Universidade Estadual Paulista
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Instituto de Geociências e Ciências Exatas

Eigenvalue Accumulation for Schrödinger Equation

A Singular Sturm-Liouville Problem in the Spectral Parameter

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This Monograph is dedicated to my parents

ANTONIO VALDECI BORIN
and
EVA APARECIDA RIBEIRO BORIN

You are everything to me.

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May the Force be with you.

Obi Wan Kenobi

Abstract

In this work we will present the Sturm-Liouville classic theory for the regular problem, showing that several properties of the eigenvalues and eigenfunctions of this problem, for example, that the eigenvalues form an infinite increasing sequence and that the eigenfunctions forms an orthonormal basis for the $C_{L_{2(\rho)}}[a,b]$ space.

In this way, we define the singular Sturm-Liouville problem that it depends continuously of a parameter λ and we prove that the eigenvalues accumulate into the endpoint $\nu \in \Lambda\mathbb{R}$ under certain conditions. We also study the case where it non-accumulate.

Lastly, we realize an application in Quantum Mechanics, where analyzing certain properties of the potential function in the system we may obtain information about the accumulation or non-accumulation of the energy.

Key-words: Sturm-Liouville Problem, Eigenvalue Accumulation , Schrödinger Equation.

Resumo

Neste trabalho apresentamos a teoria clássica de Sturm-Liouville para o problema regular, mostrando que diversas propriedades dos autovalores e das autofunções deste problema, por exemplo, que os autovalores formam uma sequência infinita e crescente e que as autofunções formam uma base ortonormal para o espaço $C_{L_{2(\rho)}}[a,b]$.

Em seguida, definimos o problema singular de Sturm-Liouville que depende continuamente de um parâmetro λ e mostramos que os autovalores acumulam no limitante superior $\nu \in \Lambda \subset \mathbb{R}$ sob certas condições. Também estudamos o caso em que eles não acumulam.

Por fim, realizamos uma aplicação em Mecânica Quântica, onde analisando certas propriedades da função potencial em que o sistema está submetido obtemos informações sobre a acumulação ou não-acumulação da energia.

Palavras-chave: Problema de Sturm-Liouville, Acumulação dos Autovalores, Equação de Schrödinger.

Contents

Chapter 1 Introduction

An important and significant application of Functional Analysis is the study of Sturm-Liouville's Problem come from Differential Equations. Several situations fall into type of problem, for example, in some cases when we apply the Separation of Variables Method into PDE's obtaining a Sturm-Liouville problem whose solutions depends an eigenfunctions series. This one may be transform into a integral equation, which in turn corresponding to a Hermitian compact operator, thus by the spectral theory of these operators many properties about the eigenfunctions and eigenvalues can be founded.

When we look for solutions on a certain interval $I = [a,b]$, we need a specific condition in the endpoints of I. This case is known as the Regular Sturm-Liouville Problem. However, in some physical problems we cannot define the system on the endpoint, then consider that the interval is defined by $I = (a,b]$, $I = [a,b)$ or $I = (a,b)$. Furthermore, the ODE may depends of a parameter that has a central role on the model of this work. In our case, we have a Singular Sturm-Liouville that depends of a parameter λ which vary in determined interval on $\mathbb{R}$. There are several papers about this, see [1], [3] [5], [13], [15], [17], [22], [23] [24], [27], [28], [32], [34], [41].

In this work, we will present a detail study based on [23], [41] of a result about the accumulation of the eigenvalues on the endpoint $\nu \in \Lambda$ and we will see that the eigenvalues are intrinsically related with the oscillation properties of the solution at $\lambda = \nu \in \Lambda$. Accordingly, this monograph is organized in the following outline:

Chapter 2: Mainly treats the main results about the Regular Sturm-Liouville theory.

Chapter 3: We discuss the Singular Sturm-Liouville problem which depends continuously of a parameter λ, we did all the prerequisites and necessary results to show the main theorem of this work, which provide conditions for the accumulation or non-accumulation of eigenvalues. In addition, we present the proof of this result on a detailed way.

Chapter 4: Immediately we delve into the application of the main result of Chapter 3 in Schrödinger Equation with its deduction and the physical meaning.

The main goal of this monograph is to gather classic results and very well known of the Sturm-Liouville Theory with the most recent results about the singular problem, in general, not raised in undergraduate course.

The figures in this work were prepared by the author in order to clarify some ideas present in the proofs of the results.

In conclusion, I wish you all a good and pleasant reading and I hope you enjoy the text.

CHAPTER

2 The Regular Sturm-Liouville Problem

In this chapter we will present the Regular Sturm-Liouville Problem, a classic problem in the differential equations theory with applications in physics. In the Sections 2.2 and 2.4 we will show some properties. In the Section 2.3, we will present an approximate determination method of the eigenvalues. In the last section, we will study the Sturm Comparison Theorems and Sturm's Separation Theorem. The results of the sections 2.1, 2.2, 2.3 and 2.4 can be found in [4], [18] and [19]. The section 2.6, in its totality, is in paper [6]. For the last section, the results were based in the references [9], [16], [25], [30] and [44].

2.1 Basic Facts

In this section we will introduce some basic definitions, in such way that in the end of the section we have the foundations necessary to define the Sturm-Liouville Problem.

In diverse cases, a physical phenomenon must satisfy some property on the boundary region where it's defined. This property, is called *boundary condition*. There are several types of boundary condition, however, we will focus particularly in two that will be defined bellow.

Definition 2.1.1 Consider $y \in C([a,b],\mathbb{R})$ and $\alpha_1, \alpha_2, \beta_1, \beta_2, \varphi_1, \varphi_2 \in \mathbb{R} \setminus \{0\}$ such that $\alpha_1^2 + \alpha^2 \neq 0$ and $\beta_1^2 + \beta^2 \neq 0$. If the function y satisfies the following conditions

$$\alpha_1 y(a) + \alpha_2 y'(a) = \varphi_1$$
$$\beta_1 y(b) + \beta_2 y'(b) = \varphi_2,$$

we say that these conditions are *linear*.

Definition 2.1.2 Let y be a function defined on interval $[a,b]$ and $\alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{R}/\{0\}$. If the function y satisfies the following conditions

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0$$
$$\beta_1 y(b) + \beta_2 y'(b) = 0,$$

we say that these conditions are *linear* and *homogeneous*.

Every boundary value problem consists of a condition and a differential equation that governing the system. Now, we will discuss about this equation of the Sturm-Liouville Problem. For convenience, we will in introduce the following differential operator.

Definition 2.1.3 — Liouville Operator. Let $J = [a,b] \subset \mathbb{R}$ the t-interval and let r, p and q be real functions on J, such that

- r is continuous, differential and strictly increasing function on J, i.e, $r \in C^1([a,b])$ with $r(t) > 0$ for all $t \in [a,b]$
- p is continuous on J, i.e., $p \in C([a,b],\mathbb{R})$
- q is continuous and strictly increasing on J, i.e, $q \in C([a,b])$ with $q(t) > 0$ for all $t \in [a,b]$.
  Given a function $y \in C^2([a,b])$ we define the following second order linear differential operators
  $$L_\lambda[y] = -(r(t)y')' + [p(t) - \lambda q(t)]y$$
  and
  $$L[y] = -[r(x)y']' + p(x)y.$$

where $'$ denotes $\frac{d}{dt}$. This operator is known as **Liouville Operator**.

Finally, we are ready to define the *Sturm-Liouville Problem*

Definition 2.1.4 — The Sturm-Liouville Problem. The **Regular Sturm-Liouville Problem**, or simply **Sturm-Liouville Problem**, consists in determining a function $y \in C^2([a,b])$, such that the following BVC (Boundary Value Condition) is verified:

$$L_\lambda[y](t) = 0 \qquad \text{or} \qquad L[y] = \lambda q(t)y, \tag{2.1}$$

for all $t \in [a,b]$, with the following linear and homogeneous boundary conditions,

$$\begin{aligned} \alpha_1 y(a) + \alpha_2 y'(a) = 0, \\ \beta_1 y(b) + \beta_2 y'(b) = 0. \end{aligned} \tag{2.2}$$

REM We use the term Singular Sturm-Liouville Problem to indicate when at least one of the functions r, p or q not satisfies one or more conditions in the endpoint of the interval.

The result bellow guarantees uniqueness of the solution to the problem in Definition 2.1.4.

Theorem 2.1.1 — Uniqueness of Sturm-Liouville Problem. If $\lambda = 0$ is not a eigenvalue of the Sturm-Liouville Problem, that is, if $Ly = 0$ with boundary conditions (2.2) has only the trivial solution $y = 0$, then the Sturm-Liouville Problem in Definition 2.1.4 has a only one solution.

Proof. Let y_1 and y_2 be distinct solutions of the Sturm-Liouville Problem, i.e., $L_\lambda[y_1] = 0$ and $L_\lambda[y_2] = 0$. Subtracting the two equation above, we obtain $L_\lambda[y_1] - L_\lambda[y_2] = 0$. Since the

Liouville Operator is linear

$$L_\lambda[y_1 - y_2] = 0.$$

As, by hypothesis, the above equation has only a trivial solution, thus

$$y_1 - y_2 = 0 \implies y_1 = y_2.$$

■

Now, we will do some considerations about this problem.

Proposition 2.1.2 Suppose that the non-homogeneous Sturm-Liouville Problem with homogeneous boundary conditions has a solution. Then, the same problem with homogeneous boundary conditions has solution too.

Proof. Indeed, if $y_0 \in C^2([a,b])$ is a function such that

$$\alpha_1 y(a) + \alpha_2 y'(a) = \varphi_1,$$
$$\beta_1 y(b) + \beta_2 y'(b) = \varphi_2.$$

so it is easy to see that $y = z + y_0$ is solution of

$$\begin{cases} L_\lambda[z] = f - L_\lambda[y_0], \\ \alpha_1 z(a) + \alpha_2 z'(a) = 0, \\ \beta_1 z(b) + \beta_2 z'(b) = 0. \end{cases}$$

■

Proposition 2.1.3 Every second order ordinary equation

$$-a_0(t)y'' + a_1(t)y' + [a_2(t) - \lambda\mu(t)]y = g(t), \tag{2.3}$$

where $a_0 \in C([a,b])$ with $a_0(t) > 0$ on the interval $t \in [a,b]$, $\mu \in C([a,b],\mathbb{R})$ can be write in the form $L_\lambda[y] = f$.

Proof. Multiplying all the terms of the Equation (2.3) by the function

$$\frac{1}{a_0(t)} r(t) = \frac{1}{a_0(t)} \exp\left[\int \frac{a_1(s)}{a_0(s)} ds\right],$$

we obtain that

$$r(t)y'' + \overbrace{\frac{a_1(t)}{a_0(t)} \exp\left[\int \frac{a_1(s)}{a_0(s)} ds\right]}^{r'(t)} y' + \frac{r(t)[a_2(t) + \lambda\mu(t)]}{a_0(t)} y = \frac{g(t)r(t)}{a_0(t)}.$$

In other words,

$$r(t)y'' + r'(t)y' + \frac{r(t)[a_2(t) + \lambda\mu(t)]}{a_0(t)} y = \frac{g(t)r(t)}{a_0(t)}.$$

By Product Rule, we have

$$[r(t)y']' + \frac{r(t)[a_2(t) + \lambda\mu(t)]}{a_0(t)} y = \frac{g(t)r(t)}{a_0(t)}.$$

Setting

$$p(t) = \frac{r(t)a_2(t)}{a_0(t)}, \qquad q(t) = \frac{r(t)\mu(t)}{a_0(t)} \qquad \text{and} \qquad f(t) = \frac{r(t)g(t)}{a_0(t)},$$

we have an equation under the form $L_\lambda[y] = f$. ■

The next definition is fundamental to the theory of this chapter.

