it has analogous properties such as

- $\langle x|x'\rangle = \delta(x-x')$ (Dirac delta orthonormality)
- $\int_{\mathbb{R}} dx|x\rangle\langle x| = I$. (completeness)

The term “matrix elements” in Proposition 2 is somewhat misleading. Since position and momentum operators have a continuous spectrum, these numbers cannot correspond to the entries of a matrix representation of X . Actually for a general operator Ω , we will call these elements position representation of Ω and denote it as $\Omega(x, x')$.

Now assume that the operator representation $\Omega(X, P)$ of Ω involves only polynomial factors of X and P . In this case (1.12) together with (1.11) implies that the position representation $\langle x|\Omega|x'\rangle$ is given by

$$\Omega(x, x') = \Omega\left(x, -i\hbar\frac{d}{dx}\right) \delta(x - x') \quad (1.13)$$

If $\Omega(x, x')$ has such a form we call it local. Because in such a case, position representation of the image of a state vector $\psi \in \mathcal{H}$ at position x is given by

$$\begin{aligned} (\Omega\psi)(x) &:= \langle x|\Omega|\psi\rangle \\ &= \int_{\mathbb{R}} dx' \langle x|\Omega|x'\rangle \langle x'|\psi\rangle \\ &= \Omega\left(x, -i\hbar\frac{d}{dx}\right) \psi(x), \end{aligned} \quad (1.14)$$

which only depends on the behavior of $\psi(x)$ in a small neighborhood of x . In other words, the image $(\Omega\psi)(x)$ at x_0 is not effected by how $\psi(x)$ behaves away from x_0 .

Since the factor $\delta(x - x')$ in the representation of $\Omega(x, x')$ kills the integral under which the representation operates, it is convenient to write

$$\Omega(x) := \Omega\left(x, -i\hbar\frac{d}{dx}\right) \quad (1.15)$$

as the position representation of Ω which applies only to the position representations of the state vectors in the position space such that

$$\Omega(x)\psi(x) = (\Omega\psi)(x). \quad (1.16)$$

Postulate 3: Observables are represented by Hermitian operators Ω . Under the assumption that Ω has a non-degenerate, discrete spectrum; if a particle is in a state represented by the state vector $|\psi\rangle$, a measurement of an observable Ω yields one of

the eigenvalues ω with probability $P(\omega) \propto |\langle \omega | \psi \rangle|^2$, and the state vector of the system will change from $|\psi\rangle$ to $|\omega\rangle$ as a result of the measurement [9].

Numbers $\langle \omega | \psi \rangle$ correspond to the coefficients of the basis representation of $|\psi\rangle$ in the eigenbasis of Ω . The scale of the proportionality can be found using the completeness of the eigenbasis of ω . Actually

$$\langle \psi | \psi \rangle = \sum_n |\langle \omega_n | \psi \rangle|^2 \propto \left\{ \begin{array}{l} \text{probability of the result of} \\ \text{the measurement to be any} \\ \text{one of the possible results!} \end{array} \right\} = 1. \quad (1.17)$$

Hence if both the state vectors $|\psi\rangle$ and $|\omega\rangle$ are normalized, i.e., they have norms $\|\psi\| = \|\omega\| = 1$, then the proportionality at the above postulate becomes equality. If $\|\psi\| \neq 1$ then it is always possible to choose a normal state vector $|\tilde{\psi}\rangle$ from the corresponding ray of $|\psi\rangle$; such that $|\tilde{\psi}\rangle = |\psi\rangle / \|\psi\|$. So from now on we will only deal with normalized state vectors without loss of generality.

An important physical quantity for physicists is the expectation value $\langle \Omega \rangle_\psi$ of an observable Ω in a state vector $|\psi\rangle$ which is equal to $\sum_n \omega_n P(\omega_n)$. Using the spectral representation of Ω we can easily see that $\langle \Omega \rangle_\psi = \langle \psi | \Omega | \psi \rangle$. Actually the latter is how we define the expectation value for a given normalized state vector and observable. Realize that Hermiticity of Ω guarantees the number $\langle \psi | \Omega | \psi \rangle$ to be real which should be the case if it really corresponds to the expectation value of a physical observable.

Postulate 4: An evolving state vector $|\psi(t)\rangle$ obeys the Schrödinger Equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle, \quad (1.18)$$

where $H(X, P) = \mathfrak{H}(x \rightarrow X, p \rightarrow P)$ is the quantum Hamiltonian operator, \mathfrak{H} is the Hamiltonian for the corresponding classical problem, and t corresponds to the physical time [9].

A physical system in which the physical states evolve is represented by the corresponding quantum Hamiltonian operator H , whose eigenvectors correspond to the

possible energy levels of the system. According to Postulate 4, state vectors evolve in time according to the Schrödinger Equation (1.18).

It is important to note that time evolution of a state vector $|\psi(t)\rangle$ should be unitary, i.e., it should satisfy the property that $\langle\psi(t)|\psi(t)\rangle = 1$. In other words if we represented a physical state by a normalized state vector $|\psi(t_0)\rangle$ at time t_0 , it should stay normalized at a later time t . This is because we want the total probability $\langle\psi(t)|\psi(t)\rangle$ to be equal to 1 for all time values t . This requirement is satisfied because of the Hermiticity of H . Taking the derivative of the square norm of $|\psi(t)\rangle$ and using the Schrodinger equation we have

$$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \frac{1}{i\hbar} (\langle\psi(t)|H|\psi(t)\rangle - \langle\psi(t)|H|\psi(t)\rangle^*) = 0. \quad (1.19)$$

From the above arguments we see that using Hermitian operators is important in Quantum Theory not only because they guarantee real eigenvalue requirement, but they also guarantee other requirements of Quantum Measurement Theory such as the reality of the expectation values and the unitarity of the time evolution.

Chapter 2

INTRODUCTION

In conventional Quantum Mechanics, observables are represented by Hermitian operators acting on a Hilbert space \mathcal{H} . The choice of the operators to be Hermitian ensures their eigenvalues to be real which is an indispensable requirement since any possible measurement of an observable corresponds to one of the eigenvalues of the corresponding operator. However Hermiticity of an operator is only a sufficient condition for the reality of its eigenvalues. There is no mathematical reason for not using a non-Hermitian operator as a representation of an observable if it has real eigenvalues. Recently there has been a great amount of research activity in trying to examine the properties of such non-Hermitian Hamiltonians. Historically first thoroughly examined non-Hermitian Hamiltonians H with real eigenvalues were the ones which are \mathcal{PT} -symmetric [1, 2] i.e.,

$$\mathcal{P}T H (\mathcal{P}T)^{-1} = \mathcal{P}T H \mathcal{P}T = H \quad (2.1)$$

where \mathcal{P} is the parity and \mathcal{T} is the time reversal operators which are defined as

$$(\mathcal{P}\psi)(x) = \psi(-x), \quad (\mathcal{T}\psi)(x) = \psi(x)^*, \quad \forall \psi \in \mathcal{H} = L^2(\mathbb{R}). \quad (2.2)$$

The observation that some \mathcal{PT} -symmetric Hamiltonians have real spectra led to the idea that these Hamiltonians might be used for a generalized Quantum Mechanics. This in turn led to a further investigation of \mathcal{PT} -symmetric Hamiltonians. However it is easy to show that \mathcal{PT} -symmetry is neither a necessary nor a sufficient condition for an operator to have real eigenvalues. In general one of the main properties of

\mathcal{PT} -symmetric Hamiltonians is that [1, 2, 3, 4]:

Either the eigenvalues of the Hamiltonian is real (\mathcal{PT} -symmetry is exact)
or there are real as well as complex-conjugate pairs of complex eigenvalues (2.3)
(\mathcal{PT} -symmetry is broken).

Since \mathcal{PT} -symmetry does not characterize the Hamiltonians with real eigenvalues, the need for finding necessary and sufficient conditions for an operator to have a real spectrum emerged. Finally in [5, 6, 7], Mostafazadeh made a complete mathematical investigation of the properties of the \mathcal{PT} -symmetric Hamiltonians (in general any Hamiltonian which has an anti-linear symmetry), and gave a characterization of the (diagonalizable) Hamiltonians with a discrete real spectrum [6].

Chapter 3

CHARACTERIZATION OF THE REALITY OF THE SPECTRUM

In this section we give some definitions and theorems stated in [5, 6] in order to characterize the Hamiltonians which have real eigenvalues. This section involves the main mathematical tool we use in this thesis, and one can consult the references for a more detailed discussion.

Definition: Let \mathcal{H} be a separable Hilbert Space, then a linear operator $H : \mathcal{H} \rightarrow \mathcal{H}$ is said to be pseudo-Hermitian if there exists a linear, Hermitian, invertible operator η such that

$$H^\dagger = \eta H \eta^{-1}. \quad (3.1)$$

As can be seen from the definition, pseudo-Hermiticity of H does not address the operator η . It is enough that there exists at least one η which satisfies (3.1). Actually there are infinitely many η which satisfy (3.1) if there exists one. If we want to emphasize the existence of a specific operator η_0 within the operators satisfying (3.1), we call H η_0 -pseudo-Hermitian.

Property (2.3) is a consequence of the requirement that H has an anti-linear symmetry, i.e., if H satisfies $[H, A] = 0$ for some invertible anti-linear operator A , then either the eigenvalues of H are real or they come in complex conjugate pairs. In [5] under the assumption that H has a discrete spectrum and that it is diagonalizable, it is proven that H is pseudo-Hermitian if and only if it satisfies (2.3). As a consequence all \mathcal{PT} -symmetric Hamiltonians are pseudo-Hermitian. The case where all eigenvalues of H are real corresponds to H to be η_+ -pseudo-Hermitian for some positive-definite operator η_+ . The latter is stated explicitly by the following theorem [6]:

Theorem 1: Let $H : \mathcal{H} \rightarrow \mathcal{H}$ be a Hamiltonian that acts in a Hilbert space \mathcal{H} , has a discrete spectrum, and admits a complete set of biorthonormal eigenvectors $\{|\psi_n\rangle, |\phi_n\rangle\}$, i.e.,

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \quad H^\dagger|\phi_n\rangle = E_n^*|\phi_n\rangle \quad (3.2)$$

$$\langle\phi_m|\psi_n\rangle = \delta_{mn}, \quad \sum_n |\psi_n\rangle\langle\phi_n| = I$$

where $E_n \in \mathbb{C} \quad \forall n \in \mathbb{N}^+$. Then the Spectrum of H is real if and only if there is an invertible linear operator $w : \mathcal{H} \rightarrow \mathcal{H}$ such that H is η_+ -pseudo-Hermitian where $\eta_+ = w^\dagger w$.