Definition 2.1.5 — Eigenvalues and Eigenfunctions of Sturm-Liouville Problem. We say that λ is a *Eigenvalue of Sturm-Liouville Problem* if the Equation (2.1) is satisfied by some function y_λ, that is usually λ-dependent, and this function is called of *eigenfunction* associated to the eigenvalue λ of Sturm-Liouville Problem.

This nomenclature is justified because defining the operator

$$M := -\frac{1}{q}L,$$

we can write the equation $Ly_\lambda + \lambda q y_\lambda = 0$ under the form $My_\lambda = \lambda y_\lambda$ that is the eigenvalue equation to the operator M.

Besides, several physical problems consist in solving Sturm-Liouville Problems, it's useful to solve non-homogeneous equations

$$L[y](t) = f(t)$$

where f is a given function, with boundary conditions like (2.2), known as the *Sturm Problem*. The reason for this comes from the fact of the Green functions of the Sturm Problem can be write in terms of eigenfunction and eigenvalues of a Sturm-Liouville Problem.

Now, we will give some physical examples

■ **Example 2.1** In Quantum Mechanics, to determine the one-dimensional wave function of a particle with mass m, imprisoned on an interval $[a,b] \subset \mathbb{R}$ by through infinite barrier of potential on $x \leq a$ e $x \geq b$, and subject to potential $V(x)$ on $[a,b]$, consist in solving the following time-independent Schrödinger equation,

$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}(x) - V(x)\psi(x) + E\psi(x) = 0,$$

on x-interval $x \in [a,b]$. Due to the infinite barrier of potential we must impose the boundary conditions $\psi(a) = 0$ and $\psi(b) = 0$. This is a Sturm-Liouville Problem with $r(x) = \frac{\hbar^2}{2m}$, $p(x) = -V(x)$, $q(x) = 1$, $\lambda = E$. ■

■ **Example 2.2** When we are solving the wave equation and the diffusion equation in polar coordinates, we obtain that the radial part result in the Bessel Equation

$$x^2y''(x)+xy'(x)+(\alpha^2x^2-\nu^2)y(x)=0.$$

This problem is a Sturm-Liouville Equation with $r(x)=x$, $p(x)=\dfrac{-\nu^2}{x}$, $q(x)=x$ and $\lambda=\alpha^2$. ■

2.2 Properties of the Eigenvalues and Eigenfunctions

In this section we will show some results about the Regular Sturm-Liouville Problem. For example, the eigenvalue are real and the eigenfunctions can be choose as real.

Before setting such properties of the Regular Sturm-Liouville Problem, it is necessary to present an identity, known as Lagrange's identity, which is basic to the study of linear boundary value problems.

Proposition 2.2.1 — Lagrange's Identity. Let L be a Liouville operator and $u,v\in C^2([a,b],\mathbb{C})$ given functions. Then

$$\int_a^b (\overline{v}L[u]-u\overline{L[v]})dt = M[u,v](b)-M[u,v](a)$$

where $M[u,v](t)=-r(t)[u'(v)\overline{v(t)}-u(t)\overline{v'(t)}]$,

Proof. The Liouville operator is given by

$$L[y]=-(r(t)y')'+p(t)y,$$

where $r\in C^1([a,b],\mathbb{R})$ and $p\in C([a,b],\mathbb{R})$. In this way $p(t)=\overline{p(t)}$ e $r(t)=\overline{r(t)}$. Then

$$\begin{aligned}\int_a^b (\overline{v}L[u]-u\overline{L[v]})dt &= \int_a^b (\overline{v}(-(ru')'+pu)-u\overline{(-(rv')'+pv)})dt\\ &= \int_a^b [-\overline{v}(ru')'+p\overline{v}u+u\overline{(rv')'}-p\overline{v}u]dt\\ &= -\int_a^b \overline{v}(ru')'dt+\int_a^b u\overline{(rv')}'dt.\end{aligned}$$

Integrating both terms on the variable t on the right side by parts, we obtain

$$\begin{aligned}\int_a^b (\overline{v}L[u] - u\overline{L[v]})dt &= \int_a^b (\overline{v}(-(ru')' + pu) - u\overline{u(-(rv')' + pv)})dt \\ &= -\left[\overline{v}(ru')\Big|_a^b - \int_a^b \overline{v}'(ru')dt\right] + \left[u\overline{(rv')}\Big|_a^b - \int_a^b u'\overline{rv'}dt\right] \\ &= \left[-\overline{v}(ru') + u\overline{(rv')}\right]_a^b + \int_a^b [\overline{v}'(ru') - u'\overline{(rv')}]dt \\ &= -r[u'\overline{v} - u\overline{v}']_a^b \\ &= M[u,v](b) - M[u,v](a),\end{aligned}$$

which is Lagrange's identity. ■

Now, we will show the following result called *Green's Lemma*

Lemma 2.2.2 — Green's Lemma. Let $u, v \in C^2([a,b])$. Suppose that these functions satisfy the Boundary Conditions (2.2). Then,

$$\langle Lu, v\rangle = \langle u, Lv\rangle,$$

that is

$$\int_a^b \overline{v}L[u]dt = \int_a^b u\overline{L[v]}dt.$$

Proof. From Lagrange's identity, we get

$$\int_a^b (\overline{v}L[u] - u\overline{L[v]})dt = M[u,v](b) - M[u,v](a)$$

So, if we show $M[u,v](b) = M[u,v](a) = 0$ we finish the proof.

Since u and v satisfy the Boundary Conditions (2.2), we have

$$\begin{cases} \alpha_1 u(a) + \alpha_2 u'(a) = 0 \\ \alpha_1 v(a) + \alpha_2 v'(a) = 0 \end{cases} \quad \text{e} \quad \begin{cases} \beta_1 u(b) + \beta_2 u'(b) = 0 \\ \beta_1 v(b) + \beta_2 v'(b) = 0. \end{cases}$$

Since, β_i and α_i are real functions, thus, follow by conjugation

$$\begin{cases} \alpha_1 \overline{u(a)} + \alpha_2 \overline{u'(a)} = 0 \\ \alpha_1 \overline{v(a)} + \alpha_2 \overline{v'(a)} = 0 \end{cases} \quad \text{e} \quad \begin{cases} \beta_1 \overline{u(b)} + \beta_2 \overline{u'(b)} = 0 \\ \beta_1 \overline{v(b)} + \beta_2 \overline{v'(b)} = 0 \end{cases}$$

writing in the matrix form

$$\begin{pmatrix} \overline{v(a)} & \overline{v'(a)} \\ u(a) & u'(a) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{e} \quad \begin{pmatrix} \overline{v(b)} & \overline{v'(b)} \\ u(b) & u'(b) \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

As $\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, for the system above be possible, we must have

$$\det \begin{pmatrix} \overline{v(a)} & \overline{v'(a)} \\ u(a) & u'(a) \end{pmatrix} = 0 \quad \text{e} \quad \begin{pmatrix} \overline{v(b)} & \overline{v'(b)} \\ u(b) & u'(b) \end{pmatrix} = 0,$$

i.e.,

$$\overline{v(a)}u'(a) - \overline{v'(a)}u(a) = 0$$

and

$$\overline{v(b)}u'(b) - \overline{v'(b)}u(b) = 0.$$

Hence, $M[u,v](a) = M[u,v](b) = 0$. ■

The Green's Lemma affirm that L is a symmetric operator with respect to the inner product defined by

$$< f, g >= \int_a^b f(x)\overline{g(x)}dx.$$

Now, from Green's Lemma, we will show finally some properties that are true for whatever the Sturm-Liouville problems.

Proposition 2.2.3 The eigenvalues of the Sturm–Liouville problem are real.

Proof. Let λ be an eigenvalue and let u be a corresponding eigenfunction, i.e., $L[u] = \lambda r(t)u(t)$. Note that

$$\overline{L[u]} = -\overline{(r(t)u'(t))' + p(t)u(t)} = -(r(t)\overline{y'(t)})' + p(t)\overline{u}(t) = L[\overline{u}],$$

that can be write as $\overline{L[u]} = L[\overline{u}]$.

Applying the Green's Lemma to the function u and $\overline{u}$, we have

$$\begin{aligned}
0 &= \int_a^b \left(\overline{u}L[u] - u\overline{L[u]}\right) dt \\
&= \int_a^b (\overline{u}L[y] - uL[\overline{u}])\, dt \\
&= \int_a^b \left(\overline{u}(t)\lambda q(t)u(t) - u(t)\overline{\lambda}r(t)\overline{u}(t)\right) dt \\
&= \int_a^b (\lambda - \overline{\lambda})q(t)u(t)\overline{u(t)}dt \\
&= (\lambda - \overline{\lambda}) \int_a^b q(t)|u(t)|^2 dt,
\end{aligned}$$

then,

$$(\lambda - \overline{\lambda}) \int_a^b q(t)|u(t)|^2 dt = 0. \tag{2.4}$$

Since $u \neq 0$ and $q > 0$, by hypothesis, $\int_a^b q(t)|u(t)|^2 dt \neq 0$. Therefore, $\lambda - \overline{\lambda} = 0$, i.e., $\lambda = \overline{\lambda}$. Hence, λ is real, so the theorem is proved.

■

Proposition 2.2.4 The eigenfunctions of the Sturm-Liouville Problem are a linear combination of real eigenfunction, corresponding to the same eigenvalue.

Proof. Let $y \in C^2$ be an eigenfunction corresponding to the eigenvalue λ. From the Proposition 2.2.3, we have $L[\bar{y}] = \overline{\lambda} q\bar{y} = \lambda q\bar{y}$. However, we can rewrite y in the following form

$$y(t) = \frac{1}{2}(y(t) + \overline{y(t)}) - \frac{i}{2}(i\overline{y(t)} - iy(t)).$$

Setting,

$$y_1 := \frac{y(t) + \overline{y(t)}}{2} \qquad \text{e} \qquad y_2 := \frac{i(\overline{y(t)} - y(t))}{2},$$

we obtain, in the compact form,

$$y(t) = y_1(t) + iy_2(t).$$

Thus,

$$\begin{aligned}
\lambda q(t)y_1(t) &= \lambda q(t)y_1\left(\frac{y(t) + \overline{y(t)}}{2}\right) \\
&= \frac{\lambda}{2}q(t)y(t) + \frac{1}{2}\lambda q(t)\overline{y(t)} \\
&= \frac{1}{2}L[y] + \frac{1}{2}L[\bar{y}] \\
&= \frac{1}{2}L[y + \bar{y}] \\
&= L[y_1].
\end{aligned}$$

Analogously

$$\lambda r(t)y_2(t) = L[y_2].$$

Hence, we always can write y as a linear combination of real eigenfunctions y_1 and y_2. ■

REM The previous proposition allows us to consider that the eigenfunctions of the Sturm-Liouville problem can be choose always as real functions.

The following theorem describe a fundamental property about the eigenfunction of Sturm-Liouville Problem.

Theorem 2.2.5 — Relationship of Orthogonality. Let y_1 and y_2 be two eigenfunctions of the Sturm-Liouville problem corresponding to distinct eigenvalues λ_1 and λ_2, respectively. Then y_1 and y_2 are orthogonal with respect inner product

$$\langle y_1, y_2 \rangle_r = \int_a^b y_1(t)\overline{y_2(t)}q(t)dt = 0.$$

This relationship is called **relationship of orthogonality**.