Proof: Let $\{|n\rangle\}$ be a complete orthonormal basis of \mathcal{H} , i.e.,

$$\langle m|n\rangle = \delta_{mn}, \quad \sum_n |n\rangle\langle n| = I, \quad (3.3)$$

and $w : \mathcal{H} \rightarrow \mathcal{H}$ and $H_0 : \mathcal{H} \rightarrow \mathcal{H}$ be defined by

$$w := \sum_n |n\rangle\langle\phi_n|, \quad H_0 := \sum_n E_n |n\rangle\langle n|, \quad (3.4)$$

then w is invertible with the inverse given by

$$w^{-1} = \sum_n |\psi_n\rangle\langle n| \quad (3.5)$$

and

$$wHw^{-1} = H_0. \quad (3.6)$$

Now suppose that the spectrum of H is real. Then, H_0 is Hermitian and taking the adjoint of both sides (3.6), we have

$$wHw^{-1} = (w^{-1})^\dagger H^\dagger w^\dagger \quad (3.7)$$

or equivalently

$$H^\dagger = w^\dagger wH(w^\dagger w)^{-1} = \eta_+ H \eta_+^{-1} \quad (3.8)$$

Then H is η_+ -pseudo-Hermitian.

Now assume H is η_+ -pseudo-Hermitian, i.e.;

$$H^\dagger = \eta_+ H \eta_+^{-1}, \quad (3.9)$$

where $\eta_+ = w^\dagger w$ for some invertible linear operator $w : \mathcal{H} \rightarrow \mathcal{H}$. First of all realize that η_+ is positive definite: it is Hermitian and for all nonzero state functions $\psi \in \mathcal{H}$, it satisfies $\langle \psi | \eta_+ | \psi \rangle = \langle \psi | w^\dagger w | \psi \rangle = \langle w\psi | w\psi \rangle > 0$ (since w is invertible as a consequence $w|\psi\rangle$ is nonzero). Now let us rewrite (3.9) as

$$H^\dagger \eta_+ = \eta_+ H. \quad (3.10)$$

If we apply a dual eigenvector $\langle \psi_n |$ from left and an eigenvector $|\psi_m\rangle$ from right to (3.10), we get

$$\begin{aligned} \langle \psi_n | H^\dagger \eta_+ | \psi_m \rangle &= \langle \psi_n | \eta_+ H | \psi_m \rangle \\ \Rightarrow E_n^* \langle \psi_n | \eta_+ | \psi_m \rangle &= E_m \langle \psi_n | \eta_+ | \psi_m \rangle \\ \Rightarrow (E_n^* - E_m) \langle \psi_n | \eta_+ | \psi_m \rangle &= 0. \end{aligned} \quad (3.11)$$

Since η_+ is positive definite, if we take $m = n$ in (3.11) we see that $E_n^* = E_n$ which implies the spectrum of H is real. \square

Note that the operator η_+ is not unique. It depends on the choice of the biorthonormal system. Also as we showed in the proof, it is positive definite. Actually we can restate *Theorem 1* such that the spectrum of H is real if and only if it is η_+ -pseudo-Hermitian for some positive definite operator η_+ .

Chapter 4

PHYSICAL ASPECTS

Positive-definiteness of η_+ is essential for us to be able to use such non-Hermitian but η_+ -pseudo-Hermitian Hamiltonians (for some positive-definite η_+) as energy operators whose eigenvectors correspond to the energy levels of a physical system. Actually in Quantum Mechanics reality of eigenvalues of a Hamiltonian operator is a necessary condition but it is by no means sufficient. The use of such Hamiltonians for the description of a physical system should also be consistent with Quantum Measurement Theory. As we explained in Chapter 1, in addition to the requirement of having real eigenvalues, there are also other requirements such as the reality of the energy expectation values $\langle \psi | H | \psi \rangle$ and unitarity of time evolution., i.e., $\langle \psi(t) | \psi(t) \rangle = 1$. Such conditions would automatically be satisfied if we were using a Hermitian Hamiltonian. However for a general non-Hermitian but η_+ -pseudo-Hermitian Hamiltonian, even if it exhibits real eigenvalues, these other requirements are not guaranteed to be satisfied. At the first glance to attempt to use such η_+ -pseudo-Hermitian Hamiltonians in the description of a physical system seems to cause fatal inconsistencies, in general. However the problem is not due to the incapability of such Hamiltonians but our insistence on using the standard inner product of the Hilbert Space. It turns out that one who wishes to use non-Hermitian Hamiltonians in the description of a quantum system should also change the usual inner product, or equivalently the standard Hilbert space \mathcal{H} in accordance with the requirements of Quantum Measurement Theory.

In order to find the “suitable” inner product we use the fact that up to the unitary equivalence, there is a unique separable Hilbert Space! In other words, any pair of separable Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 are related by a unitary operator $\mathcal{U} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$,

i.e., $\forall \psi, \phi \in \mathcal{H}_1$

$$\langle \mathcal{U}\psi | \mathcal{U}\phi \rangle_2 = \langle \psi | \phi \rangle_1 \quad (4.1)$$

where $\langle \cdot | \cdot \rangle_1$ and $\langle \cdot | \cdot \rangle_2$ are inner products of the Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 , respectively [8].

Given an η_+ -pseudo-Hermitian Hamiltonian H defined on a Hilbert space \mathcal{H} with the inner product $\langle \cdot | \cdot \rangle$, we form another Hilbert space \mathcal{H}_{phys} called physical Hilbert space which has the same structure with \mathcal{H} but its inner product differs from $\langle \cdot | \cdot \rangle$ such that

$$\langle \psi | \phi \rangle_+ := \langle \psi | \eta_+ | \phi \rangle, \quad \forall |\psi\rangle, |\phi\rangle \in \mathcal{H}. \quad (4.2)$$

Note that $\langle \cdot | \cdot \rangle_+$ is well defined as we explained in Chapter 1. In this case unitary equivalence of \mathcal{H}_{phys} and \mathcal{H} is satisfied by the unique positive definite square root ρ_+ of η_+ , which satisfies $\rho_+^2 = \eta_+$. In fact unitarity of $\rho_+ : \mathcal{H}_{phys} \mapsto \mathcal{H}$ immediately follows from the definition of $\langle \cdot | \cdot \rangle_+$:

$$\langle \psi | \phi \rangle_+ := \langle \psi | \eta_+ | \phi \rangle = \langle \rho_+ \psi | \rho_+ \phi \rangle, \quad \forall |\psi\rangle, |\phi\rangle \in \mathcal{H}. \quad (4.3)$$

It is easy to see that using H in the new inner product $\langle \cdot | \cdot \rangle_+$ is consistent with Quantum Measurement Theory unlike the initial one. Actually using Hermiticity of η_+ and η_+ -pseudo-Hermiticity of H , we see that $\langle \psi | H | \phi \rangle_+ = \langle \phi | H | \psi \rangle_+^* \quad \forall \psi, \phi \in \mathcal{H}_{phys}$. In fact H is a Hermitian operator acting in \mathcal{H}_{phys} and therefore it guarantees all the requirement of Quantum Measurement Theory when we use \mathcal{H}_{phys} as our Hilbert Space. However this is not the only way we must follow to analyze the physical system described by H . Unitary equivalence of \mathcal{H}_{phys} and \mathcal{H} implies that both Hilbert spaces can be used to represent the same physical system. However if we want to use \mathcal{H} as our Hilbert Space we should modify our Hamiltonian H and observables in a suitable way. Actually one can get the same physical quantities such as energy levels,

expectation values, probability distributions whether he uses

$$\begin{array}{ll}
 & \text{state vectors} \quad |\psi\rangle, |\phi\rangle \in \mathcal{H}_{phys} \\
 \text{picture1 :} & \text{Hamiltonian} \quad H \\
 & \text{observables} \quad O \\
 & \text{inner product} \quad \langle \cdot | \cdot \rangle_+
 \end{array} \tag{4.4}$$

or

$$\begin{array}{ll}
 & \text{state vectors} \quad \rho_+ |\psi\rangle, \rho_+ |\phi\rangle \in \mathcal{H} \\
 \text{picture2 :} & \text{Hamiltonian} \quad h := \rho_+ H \rho_+^{-1} \\
 & \text{observables} \quad o := \rho_+ O \rho_+^{-1} \\
 & \text{inner product} \quad \langle \cdot | \cdot \rangle
 \end{array} . \tag{4.5}$$

Note that at the beginning what we know about the physical system is the non-Hermitian Hamiltonian H in the first picture and the usual Hermitian observables o (such as position x and momentum p operators) in the second picture. Therefore one who wants to use the first picture should compute the non-Hermitian observables O using the usual Hermitian ones according to

$$O = \rho_+^{-1} o \rho_+, \tag{4.6}$$

and one who wants to use the second picture should compute the Hermitian Hamiltonian h using the non-Hermitian one (H) by the formula

$$h = \rho_+ H \rho_+^{-1}. \tag{4.7}$$

Each picture might be used according to the physical problem. However we should note that in the first picture observables O and in the second picture Hermitian Hamiltonian h are generally non-local operators. Non-locality of such operators might cause some computational difficulties in each picture.

Chapter 5

CALCULATION METHODS OF THE METRIC OPERATOR η_+ AND THE EQUIVALENT HERMITIAN HAMILTONIAN H

By definitions of the metric operator η_+ and w in *Theorem 1*, we can easily find that η_+ can be expressed in the form:

$$\eta_+ = \sum_n |\phi_n\rangle\langle\phi_n|. \quad (5.1)$$

After finding the functions ϕ_n , η_+ can be calculated in a suitable basis such as x or p using the representation (5.1).

There are several methods to calculate the metric operator η_+ , non-Hermitian operators O , and Hermitian Hamiltonian h for a given pseudo-Hermitian Hamiltonian H . These methods are explained in detail in [11, 15, 13, 14]. One of the methods uses the spectral representation $\eta_+ = \sum_n \epsilon_n |\epsilon_n\rangle\langle\epsilon_n|$ of η_+ , where $|\epsilon_n\rangle$ is its eigenbasis with corresponding eigenvalues ϵ_n , as well as (5.1) to calculate O and h . This method is explained in detail and applied to the \mathcal{PT} -symmetric square well problem in [11]. However it is not applicable to the Hamiltonian we examine in section 2, since spectrum of our Hamiltonian is not discrete.

The method we will use is explained in [13]. It applies to the η_+ -pseudo-Hermitian Hamiltonians of the form

$$H = H_0 + \epsilon H_1, \quad (5.2)$$

where ϵ is a real perturbation parameter, H_0 and H_1 are ϵ -independent Hermitian and anti-Hermitian operators, respectively. Also we express the metric operator η_+

and minus of its logarithm Q , which means $\eta_+ = e^{-Q}$ [15], as

$$\eta_+ = 1 + \sum_{n=1} \eta_{+n} \epsilon^n, \quad (5.3)$$

$$Q = \sum_{n=1} Q_n \epsilon^n, \quad (5.4)$$

where η_{+n} 's and Q_n 's are ϵ independent. Realizing $\rho_+ = e^{-Q/2}$, and then imposing (5.2), (5.4) into (4.7) and applying the Baker-Campbell-Hausdorff identity, which says that for any operator A, B

$$e^{-A} B e^A = B + [B, A] + \frac{1}{2!} [[B, A], A] + \frac{1}{3!} [[[B, A], A], A] + \dots, \quad (5.5)$$

we see that the Hermitian Hamiltonian h can be expressed as

$$h = H_0 + \left\{ H_1 + \frac{1}{2} [H_0, Q_1] \right\} \epsilon + \left\{ \frac{1}{2^3} [[H_0, Q_1], Q_1] + \frac{1}{2} [H_0, Q_2] \right\} \epsilon^2 + \mathcal{O}(\epsilon^3). \quad (5.6)$$

On the other hand, using the identity $\eta_+ = e^{-Q}$, and imposing (5.2) and (5.4) into η_+ -pseudo-Hermiticity condition (3.8) of H , and applying the Baker-Campbell-Hausdorff identity, we find an infinite sequence of operator equations for Q_n . The first two of the equations are

$$[H_0, Q_1] = -2H_1 \quad \text{and} \quad [H_0, Q_2] = 0. \quad (5.7)$$

In view of (5.7) and (5.6), we can rewrite h as

$$h = H_0 + \frac{1}{4} [H_1, Q_1] \epsilon^2 + \mathcal{O}(\epsilon^3). \quad (5.8)$$

Note also that if we use (5.3), (5.4), and identity $\eta_+ = e^{-Q}$, we can write Q_i in terms of η_{+j} 's. In particular Q_1 is related to η_{+1} as

$$Q_1 = -\eta_{+1}. \quad (5.9)$$

Chapter 6

 \mathcal{PT} -SYMMETRIC DELTA FUNCTION POTENTIAL

In this chapter we apply the pseudo-Hermiticity Theory to the \mathcal{PT} -symmetric delta function potential. Before starting our analysis we want to mention that there have been other studies examining the properties of complex delta function potentials [14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26]. Among these there are studies investigating some properties such as symmetries, scattering, bound state solutions, and band structures of different types of complex potentials consisting of Dirac delta functions. Our analysis focuses on the physical aspects of the \mathcal{PT} -symmetric delta function potential. A similar analysis is applied to a single Dirac delta potential with a complex coupling in [14]. In [26] spectral properties of general \mathcal{PT} -symmetric delta function potentials are studied but investigation of physical aspects of such potentials has not been made.

Our analysis and method have been established for systems with a discrete spectrum. Nevertheless we want to apply the same method to examine the physical aspects of the \mathcal{PT} -Symmetric delta function potential which has a continuous real spectrum.

Consider the Hamiltonian

$$H = \frac{p^2}{2m} + V(x) \quad (6.1)$$

where $V(x)$ is

$$V(x) = i\zeta[\delta(x - a) - \delta(x + a)], \quad \zeta, a \in \mathbb{R}^+. \quad (6.2)$$

First we study the solutions of the time-independent Schrodinger Equation,

$$H\psi = E\psi, \quad E \in \mathbb{C}. \quad (6.3)$$

Substituting (6.1) and (6.2) in (6.3) we get

$$-\frac{\hbar^2}{2m}\psi''(x) + i\zeta[\delta(x - a) - \delta(x + a)]\psi(x) = E\psi(x). \quad (6.4)$$

For simplicity we introduce the dimensionless quantities:

$$x := \frac{x}{a}, \quad z := \frac{2ma\zeta}{\hbar^2}, \quad E := \frac{2ma^2 E}{\hbar^2}, \quad (6.5)$$

and use the fact that $\delta(x/a) = a\delta(x)$ to rewrite (6.4) as

$$-\psi''(x) + iz[\delta(x-1) - \delta(x+1)]\psi(x) = E\psi(x). \quad (6.6)$$

In this case E belongs to the spectrum of the dimensionless Hamiltonian

$$H := \frac{2ma^2}{\hbar^2} H = -\frac{d^2}{dx^2} + iz[\delta(x-1) - \delta(x+1)]. \quad (6.7)$$

The solution of (6.6) has the form

$$\psi(x) = \psi_k(x) := \left\{ \begin{array}{ll} \psi_{1k}(x) := A_+ e^{ikx} + A_- e^{-ikx} & \text{for } x < -1 \\ \psi_{2k}(x) := B_+ e^{ikx} + B_- e^{-ikx} & \text{for } -1 < x < 1 \\ \psi_{3k}(x) := C_+ e^{ikx} + C_- e^{-ikx} & \text{for } x > 1 \end{array} \right\} \quad (6.8)$$

where $A_{\pm}, B_{\pm}, C_{\pm} \in \mathbb{C}$, and k is the principal square root of E ($k := \sqrt{E}$). We have the boundary conditions:

$$\begin{aligned} \psi_k(\pm 1^-) &= \psi_k(\pm 1^+) \\ \psi'_k(\pm 1^+) - \psi'_k(\pm 1^-) &= \pm iz\psi_k(\pm 1). \end{aligned} \quad (6.9)$$

The first boundary condition is the continuity requirement of ψ_k , and the second boundary condition can be achieved by integrating (6.6) on infinitesimal neighborhoods of -1 and 1 and demanding the derivative of ψ_k to be continuous. Substituting (6.8) into (6.9) we get the following two matrix equations:

$$\begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \mathcal{O} \begin{pmatrix} B_+ \\ B_- \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} C_+ \\ C_- \end{pmatrix} = \mathcal{R} \begin{pmatrix} B_+ \\ B_- \end{pmatrix} \quad (6.10)$$

where

$$\mathcal{O} := \begin{pmatrix} 1 + \frac{z}{2k} & \frac{z}{2k} e^{2ik} \\ -\frac{z}{2k} e^{-2ik} & 1 - \frac{z}{2k} \end{pmatrix} \quad \text{and} \quad \mathcal{R} := \begin{pmatrix} 1 + \frac{z}{2k} & \frac{z}{2k} e^{-2ik} \\ -\frac{z}{2k} e^{2ik} & 1 - \frac{z}{2k} \end{pmatrix}. \quad (6.11)$$

Realize that the determinants of \mathcal{O} and \mathcal{R} are 1 and they have the inverses

$$\mathcal{O}^{-1} := \begin{pmatrix} 1 - \frac{z}{2k} & -\frac{z}{2k}e^{2ik} \\ \frac{z}{2k}e^{-2ik} & 1 + \frac{z}{2k} \end{pmatrix} \quad \text{and} \quad \mathcal{R}^{-1} := \begin{pmatrix} 1 - \frac{z}{2k} & -\frac{z}{2k}e^{-2ik} \\ \frac{z}{2k}e^{2ik} & 1 + \frac{z}{2k} \end{pmatrix}, \quad (6.12)$$

respectively. The transition matrix \mathcal{S} which connects A_{\pm} to C_{\pm} according to

$$\begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \mathcal{S} \begin{pmatrix} C_+ \\ C_- \end{pmatrix}, \quad (6.13)$$

can be computed as

$$\mathcal{S} = \mathcal{O}\mathcal{R}^{-1} = \begin{pmatrix} 1 + \frac{(e^{4ik}-1)z^2}{4k^2} & \frac{iz(2k+z)\sin(2k)}{2k^2} \\ \frac{iz(2k-z)\sin(2k)}{2k^2} & 1 + \frac{(e^{-4ik}-1)z^2}{4k^2} \end{pmatrix}. \quad (6.14)$$

6.1 Analysis of the Spectrum

For all positive real k values, ψ_k is a solution of (6.6) with a real energy value E . These ψ_k 's are not square integrable but bounded functions, and have physical meanings since they represent scattering states. However mathematically there is no restriction on k not to be a complex number. If there are bounded solutions ψ_k of (6.6) with complex k , and so with complex or negative energy value E , then our system does not have a physical meaning. Therefore we want to examine the possibility of a bounded solution ψ_k of (6.6) with a k that has a nonzero imaginary part.

Suppose that ψ_k is a solution of (6.6) of the form (6.8) where the imaginary part of k is greater than 0, i.e.;

$$\text{Im}(k) > 0. \quad (6.15)$$

From (6.8) we can easily see that in order for the solution ψ_k not to blow up at infinities, the coefficients A_+ and C_- have to be zero.¹ If we insert this requirement into (6.13), together with (6.14) we see that k needs to satisfy the following condition in addition to (6.15):

$$1 + \frac{(e^{4ik} - 1)z^2}{4k^2} = 0. \quad (6.16)$$

¹Note that in this case boundedness of ψ_k automatically implies its square integrability.

Conditions (6.15) and (6.16) can be rewritten as

$$\frac{(e^u - 1)}{u^2} = G, \quad (6.17)$$

and

$$\operatorname{Re}(u) < 0, \quad (6.18)$$

where

$$u := 4ik, \quad \text{and} \quad G := \frac{1}{4z^2}. \quad (6.19)$$

If we started with a k value such that $\operatorname{Im}(k) < 0$, and force the solution ψ_k to be bounded again, we would get the same conditions (6.17) and (6.18), but then instead of (6.19) we would have $u := -4ik$.

It can be shown that there exists a critical G value G_c such that if $G > G_c$ there is no complex number u satisfying both (6.17) and (6.18) (See Appendix A). Together with (6.19) this means that there exists a critical z value z_c which ensures the reality of the spectrum and nonexistence of the energy eigenvalues. In other words just for those z values $z < z_c$ our system has a physical meaning, and when z becomes greater than z_c there appear discrete complex conjugate pairs of energy eigenvalues in addition to the continuous real spectrum.