Proof. Let u be any eigenfunction. Note that

$$\overline{L[u]} = L[\bar{u}].$$

Thus, applying the Green's Lemma to the functions y_1 and y_2, we have

$$\begin{aligned}0 &= \int_a^b \left(\overline{y_2}L[y_1] - y_1\overline{L[y_2]}\right) dt \\ &= \int_a^b \left(\overline{y_2}(t)\lambda_1 q(t)y_1(t) - y_1(t)\overline{\lambda_2}q(t)\overline{y_2}(t)\right) dt \\ &= (\lambda_1 - \lambda_2)\int_a^b y_1(t)\overline{y_2(t)}q(t)dt.\end{aligned}$$

By hypothesis, $\lambda_1 \neq \lambda_2$, therefore

$$\int_a^b y_1(t)\overline{y_2(t)}q(t)dt = 0.$$

■

2.3 Lower Bound for the Eigenvalues

The main objective of this section is show that the eigenvalues of Sturm-Liouville Problem cannot be less than a constant M that depends on the functions r, p and q and of the constants $\alpha_1, \alpha_2, \beta_1$ and β_2.

Definition 2.3.1 Let $C_{L_p(\rho)}([a,b])$ be the space of continuous functions getting to complex value defined on interval $[a,b]$. On this space, consider the norm $\|x\|_{p,\rho}$ with $x \in C([a,b])$, where

$$\|x\|_{p,\rho} = \left[\int_a^b |x(t)|^p \rho(t)dt\right]^{1/p},$$

where ρ is a strictly positive continuous function defined in $[a,b]$.

REM In the case where $p = 2$ and $\rho = 1$, we will denote this space by $C_{L_2}([a,b])$ with the norm

$$x \in C([a,b]) \longmapsto \|x\|_2 = \left[\int_a^b |x(t)|^2 r(t)dt\right]^{1/2},$$

Theorem 2.3.1 Consider the Regular Sturm-Liouville given by the Definition 2.1.4. Then there is a constant M, that depends on the functions r, p and q and on the constants $\alpha_1, \alpha_2, \beta_1$ and β_2, such that all the eigenvalues λ satisfy

$$\lambda \geq M$$

Proof. Let y be an eigenfunction correspondent to the eigenvalue λ. It is sufficient to show that there is a M such that for $\lambda < M$ and $y \in C^2([a,b],\mathbb{R})$ with $\|y\|_2 = 1$, we get

$$\int_a^b L_\lambda[y](t)y(t)dt > 0,$$

that is

$$\int_a^b [-(ry')' + py - \lambda qy]ydt > 0.$$

Thus,

$$\int_a^b [-(ry')' + py - \lambda qy]ydt = \int_a^b [-(ry')'y + py^2 - \lambda qy^2]dt$$
$$= -\int_a^b [(ry')'y + ry'^2 ry'^2]dt + \int_a^b py^2 dt - \lambda \int_a^b qy^2 dt$$
$$= -(ry')y\Big|_a^b + \int_a^b ry'^2 dt + \int_a^b py^2 dt - \lambda \int_a^b qy^2 dt. \quad (2.5)$$

In the case $y(a) = 0$, then $r(a)y'(a)y(a) = 0$. Now, consider $y(a) \neq 0$, from $\alpha_1 y(a) + \alpha_2 y'(a) = 0$ follow that

$$|r(a)y'(a)y(a)| = \left| r(a)\frac{\alpha_1}{\alpha_2} y(a)^2 \right| \leq \left|\frac{\alpha_1}{\alpha_2}\right| |r(a)| \left(\frac{1}{b-a} + 2\|y'\|_2\right).$$

Setting

$$\left|\frac{\alpha_1}{\alpha_2}\frac{r(a)}{b-a}\right| = M_1 \qquad \text{and} \qquad \left|\frac{\alpha_1}{\alpha_2} 2r(a)\right| = M_2,$$

we obtain

$$|r(a)y'(a)y(a)| \leq M_1 + M_2\|y'\|_2 \implies r(a)y'(a)y(a) \geq -M_1 - M_2\|y'\|_2. \quad (2.6)$$

Analogously, there are M_3 e M_2, such that

$$-r(b)y'(b)y(b) \geq M_3 + M_2\|y'\|_2. \quad (2.7)$$

We have already studied the first term of the right side of the Equation (2.5). Now, we will study the others three terms.

The second term is $\int_a^b r(t)y'(t)^2 dt$. As we have $r(t) > 0$, $\forall t \in [a,b]$, then $r_1 = \inf_{a \leq t \leq b} r(t) > 0$, such a way

$$\int_a^b r(t)y'(t)^2 dt \geq \int_a^b r_1 |y'(t)|^2 dt = r_1(\|y'\|_2)^2. \quad (2.8)$$

The third term is $\int_a^b p(t)y(t)^2 dt$. Since p is continuous on $[a,b]$ there is $q_1 = \inf_{a \leq t \leq b} p(t)$ such that

$$\int_a^b p(t)y(t)^2 dt \geq \int_a^b p_1 |y(t)|^2 dt = p_1(\|y\|_2)^2 = p_1$$

which implies

$$\int_a^b q(t)y(t)^2 dt \geq p_1 \quad (2.9)$$

Lastly, the fourth term is $-\lambda \int_a^b q(t)y(t)^2 dt$, since this term is continuous and strictly positive on interval $[a,b]$, we have $q_1 = \inf_{a \leq t \leq b} q(t)$ and

$$-\lambda \int_a^b q(t)y(t)^2 dr \geq -\lambda \int_a^b q_1 |y(t)|^2 dt = -\lambda q_1(\|y\|_2)^2 = -\lambda q_1$$

implies

$$-\lambda \int_a^b q(t)y(t)^2 dt \geq -\lambda q_1. \quad (2.10)$$

Hence, adding (2.6), (2.7), (2.8), (2.9) and (2.10), we obtain

$$\begin{aligned}
\int_a^b [-(ry')' + py - \lambda qy] y dt &= -(ry')y\Big|_a^b + \int_a^b ry'^2 dt + \int_a^b py^2 dt - \lambda \int_a^b qy^2 dt \\
&\geq M_3 + M_4 \|y'\|_2 - M_1 - M_2 \|y'\|_2 + r_1 (\|y'\|_2)^2 + r_1 - \lambda q_1 \\
&= M_5 + M_6 \|y'\|_2 + r_1 (\|y'\|_2)^2 - \lambda p_1 \\
&= \left(\sqrt{r_1} \|y'\|_2 + \frac{1}{2} \frac{M_6}{\sqrt{r_1}} \right)^2 - \frac{1}{4} \frac{M_6^2}{r_1} + M_5 - \lambda q_1 \\
&\geq M_7 - \lambda q_1,
\end{aligned}$$

where $M_5 = M_3 - M1 + p_1$, $M_6 = M_4 - M_2$ and $M_7 = M_5 - \frac{1}{4}\frac{M_6^2}{r_1}$. Thus

$$M_7 - \lambda q_1 > 0 \iff \lambda < \frac{M_7}{q_1} = M_8.$$

and enough to take $M = \min\{0, M_8\}$. ■

2.4 Rayleigh's Quotient

In this section, we will present an approximate determination method of the eigenvalues, known as *Rayleigh's quotient* and we will show some condition under which the Sturm-Liouville problem has only positive eigenvalues.

Let y_n be an eigenfunction with eigenvalue $\lambda \in \mathbb{R}$, i.e.,

$$(ry'_\lambda)' + py_\lambda + \lambda q y_\lambda = 0.$$

Multiplying this equality by y_λ and integrating from a to b, we obtain

$$\lambda \int_a^b y_\lambda(x)^2 q(x) dx = -\int_a^b y_\lambda(x)(ry'_\lambda)'(x) dx + \int_a^b y_\lambda(x)^2 p(x) dx. \tag{2.11}$$

Integrating the first term on the right side by parts

$$\int_a^b y_\lambda (ry'_\lambda)'(x) dx = (r y_\lambda y'_\lambda)(x)\Big|_a^b - \int_a^b (y'_\lambda(x))^2 r(x) dx.$$

Taking this result into (2.11)

$$\lambda \int_a^b y_\lambda(x)^2 q(x) dx = \int_a^b \left[(y'_\lambda(x)^2 r(x) - y_\lambda(x)^2 p(x) \right] dx + \left[r(a) y_\lambda(a) y'_\lambda(a) - r(b) y_\lambda(b) y'_\lambda(b) \right],$$

Isolating λ, we get

$$\boxed{\lambda = \frac{\displaystyle\int_a^b [y'_\lambda(x)^2 r(x) - y_\lambda(x)^2 p(x)] dx + [r(a) y_\lambda(a) y'_\lambda(a) - r(b) y_\lambda(b) y'_\lambda(b)]}{\displaystyle\int_a^b y_\lambda(x)^2 q(x) dx}} \tag{2.12}$$

The right side of the Equation (2.12) is called **Rayleigh's quotient**, whose main application consist in an approximate determination of the eigenvalues from approximation to eigenfunctions. It's extremely useful when the solutions of the Sturm-Liouville Problem can't be found analytically.

Now, we will use the following proposition to rewrite Rayleigh's quotient given by the Equation (2.12).

Proposition 2.4.1 Let y_λ be an eigenfunction corresponding to the eigenvalue λ of the Sturm-Liouville Problem, i.e,

$$\begin{cases} (ry'_\lambda)' + py_\lambda + \lambda q y_\lambda = 0, & \forall x \in [a,b] \\ \alpha_1 y_\lambda(a) + \alpha_2 y'_\lambda(a) = 0 \\ \beta_1 y_\lambda(b) + \beta_2 y'_\lambda(b) = 0. \end{cases}$$

Then, there are different constants γ_1 and γ_2, that are independents of y_λ, such that

$$r(a)y_\lambda(a)y'_\lambda(a) = \gamma_1[y_\lambda(a)]^2 \tag{2.13}$$

and

$$r(b)y_\lambda(b)y'_\lambda(b) = -\gamma_2[y_\lambda(b)]^2. \tag{2.14}$$

Proof. On the point a, y_λ satisfy

$$\alpha_1 y_\lambda(a) + \alpha_2 y'_\lambda(a) = 0.$$

First, let's suppose that $\alpha_2 \neq 0$. Multiply the equation above by $r(a)y_\lambda(a)$ we obtain

$$r(a)y'_\lambda(a)y_\lambda(a) = -\frac{\alpha_1}{\alpha_2} r(a)[y_\lambda(a)]^2.$$

In this case, we take $\gamma_1 = -r(a)\dfrac{\alpha_1}{\alpha_2}$.

If $\alpha_2 = 0$, the relation $\alpha_1 y_\lambda(a) + \alpha_2 y'_\lambda(a) = 0$ tell us that $y_\lambda(a) = 0$. Therefore, it's evident that (2.13) is satisfied, since to any constant γ_1, both sides are null. This finish the proof to the Equation (2.13). Similarly, we found $\gamma_2 = r(b)\dfrac{\beta_1}{\beta_2}$ for $\beta_2 \neq 0$ in the Equation (2.14). ■

Inserting (2.13) and (2.14) into (2.12), we may rewrite the Rayleigh's quotient as:

$$\boxed{\lambda = \frac{\displaystyle\int_a^b [y'_\lambda(x)^2 r(x) - y_\lambda(x)^2 p(x)]dx + \gamma_1[y_\lambda(a)]^2 + \gamma_2[y_\lambda(b)]^2}{\displaystyle\int_a^b y_\lambda(x)^2 q(x)dx}} \tag{2.15}$$

where

$$\gamma_1 = \begin{cases} -r(a)\dfrac{\alpha_1}{\alpha_2}, & \text{if } \alpha_2 \neq 0 \\ 0, & \text{if } \alpha_2 = 0 \end{cases} \quad \text{and} \quad \gamma_2 = \begin{cases} r(b)\dfrac{\beta_1}{\beta_2}, & \text{if } \beta_2 \neq 0 \\ 0, & \text{if } \beta_2 = 0. \end{cases}$$

What follows are an example of Rayleigh's quotient to determine an approximation eigenvalue.

■ **Example 2.3** Let $u \in C^2[0,1]$ be a solution of BVP

$$\begin{cases} u''(x) + \lambda u(x) = 0, & x \in [0,1] \\ u(0) = 0 \\ u(1) = 0 \end{cases}$$

This is a Regular Sturm-Liouville Problem on interval $[a,b] = [0,1]$ with $r(x) = 1$, $p(x) = 0$ and $q(x) = 1$ for all $x \in [0,1]$, therefore $(\alpha_1, \alpha_2) = (1,0)$ and $(\beta_1, \beta_2) = (1,0)$. This is the harmonic oscillator equation, whose eigenvalues are $\lambda_n = n^2\pi^2$ with $n = 1,2,3,4,\ldots$ and the eigenfunctions (not normalized) are $u_{\lambda_n}(x) = \sin(n\pi x)$.

For example, we take the case $n = 1$, the eigenfunction is $u_{\lambda_1}(x) = \sin(\pi x)$, where is null on $x = 0$ and $x = 1$, being positive in the rest of interval $[0,1]$ and maximum value is equal to 1 on $x = 1/2$.

The function $u_{(1)} = 4x(1-x)$ is similar to u_{λ_1}, as show the Figure 2.1, and can be considered an approximation to the function u_{λ_1}.

Replacing $u_{(1)}$ by u_{λ_1} into (2.12) or (2.15), we get an approximation to the eigenvalue $\lambda_1 = \pi^2$ given by

$$\pi^2 \cong \frac{\displaystyle\int_0^1 (1-2x)^2 dx}{x^2(1-x)^2 dx} = \frac{1/3}{1/30} = 10,$$

which provides the approximation $\pi \cong \sqrt{10} = 3,162$, which has relative error of only $0,66\%$.

■

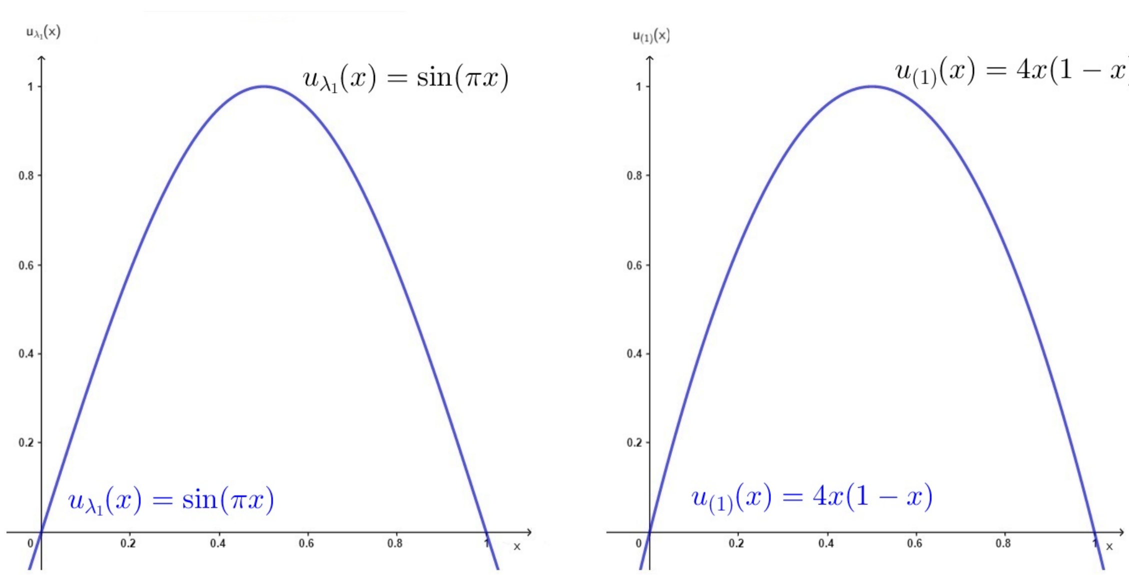

Figure 2.1: On yours left we can see $u_{\lambda_1}(x) = \sin(\pi x)$ and on right $u_{(1)} = 4x(1-x)$, that show their similarities.

This method was developed by Rayleigh in 1870, that systematized it, adding ideas of calculus of variations. The variational methods of eigenvalue determination are very utilized in computational simulation due to its simplicity and efficiency. Originally, these methods were developed to Sturm-Liouville Theory, but these results can be applied in another problem involving the determination of isolate eigenvalues, as in several applications of Quantum Mechanics, Nuclear Physics and Solid State Physics.

Finally, in several problems in physics we need that the eigenvalues of the Sturm-Liouville problem to be positive. The following proposition show that there are some conditions that imply this occurs.

> **Proposition 2.4.2** Consider the conditions of the Sturm-Liouville Problem listed previously. If the following conditions are simultaneously valid:
> (I) $p(x) < 0$, for all $x \in [a,b]$
> (II) $\alpha_1\alpha_2 \leq 0$
> (III) $\beta_1\beta_2 \geq 0$
> then the eigenvalues λ of the Sturm-Liouville Problem are strictly positive.

Proof. Let y be a eigenfunction with eigenvalue $\lambda \in \mathbb{R}$, i.e., $(ry')' + py + \lambda qy = 0$. We can show that $\lambda > 0$ if Rayleigh's quotient (2.12) is positive.

Note that the denominator of the Rayleigh's quotient (2.12) is always greater than zero, that is, $\int_a^b y(x)^2 q(x)dx > 0$, because $y(x)^2 > 0$ and $q(x) > 0$, by hypothesis. By the same argument, we have $\int_a^b (y'(x))^2 r(x)dx > 0$, so that $-\int_a^b (y(x))^2 p(x)dx$ be larger than zero we must impose the condition (I)($p(x) < 0$), thus $-\int_a^b (y(x))^2 p(x)dx > 0$.

Therefore, remains to analysis under what conditions

$$r(a)y(a)y'(a) - r(b)y(b)y'(b) \leq 0. \tag{2.16}$$

On the point a, y satisfy $\alpha_1 y(a) + \alpha_2 y'(a) = 0$. We can rewrite the equation as

$$\alpha_1^2 y(a)^2 + \alpha_2^2 y'(a)^2 + 2\alpha_1\alpha_2 y(a)y'(a) = 0,$$

then,

$$2\alpha_1\alpha_2 y(a)y'(a) = -\left[\alpha_1^2 y(a)^2 + \alpha_2^2 y'(a)^2\right]. \tag{2.17}$$

Analogously, for the point b,

$$2\beta_1\beta_2 y(b)y'(b) = -\left[\beta_1^2 y(b)^2 + \beta_2^2 y'(b)^2\right]. \tag{2.18}$$

The Equation (2.18) show that $\alpha_1\alpha_2$ e $y(a)y'(a)$ has opposite sign, and by boundary conditions, if $\alpha_1\alpha_2 = 0$ e $\beta_1\beta_2 = 0$, follow respectively, $y(a)y'(a) = 0$ and $y(b)y'(b) = 0$.

Thus, so that (2.16) be satisfied, we have that $y(a)y'(a) \geq 0$ e $y(b)y'(b) \leq 0$ and by Equations (2.17) and (2.18), this occurs if, and only if, the conditions (I) and (II) be satisfied, in another words, $\alpha_1\alpha_2 \leq 0$ and $\beta_1\beta_2 \geq 0$. Hence, so that λ be larger than zero, the conditions (I), (II) and (III) must are simultaneously valid. ■

It's important to observe that there are negative eigenvalues. However, by the Theorem 2.3.1 these not be arbitrarily negative.

REM We can also show the Theorem 2.3.1 using Rayleigh's quotient (2.12), that can be found in the page 21, where we consider all possible combinations for constants γ_1 e γ_2 which are positive real numbers or negative, show that in all cases, the eigenvalue λ given by the Rayleigh's quotient always have a lower bound.

2.5 Main Result

A very useful tool when studying a Sturm-Liouville Problem is to turn it into an integral equation using the Green function. As we will see, this can only be done by assuming that $\lambda = 0$ is not an eigenvalue of the Sturm-Liouville Problem.

Before we continue the discussion, we will give some definitions and results that will useful. The first result is known as Spectral Theorem for Hermitian Compact Operators. The proof can be found in the classical books about Operator Theory and Functional Analysis [18], [19], [20], [33].

Theorem 2.5.1 — Spectral Theorem for Hermitian Compact Operators. Let $\mathcal{P}$ be a pre-Hilbert space (or inner product space) and A a Hermitian compact operator defined on $\mathcal{P}$, $A \neq 0$. Thus, there is a sequence $\lambda_n \in \mathbb{R}$ of nonzero eigenvalues of A and a sequence e_n of corresponding eigenvectors that form an orthonormal set such that $\forall x \in \mathcal{P}$, we have:

$$Ax = \sum \lambda_n x_n e_n, \qquad \text{where } x_n =< x, e_n > .$$

Now, we will introduce to the Green function, which will be responsible for transforming ODE into an integral equation.

Definition 2.5.1 — Fundamental Solution. Let H be a symmetrical function, we called it the **fundamental solution** from Sturm-Liouville problem if it satisfies

$$L\left(\int_a^b H(x,y)f(y)dy\right) = f(x)$$

and

$$L_x[H(x,y)] = -\frac{\partial}{\partial x}\left(r(x)\frac{\partial H}{\partial x}\right) + pH = \delta(x-y).$$

Definition 2.5.2 — Green's Function. A two-variable function $G(x,y)$ with $x, y \in [a,b]$ is a **Green function** for the Sturm-Liouville problem, if G is a fundamental solution of the problem and the expression

$$\int_a^b G(x,y)f(y)dy$$

satisfy the boundary conditions (2.2).

Now we can enunciate Green's theorem for Sturm-Liouville problem.

Theorem 2.5.2 — Green's Theorem. There is a continuous function

$$G:\ [a,b]\times[a,b]\longrightarrow\mathbb{R}$$

such that $f\in C([a,b])$, $y\in C^2([a,b])$ is solution of

$$L[y]=-(ry')'+py=f \qquad \text{on } [a,b]$$

satisfying the boundary conditions (2.2), that is,

$$F_1[y]\equiv\alpha_1 y(a)+\alpha_2 y'(a)=0$$

$$F_2[y]\equiv\beta_1 y(b)+\beta_2 y'(b)=0$$

if and only if

$$y(t)=\int_a^b G(t,s)f(s)ds,$$

where the function G is a Green's Function, given by

$$G(t,s)=\begin{cases}\dfrac{y_1(t)y_2(s)}{r(s)W[y_1,y_2](s)}:=G_1(t,s), & \text{if } a\le t<s\\ \dfrac{y_2(t)y_1(s)}{r(s)W[y_1,y_2](s)}:=G_2(t,s), & \text{if } s\le t<b\end{cases}$$

where W represents the Wronskian, y_1 and y_2 are linearly independent solutions of the equation $L[y]=0$, with the conditions (2.2).