We can easily see this fact using some graphical solutions. In Figure 6.1 we simultaneously plotted the solutions of the equations $Eq1 : \operatorname{Re}\left(\frac{e^u - 1}{u^2}\right) = G_i$ and $Eq2 : \operatorname{Im}\left(\frac{e^u - 1}{u^2}\right) = 0$ on complex plane for four different G_i values $G_1 = 0.35$, $G_2 = 0.20$, $G_3 = 0.14$ and $G_4 = 0.02$. The full curve represents the solution points of $Eq1$ and the dashed curve represents the solution points of $Eq2$. So the intersection points gives us the u values which satisfies $\frac{e^u - 1}{u^2} = G_i$. First of all realize that both curves are symmetric with respect to real axis, so the intersection points are always in complex conjugate pairs. They also extend through imaginary axis repeating the finger-like shape infinitely many times. For the dashed curve the edges of these finger shaped curves always extend to the region where $\operatorname{Re}(u) < 0$. For the full curve the edges of these finger shaped curves get closer to the imaginary axis as G increases and pass through it starting from the closest ones to the real axis. This let the dashed and the

full curves intersect in the region where $Re(u) < 0$. Therefore we start to get complex conjugate pairs of energy eigenvalues $E = -u^2/4$ for those intersection points u where $Re(u) < 0$.

From Figure 6.1, we see that critical G value is $G_c \simeq 0.20$ which gives us corresponding critical z value $z_c \simeq 1.11$. Note that in our analysis we just showed the existence of z_c and numerically calculated what its value is. Actually while we were working on this thesis Haydar Uncu and Ersan Demiralp [26] investigated the bound state (square integrable) solutions of \mathcal{PT} -symmetric potential with Dirac delta functions represented as

$$V(x) = \sum_{i=1}^N [\sigma_i \delta(x - x_i) + \sigma_i^* \delta(x + x_i)] \quad (6.20)$$

where N is any integer, σ_i is an arbitrary complex valued coupling constant, and x_i is real. In the case where $N = 1$ and σ_i is purely imaginary, $V(x)$ reduces to our potential in (6.2). For this case, using complex analysis, Uncu and Demiralp showed that bound state (consequently bounded) solutions with complex eigenvalues do not exist if

$$|\sigma_i|_{x_1} \leq \frac{\sqrt{2}\pi}{4}, \quad (6.21)$$

and there are $2n$ number of them if

$$(2n - 1) \frac{\sqrt{2}\pi}{4} < |\sigma_i|_{x_1} \leq (2n + 1) \frac{\sqrt{2}\pi}{4}. \quad (6.22)$$

In our case $x_1 = 1$ and $|\sigma_i| = z$. Hence (6.21) implies that for $z \leq \sqrt{2}\pi/4 = 1.1058$, there is no bounded solution with complex eigenvalue which is in perfect match with our numerical approximation $z_c = 1.11$. Furthermore (6.22) implies that as z increases there appear bound state solutions with complex conjugate eigenvalues as we mentioned when analyzing Figure 6.1.

6.2 Finding a Biorthonormal System

From now on we will assume $z \leq z_c$. So all bounded solutions ψ_k have real k values. This automatically implies that k is positive since k is the principal square root of $k^2 = E$.

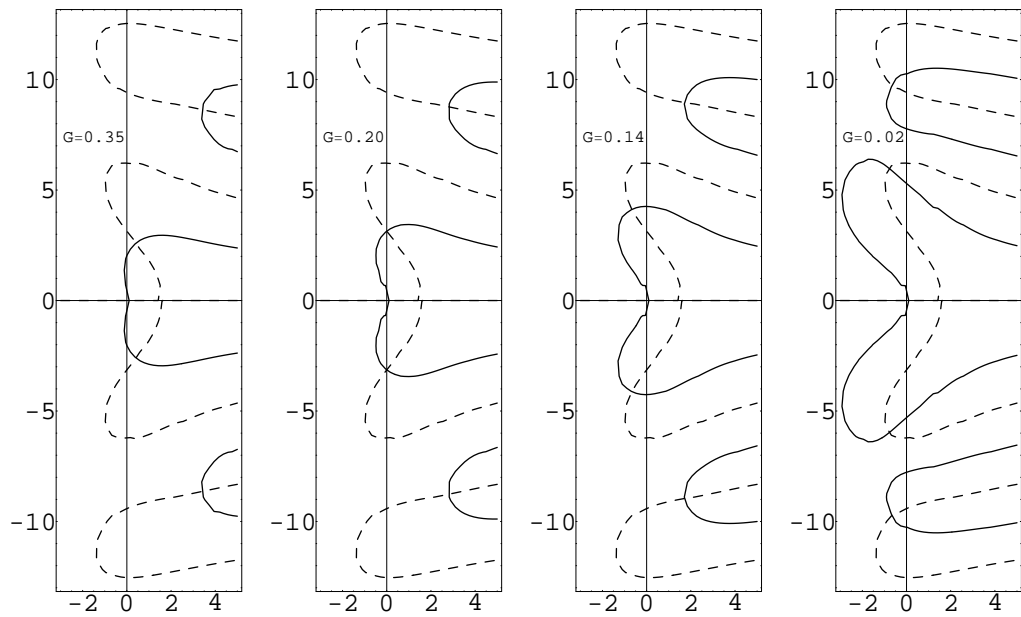


Figure 6.1: Plots of the solutions of $Eq1$ (the full curve) and $Eq2$ (the dashed curve) on complex plane for different G values $G_1 = 0.35$, $G_2 = 0.20$, $G_3 = 0.14$ and $G_4 = 0.02$. Horizontal and vertical axes represent real and imaginary axes, respectively. In the first picture, there is no intersection points in the left half plane, so we are in the safe region. For $G = 0.20$ the full curve gets closer to the imaginary axis and there is a pair of intersection points on the imaginary axis. This gives us our critical G value. In the third picture the full curve shifts to the left a little bit more and there appears a complex conjugate pair of intersection points on the left half plane and we get our corresponding complex energy eigenvalues. In the last one we see that while the first pair keeping stay in the left half plane, now there comes a new pair of intersection points to the left half plane as well.

First we want to write the eigenfunction solutions of (6.6) explicitly. As seen from (6.10), there are actually two arbitrary coefficients B_+, B_- in the expression (6.8) of eigenfunctions ψ_k . This shows that energy levels are doubly degenerate. Inserting (6.10), and (6.11) into (6.8) and choosing first that $B_+ = \frac{1}{\sqrt{2\pi}}$, $B_- = 0$, and then $B_+ = 0$, $B_- = \frac{1}{\sqrt{2\pi}}$; for each value of k , we can write two linearly independent eigenfunction solutions $\psi_{k,1}$, and $\psi_{k,2}$, respectively:

$$\psi_{k,1}(x) = \begin{cases} \frac{1}{\sqrt{2\pi}} \left\{ \left(1 + \frac{z}{2k}\right) e^{ikx} - \frac{z}{2k} e^{-2ik} e^{-ikx} \right\} & \text{for } x < -1 \\ \frac{1}{\sqrt{2\pi}} e^{ikx} & \text{for } -1 < x < 1 \\ \frac{1}{\sqrt{2\pi}} \left\{ \left(1 + \frac{z}{2k}\right) e^{ikx} - \frac{z}{2k} e^{2ik} e^{-ikx} \right\} & \text{for } x > 1 \end{cases}, \quad (6.23)$$

$$\psi_{k,2}(x) = \begin{cases} \frac{1}{\sqrt{2\pi}} \left\{ \frac{z}{2k} e^{2ik} e^{ikx} + \left(1 - \frac{z}{2k}\right) e^{-ikx} \right\} & \text{for } x < -1 \\ \frac{1}{\sqrt{2\pi}} e^{-ikx} & \text{for } -1 < x < 1 \\ \frac{1}{\sqrt{2\pi}} \left\{ \frac{z}{2k} e^{-2ik} e^{ikx} + \left(1 - \frac{z}{2k}\right) e^{-ikx} \right\} & \text{for } x > 1 \end{cases}.^2 \quad (6.24)$$

Comparing these expressions, it is seen that

$$\psi_{-k,1} = \psi_{k,2}. \quad (6.25)$$

Any eigenfunction ψ_k is a linear combination of $\psi_{k,1}$, and $\psi_{k,2}$, i.e.;

$$\psi_k = \beta_1 \psi_{k,1} + \beta_2 \psi_{k,2} \quad (6.26)$$

where in general β_1 and β_2 are complex valued coefficients which may depend on z and k . However, since our Hamiltonian is \mathcal{PT} -Symmetric, we want our eigenfunctions to be \mathcal{PT} -Symmetric, too, i.e.; we impose the condition

$$\psi_k(x) = \psi_k(-x)^* \quad (6.27)$$

²The choice of the coefficients is made under the demand that $\psi_{k,1}$ and $\psi_{k,2}$ tend to ordinary δ -function-normalized free particle solutions $\frac{1}{\sqrt{2\pi}} e^{ikx}$ and $\frac{1}{\sqrt{2\pi}} e^{-ikx}$, respectively, as coupling constant z tends to 0.

on our eigenfunctions $\psi_k(x)$. It is seen from the expressions (6.23) and (6.24) that \mathcal{PT} -Symmetry condition (6.27) is satisfied if and only if β_1 and β_2 are real. So we will only take real linear combinations of $\psi_{k,1}$, and $\psi_{k,2}$ in each degeneracy subspace.