Proof. According to the theory of ordinary differential equations, the general solution of the equation

$$L[y]=f(t) \tag{2.19}$$

is

$$y(t)=c_1y_1(t)+c_2y_2(t)+y_p(y),$$

where c_1 and c_2 are constant,the particular solution is the form $y_p(t)=v_1(t)y_1(t)+v_2(t)y_2(t)$, where $v_1(t)$ e $v_2(t)$ are time dependent functions. Therefore

$$y_p(t)=\int_a^s\frac{y_1(s)y_2(t)f(t)}{r(t)W[y_1,y_2](t)}dt+\int_s^b\frac{y_2(s)y_1(t)f(t)}{r(t)W[y_1,y_2](t)}dt.$$

So we define Green's function by

$$G(t,s)=\begin{cases}\dfrac{y_1(t)y_2(s)}{r(s)W[y_1,y_2](s)}:=G_1(t,s), & \text{if } a\le t<s,\\ \dfrac{y_2(t)y_1(s)}{r(s)W[y_1,y_2](s)}:=G_2(t,s), & \text{if } s\le t<b.\end{cases}$$

Then we can write

$$\begin{aligned}y_p(s)&=\int_a^b G_1(s,t)f(t)dt+\int_s^b G_2(s,t)f(t)dt\\&=\int_a^b G(x,t)f(t)dt\end{aligned}$$

■

Now, by Green's theorem, $y(x) = \int_a^b G(x,s)f(s)ds$ is a solution for $L[y] = f$ with the conditions (2.2) then, this solution is unique. However, under the hypothesis that $\lambda = 0$ is not an eigenvalue of the Sturm-Liouville problem, every function y that satisfies $L[y] = f$ with the boundary conditions (2.2) also satisfies $y(x) = \int_a^b G(x,s)f(s)ds$ for **any continuous function** f. Thus, for a specific f, we have the following consequence:

Corollary 2.5.3 A function y is a solution to the non-homogeneous Sturm-Liouville problem with conditions (2.2) if and only if

$$y(t) - \lambda \int_a^b G(t,s)y(s)q(s)ds = g(t),$$

where

$$g(t) = \int_a^b G(t,s)f(s)ds.$$

Proof. By Green's Theorem for the Regular Sturm-Liouville Problem, we have that y is solution of

$$L[y] = \lambda qy + f$$

satisfying (2.2) if and only if

$$y(t) = \int_a^b G(t,s)[\lambda q(s)y(s) + f(s)]ds,$$

this is,

$$y(t) - \lambda \int_a^b G(t,s)y(s)q(s)ds = g(t).$$

■

An equation like this, where function $G(t,s)q(s)$ is continuous on a closed interval, is known as the **Fredholm integral equation of the second type**. We then define an operator related to this type of integral equation.

Definition 2.5.3 — Fredholm Operator. Let us indicate by $\mathfrak{F}$ the integral operator in $C_{L_2(r)}([a,b])$ defined by

$$\mathfrak{F}[y](t) = \int_a^b G(t,s)y(s)q(s)ds.$$

We called $\mathfrak{F}$ as **Fredholm operator**.

As a consequence of the previous corollary, the homogeneous Sturm-Liouville Problem can be written as

$$y(t) = \lambda \int_a^b G(t,s)y(s)q(s)ds.$$

However, the previous equation

$$\mathfrak{F}[y] = \frac{1}{\lambda}y,$$

that is, $1/\lambda$ is an eigenvalue of the Fredholm Operator $\mathfrak{F}$. Proving the following Corollary.

Corollary 2.5.4 (a) λ is an eigenvalue of the Sturm-Liouville problem if, and only if, $1/\lambda$ is a eigenvalue of $\mathfrak{F}$.

(b) y is the eigenfunction of the Sturm-Liouville Problem corresponding to the eigenvalue λ if and only if y is a eigenfunction of the operator $\mathfrak{F}$ corresponding to the eigenvalue $1/\lambda$.

Since the kernel G is a real function and symmetrical, follows that the integral operator $\mathfrak{F}$ is Hermitian and compact, so we can apply the theory of operators and integral equations (see [18], [19], [46]), such that the results that follows are valid.

Proposition 2.5.5 Let $\mathcal{P} = C_{L_2}([a,b],\mathbb{C})$ be a pre-Hilbert space, $K: [a,b]\times[a,b] \longrightarrow \mathbb{C}$ a continuous function and $k: \mathcal{P} \longrightarrow \mathcal{P}$ the operator defined by $(kf)(t) = \int_a^b K(t,s)f(s)ds$. Then

$$\sum_{n=1}^{\infty} \lambda_n^2 \le \int_a^b \int_a^b |K(t,s)|^2 ds dt,$$

where λ_n are the nonzero eigenvalues of the operator k.

Theorem 2.5.6 Given a Hermitian continuous kernel K and an eigenvalue $\lambda \neq 0$ of the Hermitian compact operator k, associated with K, then the integral equation,

$$\lambda x(t) = y(t) + \int_a^b K(t,s)x(s)ds$$

has a solution if and only if $\int_a^b y(t)\overline{z(t)}dt = 0$ for all continuous function $z \in C([a,b],\mathbb{C})$ such that

$$\int_a^b K(t,s)z(s)ds = \lambda z(t). \tag{2.20}$$

The solutions have the form

$$x(t) = \frac{1}{\lambda}y(t) + \frac{1}{\lambda}\sum_{\lambda_n \neq \lambda} \lambda_n \frac{y_n}{\lambda - \lambda_n} e_n(t) + z(t), \tag{2.21}$$

where z is an element of $C([a,b],\mathbb{C})$ that satisfies (2.20) and $y_n = \int_a^b y(s)e_n(s)ds$.

The series (2.21) is absolutely and uniformly convergent.

For the demonstration of the next theorem, we will introduce the following notation: Let $\mathscr{D}(]a,b[)$ be the vector space of functions that mapping elements of $]a,b[\equiv (a,b)$ to complex values that are infinitely derivable and null outside a closed interval contained in $]a,b[$. Finally, we can prove the main theorem:

Theorem 2.5.7 Consider the Sturm-Liouville Problem given in the Definition 2.1.4. Then

(a) The values $\lambda \in \mathbb{C}$ such that there is a solution $y \neq 0$ of $L_\lambda[y] = 0$ satisfying $F_1[y] = F_2[y_2] = 0$, that is, the eigenvalues of the Sturm-Liouville problem form an infinite increasing sequence λ_n of real numbers such that

$$\lim_{n\to\infty} \lambda_n = +\infty \qquad \text{and} \qquad \sum_{n=1}^{\infty} \frac{1}{\lambda_n} < \infty.$$

(b) The sequence φ_n of the eigenfunctions forms an orthonormal basis of the pre-Hilbert space $C_{L_2(q)}([a,b])$.

(c) For every function $x \in C^2([a,b])$, such that

$$F_1[x] = F_2[x] = 0,$$

we have

$$x(t) = \sum_{n=1}^{\infty} x_n \varphi_n(t)$$

where

$$x_n =< x, \varphi_n >_q = \int_a^b x(t)\varphi_n(t)q(t)dt,$$

being the series uniformly and absolutely convergent in $[a,b]$.

(d) Let $\lambda \neq \lambda_n$ for all n, and $f \in C([a,b])$ the system

$$L_\lambda[y] = f, \quad \text{with } F_1[y] = F_2[y] = 0,$$

has only one solution y,

$$y(t) = \sum_{n=1}^{\infty} \frac{< f, \varphi_n >}{\lambda - \lambda_n} \varphi_n(t),$$

being the series uniformly and absolutely converging in $[a,b]$.

(e) If $\lambda = \lambda_m$, given a $f \in C([a,b])$, the system

$$L_\lambda[y] = f, \quad \text{with } F_1[y] = F_2[y] = 0,$$

has a solution if and only if $< f, \varphi_m >= 0$, this is,

$$\int_a^b f(t)\varphi_m(t)dt = 0.$$

In this case the solution is like in (d), being arbitrary component y_m of φ_m.

Proof. (c) Let $x \in C^2([a,b])$ with $F_1[x] = F_2[x] = 0$. From Green's Theorem, it follows that

$$\begin{aligned} x(t) &= \int_a^b G(t,s)L[x](s)ds \\ &= \int_a^b G(t,s)\frac{L[x](s)}{q(s)}q(s)ds \\ &= \mathfrak{F}\left[\frac{L[x]}{q}\right](t). \end{aligned}$$

Since $\mathfrak{F}$ a Hermitian compact operator, by the Spectral Theorem for Compact Hermitian Operators, we have

$$x(t) = \mathfrak{F}\left[\frac{L[x]}{q}\right](t) = \sum_{n=1}^{\infty}\frac{1}{\lambda_n}\left(\frac{L[x]}{q}\right)_n \varphi_n(t), \tag{2.22}$$

where

$$\left(\frac{L[x]}{q}\right)_n = \left\langle \frac{L[x]}{q}, \varphi_n(t)\right\rangle$$

Consider $\alpha_n =< x, \varphi_n >_q$, thus

$$\begin{aligned} \alpha_n =< x, \varphi_n >_r &= \int_a^b x(t)\varphi_n(t)q(t)dt \\ &= \int_a^b \left[\int_a^b G(t,s)L[x](s)ds\right]\varphi_n(t)q(t)dt \\ &= \int_a^b \mathfrak{F}[\varphi_n](s)L[x](s)ds \\ &= \frac{1}{\lambda_n}\int_a^b \varphi_n(s)L[x]\left(\frac{q(s)}{q(s)}\right)ds \\ &= \frac{1}{\lambda_n}\left\langle \frac{L[x]}{q}, \varphi_n\right\rangle_q \\ &= \frac{1}{\lambda_n}\left(\frac{L[x]}{q}\right)_n. \end{aligned}$$

Therefore,

$$x(t) = \sum_{n=1}^{\infty}\frac{1}{\lambda_n}\left(\frac{L[x]}{q}\right)_n \varphi_n(t) = \sum_{n=1}^{\infty}\alpha_n\varphi_n(t),$$

where the series is uniformly and absolutely convergent.

(b) For all $x \in \mathscr{D}(]a,b[)$ the conditions $F_1[x] = F_2[x] = 0$ are satisfied, so the item (c) can be applied to functions from $\mathscr{D}(]a,b[,\mathbb{C})$, this is,

$$x(t) = \sum_{n=1}^{\infty}\alpha_n\varphi_n(t),$$

where the series converges uniformly and absolutely in (a,b). Since $\mathscr{D}(]a,b[,\mathbb{C})$ is dense in $C_{L_2(q)}(]a,b[,\mathbb{C})$, given $y \in C_{L_2(q)}([a,b],\mathbb{C})$ and $\varepsilon > 0$, there is a $x \in \mathscr{D}(]a,b[,\mathbb{C})$ such as

$$\|y-x\| = \left\|y - \sum_{n=1}^{\infty}\alpha_n\varphi_n\right\| < \varepsilon.$$

Therefore, if we consider all linear combinations of φ_n, so we have that it is dense in $C_{L_2(q)}(]a,b[,\mathbb{C})$, thus the φ_n are a complete orthogonal family of $C_{L_2(q)}(]a,b[,\mathbb{C})$.

(a) Since the kernel is Hermitian, all the eigenvalues of the Sturm-Liouville Problem are real. From item (c) follows that the sequence of the eigenvalues, (λ_n), is infinity and by the Spectral Theorem for Hermitian Compact Operators, and Corollary 2.5.4 follows that $\frac{1}{\lambda_n} \longrightarrow 0$ and therefore, $\lambda_n \longrightarrow +\infty$. We still have from Corollary 2.5.4, that λ_n is an eigenvalue if, and only if $\frac{1}{\lambda_n}$ is a eigenvalue of $\mathfrak{F}$, so for the sequence $\left(\frac{1}{\lambda_n}\right)$, the Proposition 2.5.5, page 28, and from Corollary (2.5.4) follows that $\sum_{n=1}^{\infty} \frac{1}{\lambda_n} < \infty$.

(d) From Corollary 2.5.3, page 27, follows that the solution y of the Sturm-Liouville problem satisfies

$$\begin{aligned} y(t) &= \lambda \int_a^b G(t,s)y(s)q(s)ds + \int_a^b G(t,s)f(s)ds \\ &= \int_a^b G(t,s)[\lambda y(s)q(s) + f(s)]ds \\ &= \int_a^b G(t,s)\left[\lambda q(s) + \frac{f(s)}{q(s)}\right] q(s)ds, \end{aligned}$$

that is,

$$\frac{1}{\lambda}\mathfrak{F}\left[\frac{f}{q}\right] = \frac{1}{y}y - \mathfrak{F}[y].$$

Since the eigenvalues are real, replacing λ by $1/\lambda$, λ_n for $1/\lambda_n$, x by y e y for $\frac{1}{\lambda}\mathfrak{F}\left[\frac{f}{q}\right]$, we conclude that

$$\begin{aligned} y(t) &= \lambda \frac{1}{\lambda}\mathfrak{F}\left[\frac{f}{q}\right](t) + \lambda \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \frac{\frac{1}{\lambda}\mathfrak{F}\left[\frac{f}{q}\right]_n}{\frac{1}{\lambda} - \frac{1}{\lambda_n}} \varphi_n(t) \\ &= \sum_{n=1}^{\infty} \frac{< f, \varphi >}{\lambda_n}\varphi_n(t) + \lambda \sum_{n=1}^{\infty} \frac{\frac{1}{\lambda} < f, \varphi >}{\lambda_n - \lambda}\varphi_n(t) \\ &= \sum_{n=1}^{\infty} \frac{< f, \varphi_n >}{\lambda_n - \lambda}\varphi_n(t). \end{aligned}$$

where we use (2.22) and the series converges uniformly and absolutely on $[a,b]$.

(e) It follows the same way of the Theorem 2.5.6, page 28 (see [18], [19]). ■

2.6 Sturm's Theorems

It is very important from the point of view of physical applications, to determine the number of zeros which the solution has on interval $[a,b]$, this problem was first attacked by Sturm in 1936, see [40].

The principal interest of this section will be to study the zeros set of a solution y of Sturm-Liouville equation

$$-\left(r(x)y'(x)\right)' + p(x)y(x) = 0 \tag{2.23}$$

where r and p are continuous, real-valued functions defined on interval $[a,b]$ with $p > 0$.

An useful tool for the proof of the Comparison Theorem is the *Prüfer Transformation*. From the Figure 2.2, we may introduce the following "polar" coordinate

$$\begin{cases} y = \rho \sin\theta & (2.24) \\ ry' = \rho\cos\theta. & (2.25) \end{cases}$$

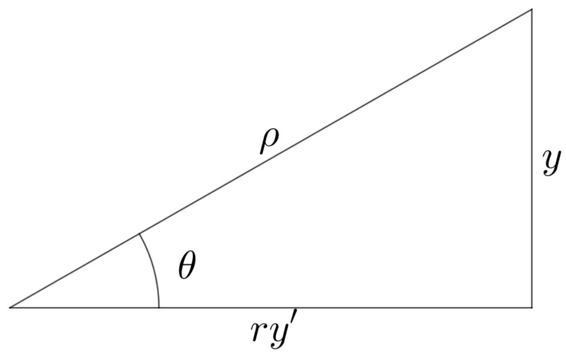

Figure 2.2: Prufer's Triangle.

We want to obtain ρ and θ as functions of the variables y and ry'. As such, dividing (2.24) by (2.25),

$$\tan\theta = \frac{y}{ry'} \implies \theta = \tan^{-1}\left(\frac{y}{ry'}\right). \tag{2.26}$$

Square (2.24) and (2.25), then adding it, we obtain

$$y^2 + (ry')^2 = \rho^2. \tag{2.27}$$

Differentiating the Equation (2.26),

$$\theta' = \frac{\left(\frac{y}{ry'}\right)'}{1 + \frac{y^2}{(ry')^2}} = \frac{\frac{y'ry' - y(ry')'}{(ry')^2}}{1 + \frac{y^2}{(ry')^2}},$$

thus

$$\theta' = \frac{y'ry' - y(ry')'}{(ry')^2 + y^2}. \tag{2.28}$$

Replacing the Equation (2.27) into (2.28) and from (2.23),

$$\theta' = \frac{y'ry' - y(ry')'}{\rho^2} \underbrace{=}_{(2.23)} \theta' = \frac{y'ry' - y(py)}{\rho^2}$$

that can be rewrite

$$\theta' - \frac{1}{r}\left(\frac{ry'}{\rho}\right)^2 - p\left(\frac{y}{\rho}\right)^2.$$

Thus, from (2.24) and (2.25),

$$\theta' = \frac{1}{r}\cos^2\theta - p\sin^2\theta.$$

Now, differentiating the equation (2.27), we get

$$2\rho\rho' = 2(ry')(ry')' + 2yy'.$$

Dividing both sides by 2ρ implies

$$\rho' = \frac{(ry')}{\rho}(ry')' + \frac{y}{\rho}y'.$$

Replacing the equations (2.24) and (2.25) into the above equation

$$\rho' = (ry')'\cos\theta + y'\sin\theta,$$

from (2.23),

$$\rho' = py\cos\theta + y'\sin\theta. \tag{2.29}$$

However, from (2.24) and (2.25), we have

$$\begin{cases} \theta = \tan^{-1}\left(\dfrac{y}{ry'}\right) \\ ry' = \dfrac{\rho}{r}\cos\theta. \end{cases} \tag{2.30}$$

In this way, replacing (2.30) into (2.29),

$$\rho' = \left(\frac{1}{r} + p\right)\rho\cos\theta\sin\theta.$$

Definition 2.6.1 — Prüfer Transformation. Let y be a nontrivial real-valued solution of (2.23) and let

$$\begin{cases} y = \rho\sin\theta \\ \rho^2 = y^2 + (ry'). \end{cases}$$

These relations transform the Equation (2.23) into

$$\begin{cases} \theta' = \dfrac{1}{r}\cos^2\theta - p\sin^2\theta, & (2.31) \\ \rho' = \left(\dfrac{1}{r} + p\right)\rho\cos\theta\sin\theta. & (2.32) \end{cases}$$

REM Note that any solution of (2.31) exist on the whole interval, where p, q are continuous similar to (2.23).

Note that if y is null then θ assume value $m\pi$, where m is an integer number.

Lemma 2.6.1 Let y be a nontrivial real-valued solution of (2.23) with $r(x) > 0$ and $p(x)$ real valued and continuous on $[a,b]$. Consider that $y(x)$ has exactly $ngeq1$ zeros, $z_1 < z_2 < \cdots < z_n$ on $a < x \leq b$. Let $\theta(x)$ be a continuous function given by (2.26) with $0 < \theta(a) < \pi$. Then,
(i) $\theta(z_k) = k\pi$
(ii) $\theta(x) > k\pi$ for $z_k < x \leq b$.
for $k \in 1,\ldots,n$.

Proof. Let's show the case (i). Since θ and θ' do not vanish simultaneously follows from (2.27), that $\rho(x)^2 > 0$ on interval (a,b). In this way, we can assume $\rho(x) > 0$. As consequence, follow from (2.24), that $y = \rho \sin\theta$ vanishes only when $\theta(x)$ is an integer multiple of π.

To prove the case (ii) observe from the first case, for a x-value, $y = 0$ if only if $\theta = m\pi$, for some integer number m. Thus, from (2.31), follow that

$$\theta' = \frac{1}{p} > 0.$$

In this way, $\theta(x)$ is increasing in the neighborhood of x where $\theta(x) = m\pi$. Hence, if $a < x_0 < b$ and $m\pi < \theta(x_0)$, then $\theta(x) > m\pi$ for $x_0 < x \leq b$. This proves the case (ii). ■

For the theorems that follows in this monograph, consider two Sturm-Liouville equations

$$\begin{aligned} -(r_1(x)y'(x))' + p_1(x)y_1(x) = 0 \\ -(r_2(x)y'(x))' + p_2(x)y_1(x) = 0, \end{aligned}$$

denoted by (SLE$_1$) and (SLE$_2$), respectively. Let $r_j(x), p_j(x)$ be real-valued continuous function on an interval I and $r_j > 0$ for $j = 1,2$. Thus, we may define

Definition 2.6.2 — Sturm Majorant. Under the above condition, if $r_1 \geq r_2$ and $p_1 \geq p_2$ on I, then, the Equation (SLE$_1$) is said to be a **Sturm Majorant** for Equation (SLE$_2$) on I, and will be denoted by (SLE$_1$) $\succeq$ (SLE$_2$).

REM We say also, (SLE$_2$) is a *Sturm minorant* for (SLE$_1$).

Definition 2.6.3 — Strict Sturm Majorant. If, in addition the previous conditions, either

$$r_1(x) > r_2(x) \qquad \text{or} \qquad p_1(x) > p_2(x)$$

for some $x \in I$. Then (SLE$_1$) is said to be a **strict Sturm Majorant** for Equation (SLE$_2$) on I and denoted by (SLE$_1$) $\succ$ (SLE$_2$).

Finally, we will show the Sturm's Comparison theorem in two different cases that will depend on the endpoints.

Theorem 2.6.2 — Sturm's First Comparison Theorem. Let (SLE_1) be a Sturm Majorant for (SLE_2), i.e., (SLE_1) $\succeq$ (SLE_2) on an interval $[a,b]$. Consider $y_2(x)$ a nontrivial solution of (SLE_2) with exactly n zeros $z_1 < z_2 < \cdots < z_n$ on $(a,b]$ and y_1 is a nontrivial real solution of (SLE_1) satisfying

$$\frac{r_1(a)y_1'(a)}{y_1(a)} \leq \frac{r_2(a)y_2'(a)}{y_2(a)} \tag{2.33}$$

where the quotient is considered to be $+\infty$ when $y_i(a) = 0$, $i \in 1,2$.

Then y_1 has at least n zeros on $(a, z_n]$. Furthermore, the result also holds if either (SLE_1) $\succ$ (SLE_2) or the inequality in (2.33) is strict.

The idea of the proof is to use the Prüfer Transformation (see page 33) and its properties to show that $\theta_2(x) \leq \theta_1(x)$, $\forall x \in [a,b]$. When $x = z_n$ we have $\theta_2(z_n) = n\pi \leq \theta_1(z_n)$ and applying the Lemma 2.6.1 the result follows.

Proof. The inequality (2.33) motivates us to use the Prüfer Transformation. Thus, let

$$\theta_i(x) = \tan^{-1}\left(\frac{y_i(x)}{r_i(x)y_i'(x)}\right), \qquad \text{for } i = 1,2$$

and, from (2.33), we have

$$\theta_2(a) \leq \theta_1(a). \tag{2.34}$$

From da Definition 2.6.1 of the Prüfer Transformation, θ must satisfy (2.31), i.e.,

$$\theta_i' = \frac{1}{r_i}\cos^2\theta_i - p_i \sin^2\theta_i \equiv f_i(x,\theta_i). \tag{2.35}$$

Since $\cos^2\theta$ and $\sin^2\theta$ are uniformly bounded, the function $f_i(x,\theta_i)$ is smooth as function of the variable θ_i, $i = 1,2$, then the solution of (2.35) is unique and determined by their initial conditions.

Since (SLE_1) is a Sturm majorant for (SLE_2), it follows that

$$f_1(x,\theta) \leq f_2(x,\theta)$$

for $a \leq x \leq b$ and all θ. From (2.35) and Corollary III.4.2 ([16]), we get

$$\theta_2(x) \leq \theta_1(x), \qquad \forall x \in [a,b].$$

Hence, since $\theta_2(z_n) = n\pi$ this implies that $n\pi \leq \theta_1(z_n)$. Then, by the Lemma 2.6.1, y_1 has at least n zeros on $(a, z_n]$. This show the first assertion.

In the case where either (SLE_1) $\succ$ (SLE_2) or the inequality in (2.33) is strictly, the proof is analogous, since $\theta_2(a) < \theta_1(a)$ or $f_2(x,\theta) < f_1(x,\theta)$ on interval $[a,b]$, then, by the same argument in the first part, y_1 has at least n zeros on (a, z_n). This completes the proof. ■

Now, studying the same result, however on the another endpoint. Thus, we obtain the following assertion.