Construction of the metric operator η_+ involves $\{\phi_k\}_{k>0}$ where ϕ_k is the solution of the eigenfunction equation $H^\dagger\phi_k = E_k\phi_k$ where $E_k = k^2$. Since the expression of H^\dagger is as the expression of H with z replaced by $-z$, we can obtain the expression for ϕ_k by changing z to $-z$ in the expression for ψ_k . This yields

$$\phi_{k,1}(x) := \left\{ \begin{array}{ll} \frac{1}{\sqrt{2\pi}} \left\{ \left(1 - \frac{z}{2k}\right) e^{ikx} + \frac{z}{2k} e^{-2ik} e^{-ikx} \right\} & \text{for } x < -1 \\ \frac{1}{\sqrt{2\pi}} e^{ikx} & \text{for } -1 < x < 1 \\ \frac{1}{\sqrt{2\pi}} \left\{ \left(1 - \frac{z}{2k}\right) e^{ikx} + \frac{z}{2k} e^{2ik} e^{-ikx} \right\} & \text{for } x > 1 \end{array} \right\}, \quad (6.28)$$

and

$$\phi_{k,2}(x) := \left\{ \begin{array}{ll} \frac{1}{\sqrt{2\pi}} \left\{ -\frac{z}{2k} e^{2ik} e^{ikx} + \left(1 + \frac{z}{2k}\right) e^{-ikx} \right\} & \text{for } x < -1 \\ \frac{1}{\sqrt{2\pi}} e^{-ikx} & \text{for } -1 < x < 1 \\ \frac{1}{\sqrt{2\pi}} \left\{ -\frac{z}{2k} e^{-2ik} e^{ikx} + \left(1 + \frac{z}{2k}\right) e^{-ikx} \right\} & \text{for } x > 1 \end{array} \right\}. \quad (6.29)$$

Again every \mathcal{PT} -Symmetric solution of $H^\dagger\phi_k = E_k\phi_k$ can be written as a linear combination of $\phi_{k,1}$ and $\phi_{k,2}$:

$$\phi_k = \alpha_1\phi_{k,1} + \alpha_2\phi_{k,2} \quad (6.30)$$

where α_1 and α_2 are real valued coefficients which may depend on z and k . In the non-degenerate case, system of functions $\{\psi_k, \phi_k\}_{k>0}$ automatically gives us a biorthonormal system after suitable normalization. However in the degenerate case, in order to satisfy biorthonormality, we should choose two proper pairs of eigenfunctions $\tilde{\psi}_{k,1}, \tilde{\psi}_{k,2}$; and $\tilde{\phi}_{k,1}, \tilde{\phi}_{k,2}$ in each degeneracy subspace spanned by $\psi_{k,1}, \psi_{k,2}$; and $\phi_{k,1}, \phi_{k,2}$.

$\phi_{k,2}$ respectively, which satisfy the following conditions:

$$\begin{aligned}\langle \tilde{\psi}_{l,1} | \tilde{\phi}_{k,1} \rangle &= \delta(k-l) & \langle \tilde{\psi}_{l,1} | \tilde{\phi}_{k,2} \rangle &= 0 \\ \langle \tilde{\psi}_{l,2} | \tilde{\phi}_{k,1} \rangle &= 0 & \langle \tilde{\psi}_{l,2} | \tilde{\phi}_{k,2} \rangle &= \delta(k-l).\end{aligned}\tag{6.31}$$

This condition can be rewritten in a matrix form

$$\begin{pmatrix} \langle \tilde{\psi}_{l,1} | \\ \langle \tilde{\psi}_{l,2} | \end{pmatrix} \cdot (|\tilde{\phi}_{k,1}\rangle, |\tilde{\phi}_{k,2}\rangle) = \delta(k-l)I\tag{6.32}$$

where (\cdot) stands for the usual matrix product and I is 2×2 identity matrix. In order to construct an appropriate biorthonormal system we first compute the inner products $\langle \psi_{l,i} | \phi_{k,j} \rangle$, $i, j \in \{1, 2\}$:

$$\langle \psi_{l,i} | \phi_{k,j} \rangle = \int_{-\infty}^{\infty} \langle \psi_{l,i} | x \rangle \langle x | \phi_{k,j} \rangle dx = \int_{-\infty}^{\infty} \psi_{l,i}^*(x) \phi_{k,j}(x) dx\tag{6.33}$$

Inserting (6.23), (6.24) and (6.28), (6.29) into (6.33) and using the facts that $\delta(k \pm l) = \lim_{\rho \rightarrow \infty} \frac{\sin(\rho(k \pm l))}{\pi(k \pm l)}$ and $k + l > 0$, we find

$$\begin{aligned}\langle \psi_{l,1} | \phi_{k,1} \rangle &= \left(1 - \frac{z^2}{2k^2}\right) \delta(k-l) & \langle \psi_{l,1} | \phi_{k,2} \rangle &= \left(\frac{z}{k} - \frac{z^2}{2k^2}\right) \delta(k-l) \\ \langle \psi_{l,2} | \phi_{k,1} \rangle &= -\left(\frac{z}{k} + \frac{z^2}{2k^2}\right) \delta(k-l) & \langle \psi_{l,2} | \phi_{k,2} \rangle &= \left(1 - \frac{z^2}{2k^2}\right) \delta(k-l).\end{aligned}\tag{6.34}$$

We can rewrite (6.34) in matrix form as

$$\begin{pmatrix} \langle \psi_{l,1} | \\ \langle \psi_{l,2} | \end{pmatrix} \cdot (|\phi_{k,1}\rangle, |\phi_{k,2}\rangle) = \delta(k-l)J\tag{6.35}$$

where

$$J = \begin{pmatrix} 1 - \frac{z^2}{2k^2} & \frac{z}{k} - \frac{z^2}{2k^2} \\ -\frac{z}{k} - \frac{z^2}{2k^2} & 1 - \frac{z^2}{2k^2} \end{pmatrix}.\tag{6.36}$$

Note that J is invertible for all z , $k > 0$ with the inverse

$$J^{-1} = \begin{pmatrix} 1 - \frac{z^2}{2k^2} & -\frac{z}{k} + \frac{z^2}{2k^2} \\ \frac{z}{k} + \frac{z^2}{2k^2} & 1 - \frac{z^2}{2k^2} \end{pmatrix}.\tag{6.37}$$

So comparing (6.32) and (6.35), and using the fact that J has an inverse, we can see that an initial choice for our biorthonormal system $\{\tilde{\phi}_{l,i}^{initial}, \tilde{\psi}_{k,j}^{initial}\}$, $i, j \in \{1, 2\}$ would be

$$\begin{pmatrix} \tilde{\psi}_{l,1}^{initial} \\ \tilde{\psi}_{l,2}^{initial} \end{pmatrix} = J^{-1} \begin{pmatrix} \psi_{l,1} \\ \psi_{l,2} \end{pmatrix} \text{ and } \begin{pmatrix} \tilde{\phi}_{k,1}^{initial} \\ \tilde{\phi}_{k,2}^{initial} \end{pmatrix} = \begin{pmatrix} \phi_{k,1} \\ \phi_{k,2} \end{pmatrix}. \quad (6.38)$$

However this initial choice is not a proper biorthonormal system. By “not proper” we mean that the metric operator $\eta_+^{initial}$ constructed from this initial system fails to satisfy some necessary properties such as boundedness and squarability ($(\eta_+^{initial})^2$ does not exist). Therefore we need to switch to a new, proper biorthonormal system. This can be done by realizing the fact that any other system $\{\tilde{\phi}_{l,i}, \tilde{\psi}_{k,j}\}$ in the form

$$\begin{pmatrix} \tilde{\psi}_{k,1} \\ \tilde{\psi}_{k,2} \end{pmatrix} = (K^\dagger)^{-1} \begin{pmatrix} \tilde{\psi}_{k,1}^{initial} \\ \tilde{\psi}_{k,2}^{initial} \end{pmatrix}; \quad \begin{pmatrix} \tilde{\phi}_{k,1} \\ \tilde{\phi}_{k,2} \end{pmatrix} = K \begin{pmatrix} \tilde{\phi}_{k,1}^{initial} \\ \tilde{\phi}_{k,2}^{initial} \end{pmatrix} \quad (6.39)$$

can be chosen as a biorthonormal system for our Hamiltonian where K is any invertible complex valued 2×2 matrix possibly depending on k and z . However we have a requirement such that KK^\dagger must tend to identity as z tends to zero to ensure that the Hermitian limit of the metric operator is identity.

Here we do not have a systematic procedure to calculate K which will give us a non-problematic metric operator. However looking for a more symmetric choice of the biorthonormal system we are able to find a K which at least fixes the first order problems in the metric operator.

To obtain a more symmetric choice realize that J^{-1} has a square root, namely

$$J^{-\frac{1}{2}} := -i \begin{pmatrix} \frac{z}{2k} & 1 - \frac{z}{2k} \\ -1 - \frac{z}{2k} & \frac{z}{2k} \end{pmatrix}. \quad (6.40)$$

We claim that K would be in the form

$$K = iJ^{-\frac{1}{2}} + \mathcal{O}(z^2). \quad (6.41)$$

Note that such a choice of K is in agreement with the requirement KK^\dagger is identity in the Hermitian limit; and comparing (6.38) and (6.39), it is easy to see that it gives

us a more symmetric choice of the biorthonormal system such that

$$\begin{pmatrix} \tilde{\psi}_{k,1} \\ \tilde{\psi}_{k,2} \end{pmatrix} = -i(J^{-\frac{1}{2}})^T \begin{pmatrix} \psi_{k,1} \\ \psi_{k,2} \end{pmatrix} + \mathcal{O}(z^2) \quad (6.42)$$

and

$$\begin{pmatrix} \tilde{\phi}_{l,1} \\ \tilde{\phi}_{l,2} \end{pmatrix} = iJ^{-\frac{1}{2}} \begin{pmatrix} \phi_{l,1} \\ \phi_{l,2} \end{pmatrix} + \mathcal{O}(z^2). \quad (6.43)$$

More explicitly, we have³

$$\begin{aligned} \tilde{\psi}_{k,1} &= -\frac{z}{2k}\psi_{k,1} + \left(1 + \frac{z}{2k}\right)\psi_{k,2} + \mathcal{O}(z^2), \\ \tilde{\psi}_{k,2} &= \left(-1 + \frac{z}{2k}\right)\psi_{k,1} - \frac{z}{2k}\psi_{k,2} + \mathcal{O}(z^2); \end{aligned} \quad (6.44)$$

$$\begin{aligned} \tilde{\phi}_{k,1} &= \frac{z}{2k}\phi_{k,1} + \left(1 - \frac{z}{2k}\right)\phi_{k,2} + \mathcal{O}(z^2), \\ \tilde{\phi}_{k,2} &= \left(-1 - \frac{z}{2k}\right)\phi_{k,1} + \frac{z}{2k}\phi_{k,2} + \mathcal{O}(z^2). \end{aligned} \quad (6.45)$$

6.3 Construction of the Metric Operator

Now we are ready to construct the metric operator η_+ . To construct η_+ , we are going to use the continuous and degenerate analog of equation (5.1) which is

$$\eta_+ = \int_0^\infty dk \left[|\tilde{\phi}_{k,1}\rangle\langle\tilde{\phi}_{k,1}| + |\tilde{\phi}_{k,2}\rangle\langle\tilde{\phi}_{k,2}| \right]. \quad (6.46)$$

What we want to find is the position representation of the metric operator

$$\begin{aligned} \eta_+(\mathbf{x}, \mathbf{y}) &= \langle\mathbf{x}|\eta_+|\mathbf{y}\rangle \\ &= \int_0^\infty dk \left[\langle\mathbf{x}|\tilde{\phi}_{k,1}\rangle\langle\tilde{\phi}_{k,1}|\mathbf{y}\rangle + \langle\mathbf{x}|\tilde{\phi}_{k,2}\rangle\langle\tilde{\phi}_{k,2}|\mathbf{y}\rangle \right] \\ &= \int_0^\infty dk \left[\tilde{\phi}_{k,1}(\mathbf{x})\tilde{\phi}_{k,1}^*(\mathbf{y}) + \tilde{\phi}_{k,2}(\mathbf{x})\tilde{\phi}_{k,2}^*(\mathbf{y}) \right]. \end{aligned} \quad (6.47)$$

Examining the equations (6.28), (6.29), and (6.45) we see that $\tilde{\phi}_{-k,1}(\mathbf{x}) = -\tilde{\phi}_{k,2}(\mathbf{x})$. This means that the integrand of (6.46) is an even function of k which enables us to extend the integral from $-\infty$ to $+\infty$. So we are going to express $\eta_+(\mathbf{x}, \mathbf{y})$ in the form:

³Realize that there happened a switch between eigenfunctions in the sense that while $\psi_{k,1}$ and $\psi_{k,2}$ were tending to ordinary normalized free particle solutions $\frac{1}{\sqrt{2\pi}}e^{ikx}$ and $\frac{1}{\sqrt{2\pi}}e^{-ikx}$, respectively, now $\tilde{\psi}_{k,1}$ and $\tilde{\psi}_{k,2}$ tend to $\frac{1}{\sqrt{2\pi}}e^{-ikx}$ and $\frac{1}{\sqrt{2\pi}}e^{ikx}$, respectively, as coupling constant z tends to 0.

$$\eta_+(x, y) = \frac{1}{2} \int_{-\infty}^{\infty} dk \left[\tilde{\phi}_{k,1}(x) \tilde{\phi}_{k,1}^*(y) + \tilde{\phi}_{k,2}(x) \tilde{\phi}_{k,2}^*(y) \right]. \quad (6.48)$$

Since $\tilde{\phi}_{k,\cdot}(x)$ has three different representations in three different regions for $x < -1$, $-1 < x < 1$, and $x > 1$, in order to find $\eta_+(x, y)$, we need to consider the integral (6.48) in 9 different regions. However Hermiticity of η_+ , i.e.; $\eta_+^*(x, y) = \eta_+(y, x)$, reduces the necessity to examine all 9 cases to just 5. Then using the Hermiticity we are able to find the representation of $\eta_+(x, y)$ for other 4 cases.

Using (6.28), (6.29), (6.45), (6.48), and the identity $\frac{1}{2\pi} \int_{-\infty}^{\infty} dk \frac{e^{ik\alpha}}{k^n} = \frac{i^n \alpha^{n-2} |\alpha|}{2(n-1)!}$ and after tedious calculations and surprising simplifications, we find the metric operator $\eta_+(x, y)$ as

$$\eta_+(x, y) = \delta(x - y) + \eta_{+1}(x, y)z + \mathcal{O}(z^2), \quad (6.49)$$

in which

$$\eta_{+1}(x, y) = \frac{i}{2} \text{sign}(y - x) [\Theta(x + y - 2) - \Theta(x + y + 2)], \quad (6.50)$$

where

$$\text{sign}(x) = \left\{ \begin{array}{ll} -1 & \text{for } x < 0 \\ 1 & \text{for } x > 0 \\ 0 & \text{for } x = 0 \end{array} \right\}, \quad (6.51)$$

and

$$\Theta(x) = \left\{ \begin{array}{ll} 0 & \text{for } x \leq 0 \\ 1 & \text{for } x > 0 \end{array} \right\}. \quad (6.52)$$

It is easy to check that $\eta_+(x, y)$ is Hermitian and at the Hermitian limit $z \rightarrow 0$, $\eta_+(x, y) \rightarrow \delta(x, y)$. However boundedness of $\eta_{+1}(x, y)$ so of η_+ is not that much clear and we therefore give a detailed proof in Appendix B.

Before finishing this section we want to mention that while we were working on this thesis, Mostafazadeh achieved a differential realization of pseudo-Hermiticity in [14]. He used the fact that when it is realized in the \vec{x} -basis, pseudo-Hermiticity condition (3.1) for a general Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + v(\vec{x}) \quad (6.53)$$

acting on $L^2(\mathbb{R}^n)$ gives a partial differential equation for the metric operator $\eta(x, y)$, namely

$$\left(-\nabla_x^2 + \nabla_y^2 + \frac{2m}{\hbar^2} [v(\vec{x})^* - v(\vec{y})] \right) \eta(x, y) = 0, \quad (6.54)$$

where $\nabla_x^2 = \sum_j^n \partial/\partial x_j^2$. Using (6.54) he found a perturbative calculation method for $\eta(x, y)$ without making any spectral analysis. He applied this method to some toy models including our Hamiltonian. He found that for the potential type $v(x) = i \sum_{n=1}^N z_n [\delta(x - a_n) - \delta(x - a_n)]$, where $N \in \mathbb{Z}^+$, $z_n, a_n \in \mathbb{R}$, most general metric operator $\eta(x, y)$ which reduces to the identity in the Hermitian limit is given by

$$\eta(x, y) = \delta(x - y) + \sum_{n=1}^N z_n \eta_{1n}(x, y) + \mathcal{O}(z_n^2), \quad (6.55)$$

where

$$\eta_{1n}(x, y) := w_{n+}(x - y) + w_{n-}(x + y) + \frac{i}{2} \Theta(x + y - 2a_n) \text{sign}(y - x), \quad (6.56)$$

and $w_{n\pm} : \mathbb{R} \mapsto \mathbb{C}$ is any arbitrary function satisfying $w_{n\pm}(x)^* = w_{n\pm}(\mp x)$. Note that when we take $N = 1$, $a_1 = 1$ and $w_{1\pm} = 0$, it reduces to our metric operator $\eta_+(x, y)$.

6.4 Physical Analysis

After getting our metric operator $\eta_+(x, y)$ we are ready to analyze the physical system we have. As we explained in subsection 1.2 we can use whichever picture we want, picture 1 or picture 2. Here we choose to use picture 2, i.e., we want to work on usual Hilbert Space $\mathcal{H} = L^2(\mathbb{R})$ with the conventional inner product. So what we need to do is just to calculate the corresponding dimensionless Hermitian Hamiltonian $h := \rho_+ H \rho_+^{-1}$. In order to calculate h we are going to use the perturbative method explained in Chapter 5. Realize that in our dimensionless Hamiltonian H our real perturbation parameter is z , and H is in the form

$$H = H_0 + zH_1, \quad (6.57)$$

where H_0 is the Hermitian and H_1 is the anti-Hermitian parts of H whose position representations are

$$H_0(x, y) = \langle x | H_0 | y \rangle := -\frac{d^2}{dx^2} \delta(x - y), \quad (6.58)$$

and

$$H_1(x, y) = \langle x|H_1|y \rangle := -i\delta(x - y) [\delta(x - 1) - \delta(x + 1)], \quad (6.59)$$

respectively. So, following the argument of Chapter 5 and using (5.8) and (5.9) we see that we can express our dimensionless Hermitian Hamiltonian as

$$h = H_0 - \frac{1}{4}[H_1, \eta_{+1}]z^2 + \mathcal{O}(z^3), \quad (6.60)$$

where η_{+1} is the operator whose position representation is $\eta_{+1}(x, y)$. Now using (6.50), (6.58), (6.59) and (6.60) we can write the position representation $h(x, y)$ of h up to second order in z according to

$$\begin{aligned} h(x, y) = \langle x|h|y \rangle = & -\frac{d^2}{dx^2} + \frac{z^2}{8}\{\delta(x + 1)[\Theta(y + 1) - \Theta(y - 3)] \\ & + \delta(x - 1)[\Theta(y + 3) - \Theta(y - 1)] + \delta(y + 1)[\Theta(x + 1) - \Theta(x - 3)] \\ & + \delta(y - 1)[\Theta(x + 3) - \Theta(x - 1)]\} + \mathcal{O}(z^3). \end{aligned} \quad (6.61)$$

This is the position representation of the dimensionless Hermitian Hamiltonian h . The position representation of dimensional Hermitian Hamiltonian $h = \rho H \rho^{-1}$ (up to second order in ζ) can be found by substituting first two identities of (6.5) into (6.62) and multiply it by $\frac{\hbar^2}{2ma^2}$. Using the identities $\delta(x/a) = a\delta(x)$ and $\Theta(x/a) = \Theta(x)$ for $a > 0$ we then get

$$\begin{aligned} h(x, y) = \langle x|h|y \rangle = & -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{ma\zeta^2}{4\hbar^2} \{\delta(x + a)[\Theta(y + a) - \Theta(y - 3a)] \\ & + \delta(x - a)[\Theta(y + 3a) - \Theta(y - a)] + \delta(y + a)[\Theta(x + a) - \Theta(x - 3a)] \\ & + \delta(y - a)[\Theta(x + 3a) - \Theta(x - a)]\} + \mathcal{O}(\zeta^3). \end{aligned} \quad (6.62)$$

In view of this relation h acts on a wave function $\psi(x)$ in $L^2(\mathbb{R})$ as follows:

$$\begin{aligned} (h\psi)(x) = & -\frac{\hbar^2}{2m}\psi''(x) + \frac{ma\zeta^2}{4\hbar^2} \{\delta(x + a) \int_{3a}^{-a} \psi(y)dy - \delta(x - a) \int_{-3a}^a \psi(y)dy \\ & + [\Theta(x + a) - \Theta(x - 3a)]\psi(-a) - [\Theta(x - a) - \Theta(x + 3a)]\psi(a)\} + \mathcal{O}(\zeta^3). \end{aligned} \quad (6.63)$$

6.5 Energy Expectation Value of Some Gaussian Wave Packets

We can analyze the physical aspects of our system in exactly the same way as in conventional Quantum Mechanics. The only unusual feature of our system is the fact

that our Hamiltonian is non-local. This non-locality and the complicated appearance of $h(x, y)$ in (6.62), do not however cause any difficulties in computing certain physical quantities for our system. For example we can evaluate the energy expectation values of two kinds of Gaussian wave packets. First, we consider a Gaussian wave packet that stays at the center with a nonzero mean momentum. Next we examine a Gaussian wave packet with zero mean momentum but nonzero mean position. The position representation of the first wave packet is

$$G_1(x) = \frac{1}{(\pi\sigma)^{1/4}} e^{-\frac{x^2}{2\sigma^2} + ik_0x}, \quad (6.64)$$

and of the second one is

$$G_2(x) = \frac{1}{(\pi\sigma)^{1/4}} e^{-\frac{(x-x_0)^2}{2\sigma^2}}, \quad (6.65)$$

where $\sigma > 0$ is the width and $x_0, k_0 \in \mathbb{R}$.