Theorem 2.6.3 — Sturm's Second Comparison Theorem. Let (SLE_1) be a Sturm Majorant for (SLE_2), i.e., (SLE_1) $\succeq$ (SLE_2) on an interval $[a,b]$. Consider $y_1(x)$ a nontrivial solution of (SLE_1) with exactly n zeros $z_1 < z_2 < \cdots < z_n$ on $(a,b]$ and y_2 is a nontrivial real solution of (SLE_2) satisfying

$$\frac{r_1(b)y_1'(b)}{y_1(b)} \leq \frac{r_2(b)y_2'(b)}{y_2(b)} \tag{2.36}$$

where the quotient is considered to be $-\infty$ when $y_i(b) = 0$, $i \in 1,2$.

Then y_2 has at least n zeros on $[z_1, b)$. Furthermore, the result also holds if either (SLE_1) $\succ$ (SLE_2) or the inequality in (2.36) is strict.

Proof. The proof of this result is totally analogues to the previous Theorem, just note that the assumption of the zeros set of y_2 implies the transformation of the equation (2.36) in $n\pi \leq \theta_2(b) \leq \theta_1(b) \leq (n+1)\pi$. ■

The following result is a corollary of the Sturm's First Comparison Theorem, known as *Sturm's Separation Theorem.*

Theorem 2.6.4 — Sturm's Separation Theorem. Let (SLE_1) be a Sturm Majorant for (SLE_2), i.e., (SLE_1) $\succeq$ (SLE_2) and $y_1(x)$, $y_2(x)$ be nontrivial real-valued solutions of (SLE_1) and (SLE_2), respectively. Suppose that y_1 vanish at $z_1, z_2 \in [a,b]$, with $z_1 < z_2$. Then y_2 has at least one zero on $[z_1, z_2]$.

Proof. We may assume that $\theta_2(z_1) = 0$ and $\theta_2(z_2) = \pi$ and $0 < \theta_1(z_1) < \pi$. From the proof of Sturm's Fist Theorem it follows that

$$\theta_2(x) < \theta_1(x),$$

for $z_1 < x < z_2$. Then exist $z_1 < z_1^* < z_2$, in such a way $\theta_1(z_1^*) = \pi$, i.e., there are at least one zero of y_1 on the interval $[z_1, z_2]$. Thus the assertion is proved. ■

Corollary 2.6.5 In particular, if $p_1(x) \equiv p_2(x) \equiv p(x)$, $q_1(x) \equiv q_2(x) \equiv q(x)$, and $y_1(x)$, $y_2(x)$ are two independent solutions of the same Sturm-Liouville Equation, then, the zeros of y_1 separate and are separated by those of y_2.

The main utility of the Sturm's Comparison Theorem is it may used to show that a second order linear equation (sometimes nonlinear) is oscillatory. For this purpose, we will close the Chapter with an important application of Sturm's Comparison Theorem to obtain the zero set of nontrivial solution Bessel's Equation.

Consider the following Bessel's Equation

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0 \tag{2.37}$$

where ν is a real positive parameter ($\nu \geq 0$). For $x > 0$, setting the change of variables $y = \dfrac{u}{\sqrt{x}}$, transform the Equation (2.37) into

$$u'' + \left(1 + \frac{1-4\nu^2}{4x^2}\right)u = 0 \qquad \text{for } x > 0 \tag{2.38}$$

Now, for the study about the zeros of the Equation (2.38), we need consider the values of ν.

[$0 < \nu < 1/2$] In this case, we will use the Sturm Comparison Theorem to compare (2.38) with

$$y'' + y = 0, \tag{2.39}$$

which has a solution $\sin x$ with zeros at $x = n\pi$, $n \in \mathbb{N}$. Therefore, a solution u of (2.38) has at least one zero on each of the open intervals $((n-1)\pi, n\pi)$, $n \in \mathbb{N}$

[$\nu > 1/2$] Once again, we will utilize the Sturm's Comparison Theorem with (2.38) and (2.39) and conclude that between any two consecutive zeros, α and β of y, there exist at least one zero of $\sin x$. Thus, we have $\alpha < n\pi < \beta$ for some $n \in \mathbb{N}$.

REM In the course of the work, this argument of comparing some equation with (2.39) will be employed.

CHAPTER

3 The Singular Sturm-Liouville Problems in Spectral Parameter

In this chapter we will investigate the Singular Sturm-Liouville problems with spectral parameter, that is, the coefficients depend continuously on the spectral parameter λ in an interval Λ. The focus is to show that the accumulation/non-accumulation of eigenvalues at endpoint ν of Λ is determined by oscillatory properties of the equation at the boundary $\lambda = \nu$. In the two first sections we will define the problem with spectral parameter and some basic results. In the Section 3.3 we will prove two lemmas that will be auxiliary in the proof of the main result of the last section.

3.1 Basic Definitions

In the previous chapter we saw that the Sturm-Liouville equation has a parameter $\lambda \in \mathbb{R}$. Now we will vary λ on some interval $\Lambda \subset \mathbb{R}$.

Definition 3.1.1 — The Parameter Dependent Sturm-Liouville Equation. We called of a *parameter dependent Sturm-Liouville equation*, a family of equations

$$-(r(x;\lambda)f(x)')' + p(x;\lambda)f(x) = 0, \qquad x \in I \subset \mathbb{R}$$

denoted by (SLE)(λ), $\lambda \in \Lambda \subset \mathbb{R}$ and $r, p : I \times \Lambda \longrightarrow \mathbb{R}$ are continuous functions with $r > 0$.

REM The Sturm-Liouville equation $-(r(x)f(x)')' + p(x)f(x) = 0$, will be denoted simply by (SLE).

The result bellow guarantees the existence and uniqueness of the solution to the problem in Definition 3.1.1, as well as the continuous dependence on λ.

Theorem 3.1.1 — Existence-Uniqueness. If $\chi : \Lambda \longrightarrow I$, and $\alpha, \beta : \Lambda \longrightarrow \mathbb{C}$ are continuous functions, then, for each value of the parameter λ in Λ, the initial value problem

$$-(r(x;\lambda)f(x)')' + p(x;\lambda)f(x) = 0, \qquad x \in I$$

$$f(\chi(\lambda)) = \alpha(\lambda), \qquad f'(\chi(\lambda)) = \beta(\lambda)$$

has a unique solution $y(\cdot;\lambda)$ on I, and $y(\cdot;\lambda) \longrightarrow y(\cdot;\lambda_0)$, $\dfrac{\partial y(\cdot;\lambda)}{\partial x} \longrightarrow \dfrac{\partial y(\cdot;\lambda_0)}{\partial x}$ locally uniformly on I as $\lambda \longrightarrow \lambda_0 \in \Lambda$; in particular, $y, \dfrac{\partial y}{\partial x} : I \times \Lambda \longrightarrow \mathbb{C}$ are continuous.

The proof will be omitted, however, it follows in such way that we need to transform the initial value problem into a linear first order problem and then apply the standard Picard-Lindelöf method [see [7]].

Now consider the following Sturm–Liouville problem:

Problem 3.1.2 — λ-Nonlinear Singular Sturm–Liouville Problems. The problem consist of a family of parameter dependent Sturm-Liouville equations

$$-(r(x;\lambda)f(x)')' + p(x;\lambda)f(x) = 0,$$

on an x-interval $I = (a,b)$ $(-\infty \leq a < b \leq \infty)$ or $I = [a,b)$ $(-\infty < a < b \leq \infty)$ where the parameter λ varies in an interval $\Lambda = (\mu, \nu)$, $-\infty \leq \mu < \nu \leq \infty$. In case $I = [a,b)$, we also consider a λ-dependent boundary condition

$$\alpha(\lambda)f(a) + \beta(\lambda)f'(a) = 0 \tag{3.1}$$

where it will always be assumed that

- $\alpha, \beta : \Lambda \longrightarrow \mathbb{R}$ are continuous,
- $\alpha^2(\lambda) + \beta^2(\lambda) \neq 0$ for all $\lambda \in \Lambda$,
- either $\beta \equiv 0$ or β is never zero on Λ.

Definition 3.1.2 — Limit-Equation. If the limits

$$r(x;\nu) := \lim_{\lambda \longrightarrow \nu} r(x;\lambda) > 0, \qquad p(x;\nu) := \lim_{\lambda \longrightarrow \nu} p(x;\lambda)$$

exist for all x in a subinterval J of I and define continuous functions $r(\cdot;\lambda)$ and $p(\cdot;\lambda)$ on J, then the Sturm-Liouville equation

$$-(r(x;\nu)f(x)')' + p(x;\nu)f(x) = 0,$$

will be called the *limit-equation* for $\lambda \longrightarrow \nu$ on J and denoted by (SLE)(ν) (on J).

In the next section we will give two concepts about the solution of this problem.

3.2 Oscillatory Equations and Principal Solutions

We begin this section defining oscillation and disconjugate solution of Problem 3.1.2 which we will use throughout this chapter.

Definition 3.2.1 — Oscillatory and Nonoscillatory. If one or every nontrivial real valued solution of (SLE)(λ) has infinitely many zeros on I, then we say that (SLE)(λ) is **oscillatory**. Conversely, when the nontrivial solution has at most a finite number of zeros on I, it is said to *nonoscillatory*.

Definition 3.2.2 — Disconjugate. In the case where every nontrivial real valued solution of (SLE) has at most one zero on I, then, we called (SLE)(λ) of **disconjugate**.

The following lemma is a simple corollary to the First Comparison Theorem;

Lemma 3.2.1 If the function $p \geq 0$ on I then (SLE)(λ) is disconjugate on I.

In the singular problem we have no boundary condition. Thus, in this kind of problem, the solution needs to be *principal* on the endpoint.

Definition 3.2.3 — Principal Solution. Suppose (SLE) is defined on a half-open interval $I = [a,b)$ and is nonoscillatory at b, i.e., it is nonoscillatory on $[x_0,b)$ for some $x_0 \in [a,b)$. Then, a nontrivial real valued solution y is referred to as **principal** or **nonprincipal at** b according as the integral

$$\int^b \frac{ds}{r(s)y(s)^2}$$

diverges or converges, respectively. The lower limit of integration of above equation being any point beyond the last zero of y.

Another way of characterize a principal solution y at b is when it satisfy the following condition

$$\lim_{x\to b} \frac{y(x)}{u(x)} = 0,$$

for any nontrivial solution u independent of y.

REM Principal Solutions are unique up to constant multiple.

Motivated by the results in the previous section about the Comparison Theorem, we can formulate this one for the principal solutions.

Theorem 3.2.2 — Comparison Theorem for Principal Solutions. Let $(\text{SLE}_1) \succeq (\text{SLE}_2)$ on $I = [a,b)$ and let (SLE_2) be disconjugate on I. Then, for any nontrivial real valued solution y of (SLE_2) there are a principal solution w and a nonprincipal solution v of (SLE_1) such that

$$\frac{r_1 w'}{w} \leq \frac{r_2 y'}{y} \leq \frac{r_1 v'}{v}$$

for all points of I beyond the last zero of y.

The proof of following results will be omitted, however the first Lemma can be found in [30] and the remaining found in [24].

Lemma 3.2.3 If (SLE) is disconjugate on $I = (a,b)$, then a solution which is principal at b (or a) has no zeros on I.

Lemma 3.2.4 — Principal Solutions and Boundary Conditions. Let p be given by the Definition 3.1.1:

(I) If $p(\cdot) \geq \varepsilon$ on $I = [x_0, b)$ for some $\varepsilon > 0$, then any solution of (SLE) which is principal at b is also in $L^2[x_0, b)$. If, in addition, (SLE) is in the limit point case at b, then the space of L^2-solutions at b is just $\mathbb{C} \cdot f$ where f is any principal solution at b.

(II) If $p(\cdot) \geq 0$ on $I = [x_0, b)$ and

$$\int_I p(x)dx = \infty,$$

then a nontrivial real solution w of (SLE) is principal at b if and only if $w(x) \longrightarrow 0$ as $x \longrightarrow b$.