The reason why we choose these Gaussian wave packets is that they represent some localized particles in the actual physical space. Note that if we had chosen to work in picture 1 instead of picture 2, we would have to calculate $\rho^{-1}G_1$ and $\rho^{-1}G_2$ to find the mathematical representations of these localized particles in the first picture. This again shows that despite the fact that H is local in the first picture (unlike h in the second one), it might still be much harder to work in picture 1 because the only thing we know in the first picture is H itself and every other mathematical representation of the actual physical system has to be calculated by transforming the corresponding known representations from the second picture. Moreover this is not just a problem about calculation, it is also a problem about intuition. In the first picture, the relation between physical entities and their mathematical representations is not intuitively clear except maybe H whereas in the second picture this fuzzyness in intuition may only occur for h .

Now we proceed with finding the corresponding energy expectation values

$$E_1 := \langle G_1 | h | G_1 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G_1(x) h(x, y) G_1^*(y) dx dy \quad (6.66)$$

and

$$E_2 := \langle G_2 | h | G_2 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G_2(x) h(x, y) G_2^*(y) dx dy. \quad (6.67)$$

Substituting (6.62), (6.64) into (6.66), and (6.62), (6.65) into (6.67), and using the properties of delta and theta functions and performing the necessary integrations we obtain

$$E_1 = \frac{\hbar^2}{2m} (k_0^2 + \frac{1}{2\sigma^2}) + \frac{m\zeta^2}{4\hbar^2} B_1 + \mathcal{O}(\zeta^3) \quad (6.68)$$

and

$$E_2 = \frac{\hbar^2}{2m} (\frac{x_0^2}{\sigma^4} + \frac{3}{4\sigma^2}) + \frac{m\zeta^2}{4\hbar^2} B_2 + \mathcal{O}(\zeta^3) \quad (6.69)$$

where

$$B_1 := 2\sqrt{2} e^{-\frac{1}{2}(\frac{a^2}{\sigma^2} + k_0^2 \sigma^2)} \operatorname{Re} \left(e^{iak_0} \left(\operatorname{Erf}[\frac{3a - ik_0 \sigma^2}{\sqrt{2}\sigma}] + \operatorname{Erf}[\frac{a + ik_0 \sigma^2}{\sqrt{2}\sigma}] \right) \right), \quad (6.70)$$

$$B_2 := \sqrt{2} e^{-\frac{(a+x_0)^2}{2\sigma^2}} \times \left(\operatorname{Erf}[\frac{a+x_0}{\sqrt{2}\sigma}] + e^{\frac{2ax_0}{\sigma^2}} \left(-\operatorname{Erf}[\frac{-a+x_0}{\sqrt{2}\sigma}] + \operatorname{Erf}[\frac{3a+x_0}{\sqrt{2}\sigma}] \right) + \operatorname{Erf}[\frac{3a-x_0}{\sqrt{2}\sigma}] \right). \quad (6.71)$$

Here $\operatorname{Erf}[z]$ is the error function defined as $\operatorname{Erf}[z] := \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$ for $z \in \mathbb{C}$. Actually B_1 and B_2 are more important for us than actual expectation values since they represent the non-Hermiticity effects on the energy expectation values of Gaussian wave packets. In order to see these effects we plotted several graphs of B_1 and B_2 keeping all variables constant except central position and momentum.

In Figures 6.2 and 6.3 we see some plots of B_1 versus k_0 , and B_2 versus x_0 for various values of σ . It is clearly seen from both of the figures that the effect of non-Hermiticity diminishes as σ goes to 0 or ∞ , and it attains its maximum around $\sigma = 2a$. Also in Figure 6.2, we see that non-Hermiticity effect decays rapidly for the central momentum values $p_0 = \hbar k_0$ outside the region $[-\hbar a^{-1}, \hbar a^{-1}]$. There is also an oscillation pattern for $\sigma > 1$ in addition to the decay, which seems to have a period $T = \pi/2a$ regardless of the value of σ .

In the Figure 6.3 local effects of non-Hermiticity can be seen more clearly. For small values of σ non-Hermiticity effect exists for only those stationary packets which have central position around a and $-a$ with an effective region $[-a - \sigma, -a + \sigma]$ and

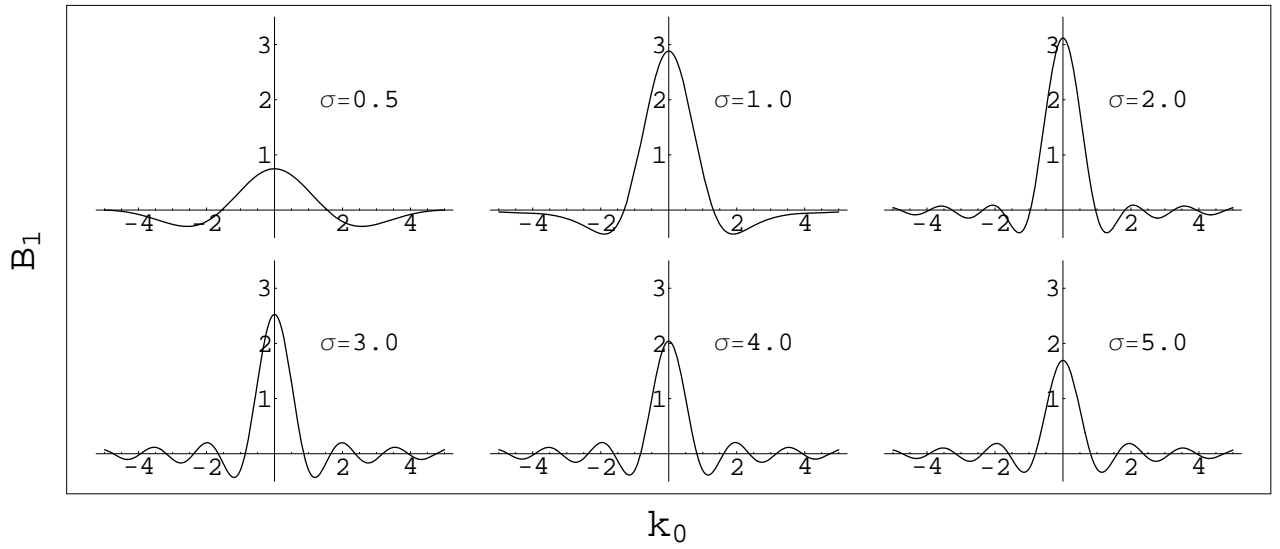


Figure 6.2: Plots of B_1 as a function of k_0 for $\sigma = 0.5$, $\sigma = 1$, $\sigma = 2$, $\sigma = 3$, $\sigma = 4$ and $\sigma = 5$ in units where $a = 1$.

$[a - \sigma, a + \sigma]$. As σ increases these effective regions extend and superpose on to each other.

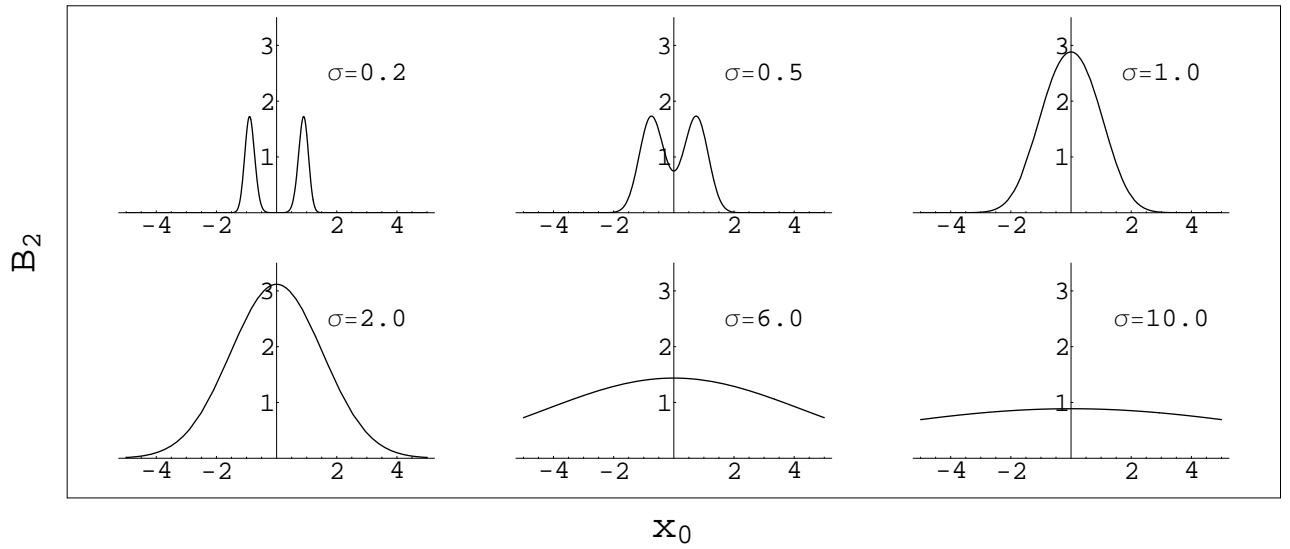


Figure 6.3: Plots of B_2 as a function of x_0 for $\sigma = 0.2$, $\sigma = 0.5$, $\sigma = 1$, $\sigma = 2$, $\sigma = 6$ and $\sigma = 10$ in units where $a = 1$.

Chapter 7

CONCLUSION

In this thesis we explained how we can use some non-Hermitian but pseudo-Hermitian Hamiltonians in Quantum Mechanics. We showed that for a Hamiltonian with discrete spectrum, its η_+ -pseudo-Hermiticity for some positive definite η_+ is equivalent to the reality of its spectrum. We then showed how we can change our Hilbert space or equivalently our inner product and other mathematical objects such as mathematical representation of physical observables and states to be consistent with Quantum Measurement Theory. We also addressed the unitary equivalence of separable Hilbert Spaces and suggested another picture in which we use conventional inner product and usual mathematical representations but we transform the initial non-Hermitian Hamiltonian H to the corresponding Hermitian Hamiltonian $h = \rho_+ H \rho_+^{-1}$.

Next we applied our theory to the \mathcal{PT} -Symmetric delta function potential with a real coupling constant ζ . We proved the existence of a critical ζ value ζ_c which ensures the reality of the spectrum of this system. After we ensured the reality of the spectrum we mimicked the method we explained for discrete systems to find an appropriate metric operator η_+ and the corresponding Hermitian Hamiltonian h for a system which has a continuous spectrum. In the non-degenerate case eigenfunctions of H and H^\dagger automatically give a biorthonormal system. However in the doubly degenerate case we deal with here, it is not clear how to choose biorthonormal pairs in each degeneracy subspace. We decided to make a symmetric choice for our biorthonormal system with respect to our initial eigenfunctions which reduce to usual free particle solutions as coupling constant tends to zero. After making our choice, we calculated η_+ up to first order in $z = \frac{2m a \zeta}{\hbar^2}$. What we found is that it reduces to the identity in the

Hermitian limit and it is a bounded operator up to our perturbation limit. This is quite remarkable because an arbitrary choice for the biorthonormal system would in general lead to an unbounded η_+ .

After getting the metric operator η_+ up to first order in z , we were able to calculate the corresponding Hermitian Hamiltonian h up to second order in z . We calculated h since we chose to work on usual inner product space \mathcal{H} with the conventional inner product. The reason why we made this choice is that in this picture mathematical representations of physical entities are easier to form and the results we obtain are easy to interpret. For example magnitude square of a state function in position basis represents the probability density of finding the physical particle at the corresponding space region in the actual physical world. This is in contrast to the first picture where we use the Hilbert Space \mathcal{H}_{phys} instead of the usual Hilbert Space $\mathcal{H} = L^2(\mathbb{R})$.

To get some idea about the physical system our Hamiltonian describes, we chose two Gaussian wave packets, one of which stays at the center in position space but has varying mean momentum and the other has zero mean momentum but varying mean position. We looked at the non-Hermiticity effect on the energy expectation values of these localized functions. The result showed that despite the non-local appearance of $h(x, y)$ it behaves like a local operator. Actually we do not see almost any effect of h on the expectation value of wave packets which are localized around any position but a and $-a$. This is what we expect in a sense since the corresponding position representation of our Hamiltonian in H_{phys} only has Dirac delta potentials which are ultra local.

Appendix A

EXISTENCE OF A CRITICAL G VALUE G_C

Theorem: Let u be a complex number which satisfies the conditions

$$\frac{-1 + e^u}{u^2} = G, \quad \text{and} \quad \text{Re}(u) < 0 \quad (\text{A.1})$$

where G is a positive real number and $\text{Re}(u)$ represents the real part of u . Then G cannot be arbitrarily large, i.e. ; there exists a critical G_c such that $\forall G > G_c$, $\nexists u$ which satisfies (A.1).

Proof: Suppose that there does not exist such a critic G_c . Then $\forall M_k > 0$, where k and $M_k \in \mathbb{N}$, $\exists G_k$ such that $G_k > M_k$ and $\exists u_k \in \mathbb{C}$ such that

$$\frac{-1 + e^{u_k}}{u_k^2} = G_k, \quad \text{and} \quad \text{Re}(u_k) < 0. \quad (\text{A.2})$$

Let $M_1 = 1$, then find a G_1 and u_1 which satisfy (A.2). Then choose an $M_2 > G_1$ and find a G_2 and u_2 which satisfy (A.2). Follow the same procedure for $k = 2, 3, 4, \dots$ as well. In this way we can construct two sequences $\{G_n\}_{n \in \mathbb{N}}$ and $\{u_n\}_{n \in \mathbb{N}}$. The sequence $\{G_n\}_{n \in \mathbb{N}}$ diverges to infinity by construction.

Now let $x_n = \text{Re}(u_n) < 0$, and $y_n = \text{Im}(u_n)$, so $u_n = x_n + iy_n$. Then we can rewrite (A.2) as

$$\frac{-1 + e^{x_n + iy_n}}{u_n^2} = \frac{-1 + e^{x_n} e^{iy_n}}{u_n^2} = G_n \quad (\text{A.3})$$

Since G_n is real this also means that

$$\frac{|-1 + e^{x_n} e^{iy_n}|}{|u_n|^2} = G_n \quad (\text{A.4})$$

Together with the fact that $e^{x_n} < 1$ the last equality implies

$$G_n \leq \frac{2}{|u_n|^2} \Rightarrow |u_n| \leq \frac{\sqrt{2}}{\sqrt{G_n}} \quad (\text{A.5})$$

So we get

$$0 \leq \lim_{n \rightarrow \infty} |u_n| \leq \lim_{n \rightarrow \infty} \frac{\sqrt{2}}{\sqrt{G_n}} = 0 \Rightarrow \lim_{n \rightarrow \infty} |u_n| = 0 \Rightarrow \lim_{n \rightarrow \infty} u_n = 0. \quad (\text{A.6})$$

Now let us rewrite (A.2) as

$$\frac{-1 + e^{u_n}}{u_n} = G_n u_n. \quad (\text{A.7})$$

Hence

$$\lim_{n \rightarrow \infty} \frac{-1 + e^{u_n}}{u_n} = \lim_{n \rightarrow \infty} G_n u_n, \quad (\text{A.8})$$

as well. Using the fact that $\lim_{n \rightarrow \infty} u_n = 0$ and applying the L'Hospital Rule, it can be easily seen that the left hand side of (A.8) is 1. Hence we get

$$\lim_{n \rightarrow \infty} G_n u_n = 1, \quad (\text{A.9})$$

which also implies that

$$\lim_{n \rightarrow \infty} G_n x_n = 1. \quad (\text{A.10})$$

However the fact that $G_n > 0$ and $x_n < 0$, $\forall n \in \mathbb{N}$, implies that

$$G_n x_n < 0 \quad \forall n \in \mathbb{N}. \quad (\text{A.11})$$

Equation (A.10) together with (A.11) leads to a clear contradiction. \square

Appendix B

BOUNDEDNESS OF η_{+1}

Consider the absolute value of $\eta_{+1}(x, y)$ of (6.50):

$$|\eta_{+1}(x, y)| = \begin{cases} \frac{1}{2} & \text{if } -2 < x + y < 2 \\ 0 & \text{otherwise} \end{cases}. \quad (\text{B.1})$$

This implies that

$$\int_{-\infty}^{\infty} |\eta_{+1}(x, y)| dy = \int_{-\infty}^{\infty} |\eta_{+1}(x, y)| dx = 2. \quad (\text{B.2})$$

Also consider the map $G : \mathbb{R}^2 \mapsto \mathbb{R}^2$ defined as

$$G(\mathbf{u}, \mathbf{v}) := \left(\frac{\mathbf{u} + \mathbf{v}}{2}, \frac{\mathbf{u} - \mathbf{v}}{2} \right). \quad (\text{B.3})$$

Then the composition function $|\eta_{+1}(G(\mathbf{u}, \mathbf{v}))|$ does not depend on \mathbf{v} :

$$|\eta_{+1}(G(\mathbf{u}, \mathbf{v}))| = \begin{cases} \frac{1}{2} & \text{if } -2 < \mathbf{u} < 2 \\ 0 & \text{otherwise} \end{cases}. \quad (\text{B.4})$$

Note also that G is a one to one and onto map with Jacobian $J_G(\mathbf{u}, \mathbf{v}) = (\text{Determinant of } G'(\mathbf{u}, \mathbf{v})) = -2$.

We need to show that $\exists c > 0$ such that $\forall \psi \in \mathcal{H}, \|\eta_{+1}\psi\| \leq c\|\psi\|$ or equivalently

$\|\eta_{+1}\psi\|^2 \leq c^2\|\psi\|^2$. Actually

$$\|\eta_{+1}\psi\|^2 = \int_{-\infty}^{\infty} dx \left| \int_{-\infty}^{\infty} dy \eta_{+1}(x, y)\psi(y) \right|^2 \quad (\text{B.5})$$

$$\leq \int_{-\infty}^{\infty} dx \left(\int_{-\infty}^{\infty} dy |\eta_{+1}(x, y)| |\psi(y)| \right)^2 \quad (\text{B.6})$$

$$= \int_{-\infty}^{\infty} dx \left(\int_{-\infty}^{\infty} dy |\eta_{+1}(x, y)|^{\frac{1}{2}} |\eta_{+1}(x, y)|^{\frac{1}{2}} |\psi(y)| \right)^2 \quad (\text{B.7})$$

$$\leq \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy |\eta_{+1}(x, y)| \cdot \int_{-\infty}^{\infty} dy |\eta_{+1}(x, y)| |\psi(y)|^2 \quad (\text{B.8})$$

$$= 2 \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy |\eta_{+1}(x, y)| |\psi(y)|^2 \quad (\text{B.9})$$

$$= 2 \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv |J_G(u, v)| |\eta_{+1}(G(u, v))| |\psi(G(u, v))|^2 \quad (\text{B.10})$$

$$= 4 \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv |\eta_{+1}(G(u, v))| |\psi((u-v)/2)|^2 \quad (\text{B.11})$$

$$= 4 \int_{-\infty}^{\infty} du |\eta_{+1}(G(u, v))| \int_{-\infty}^{\infty} dv |\psi((u-v)/2)|^2 \quad (\text{B.12})$$

$$= 8\|\psi\|^2. \quad (\text{B.13})$$

At first step (B.5) we used the Hermiticity of $\eta_{+1}(x, y)$. At step (B.9) we used the Schwartz inequality. Also at step (B.10) it should be understood that when we write $\psi(G(u, v))$ what we actually mean is $\psi(\pi_2(G(u, v)))$ where $\pi_2 : \mathbb{R}^2 \mapsto \mathbb{R}$ is the projection function defined as $\pi_2(x, y) = y$. \square

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