Lemma 3.2.5 — Continuous Families of Principal Solutions. Suppose that for (SLE)(λ) there is a continuous function $B: \Lambda \to I = (a,b)$ such that $p(x;\lambda) \geq 0$ on $[B(\lambda), b)$ and

$$\int^b p(x;\lambda)dx = \infty$$

for every λ. Then there is a family $\{w(\cdot;\lambda) \mid \lambda \in \Lambda\}$ of solutions of (SLE)(λ) principal at b such that w, $\dfrac{\partial w}{\partial x}$ are continuous on $I \times \Lambda$.

Of course that the last two lemmas also holds for the left endpoint.

3.3 Background to Main Result

The proof of the main result will be summarized in the lemmas bellow. For the rest of chapter we will made the following assumptions

(D) When a (respectively b) is a singular endpoint, there is a continuous function $A: \Lambda \longrightarrow (a,b)$ (respectively $B: \Lambda \longrightarrow (a,b)$) such that (SLE)($\lambda$) is disconjugate on $(a, A(\lambda)]$ (respectively $[B(\lambda), b)$) for every $\lambda \in \Lambda$.

(PS) In the case where a (respectively b) is a singular endpoint, there are a family of solutions $\{v(.\cdot;\lambda) \mid \lambda \in \Lambda\}$ (respectively $\{w(.\cdot;\lambda) \mid \lambda \in \Lambda\}$) of (SLE)($\lambda$) such that $v(.\cdot;\lambda)$ (respectively $w(.\cdot;\lambda)$) is principal at a (respectively b) for each λ and v, $\dfrac{\partial v}{\partial x}$ (respectively w, $\dfrac{\partial w}{\partial x}$) are continuous on $I \times \Lambda$.

(MC1) For any $\lambda_1, \lambda_2 \in \Lambda$ such that $\lambda_1 < \lambda_2$ and (SLE)(λ_1) $\succeq$ (SLE)(λ_2). Then for any subinterval of I like $J = (c,b)$ (or $J = (a,c)$ when a is also a singular endpoint) we have (SLE)(λ_1)$|_J$ $\succ$ (SLE)(λ_2)$|_J$.

(MC2) In the case $I = [a,b)$, then $\lambda \mapsto \dfrac{r(a;\lambda)\alpha(\lambda)}{\beta(\lambda)}$ is increasing on Λ (as an extended real valued function).

We first consider only the special case where the following conditions holds:

(a) The x-interval is $I = (-\infty, b)$,

(b) The hypotheses (D) and (PS) hold for the endpoint b of I,

(c) The limits,

$$\lim_{x\to-\infty} \sup r(x;\lambda) < \infty \qquad \text{and} \qquad \lim_{x\to-\infty} \sup p(x;\lambda) < 0$$

holds for each $\lambda \in \Lambda$

Lemma 3.3.1 Suppose that (a)-(c) occurs and let $B(\cdot)$ be as in (D) and $w(\cdot;\cdot)$ as in (PS).

(i) The set of all zeros of $w(\cdot;\cdot)$ on $(-\infty,b) \times \Lambda$ consists of an infinite sequence $\{z_n : \Lambda \longrightarrow (-\infty,b)\}_{n=1}^{\infty}$ of continuous curves such that $z_{n+1}(\cdot) < z_n(\cdot) \le B(\cdot)$ on Λ for every n.

(ii) Consider that (MC1) holds, then the zero curves of w are strictly increasing in λ and, for any fixed $x_0 \in (-\infty,b)$,

$$\frac{r(x_0;\cdot)w'(x_0,\cdot)}{w(x_0;\cdot)}$$

is strictly increasing on any subinterval Λ_0 of Λ such that no zero curves of w intersect $\{x_0\} \times \Lambda_0$.

Proof. By the assumption in (c), for a given $\lambda \in \Lambda$ there are $\varepsilon, \delta > 0$ such that

$$-\varepsilon f'' - \delta f = 0 \tag{3.2}$$

where

$$\lim_{x\to-\infty} \sup r(x;\lambda) = \varepsilon \qquad \text{and} \qquad \lim_{x\to-\infty} \sup p(x;\lambda) = -\delta.$$

The equation (3.2) is a Sturm majorant for (SLE)(λ) near $-\infty$ and since this equation is obviously oscillatory, because is a classic harmonic oscillator's equation, it follows that $w(\cdot;\lambda)$ has infinitely many zero which of course cannot accumulate at any finite point.

Since the solutions $w(\cdot;\lambda)$ are assumed to be principal at b and (SLE) (λ) is disconjugate on $(B(\lambda),b)$, by the Lemma 3.2.3, they can have no zeros on the interior of the interval $[B(\lambda),b)$. Thus, consider $z_n(\lambda)$ as being the n'th zero of $w(\cdot,\lambda)$ to the left of $B(\lambda)$.We can see that $z_n(\lambda)$ is well-defined and since w is oscillatory, $w(z_n(a),a) = 0$, where $z_n(a) < B(a)$.

The continuity of z_n at a given $\lambda_0 \in \Lambda$ follows from the Implicit Function Theorem, since $w, \dfrac{\partial w}{\partial x} : (-\infty,b) \times \Lambda \longrightarrow \mathbb{R}$ are continuous and $\dfrac{\partial w}{\partial x}$ is not null at zeros of w, by the Implicit Function Theorem for each $j \in \{1,\dots,n\}$ there exist an open bounded rectangle $R_j = I_j \times \Lambda_j \subset (-\infty,b) \times \Lambda$ centered at $(z_j(\lambda_0);\lambda_0)$ with $\overline{\Lambda_j} \subset \Lambda$, as shown in Figure 3.1, and exist a unique continuous function $h_j:\ \Lambda \longrightarrow I_j$ such that $h_j(\lambda_0) = z_j(\lambda_0)$ and $w(h_j(\lambda);\lambda) = 0$, for all $\lambda \in \Lambda_j$.

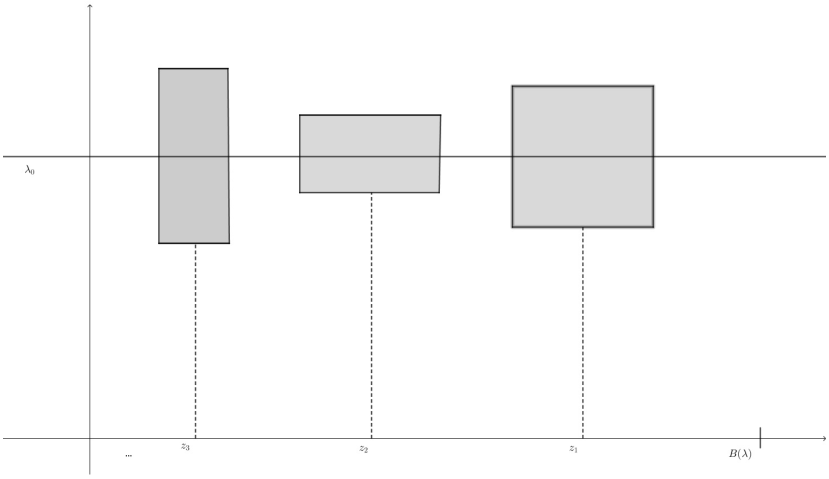

Figure 3.1: The figure illustrates the rectangles R_j cited above.

The rectangles may be taken sufficiently small that they are disjoint and such that h_j exhausts the set of zeros of w in R_j. Write $I_j = (a_j, b_j)$ and choose an upper bound $M < b$ for $B(\cdot)$ on the compact interval $\cap_1^n \overline{\Lambda_j}$ such that also $M > b_1$. In particular, $w(\cdot;\lambda_0)$ has no zeros on (M,b) for $\lambda \in \cap_1^n \Lambda_j$. Because $w(\cdot,\lambda_0)$ also has no zeros on the compact set

$$K := [b_n, a_{n-1}] \cup [b_{n-1}, a_{n-2}] \cup \cdots [b_2, a_1] \cup [b_1, M]$$

and $w(\cdot;\lambda) \longrightarrow w(\cdot;\lambda_0)$ locally uniformly as $\lambda \longrightarrow \lambda_0$, then, there is a neighborhood $\Lambda_0 \subset \cap_1^n \Lambda_j$ of λ_0 such that w has no zeros on $K \times \Lambda_0$, as shown the Figure 3.2.

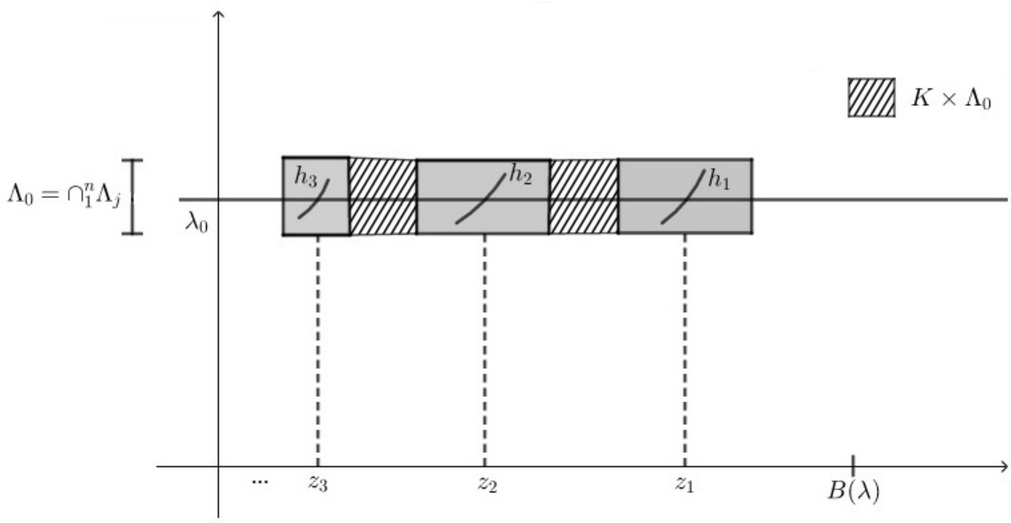

Figure 3.2: The figure illustrates the neighborhood Λ_0 where w has no zeros on $K \times \Lambda_0$.

Therefore, the only zeros of w in $(a_n, b) \times \Lambda_0$ are just those given by the functions $h_1, h_2, \ldots, h_n$ and, since the z_j are defined by counting zeros from right to left, $z_j \equiv h_j$ on Λ_0, where $1 \le j \le n$.

By the same arguments, we concluded that z_n, where $n \in \{1, 2, \ldots\}$ is a continuous curve.

Now, we will prove the part (ii). For $\lambda_1 < \lambda_2$ in Λ consider the equations (SLE)(λ_1) $\succeq$ (SLE)(λ_2) and choose a bound $B(\cdot) < d < b$ on $[\lambda_1, \lambda_2]$ so that, by (D), both equations are disconjugate on (B,b), since this is valid also in a subinterval, thus both equations are disconjugate on [d,b).

By the Comparison Theorem for Principal Solutions (Theorem 3.2.2), there is a principal solution u of (SLE)(λ_1) on [d,b) such that

$$\frac{r(x;\lambda_1)\, u'(x)}{u(x)} \leq \frac{r(x;\lambda_2)\, w'(x;\lambda_2)}{w(x;\lambda_2)}, \qquad \forall x \geq d.$$

Since $w(\cdot;\lambda_1)$ is a principal solution on $[d,b)$ and such solutions are unique up to a constant multiple, we have

$$\frac{r(x;\lambda_1)\, w'(x;\lambda_1)}{w(x;\lambda_1)} \leq \frac{r(x;\lambda_2)\, w'(x;\lambda_2)}{w(x;\lambda_2)}, \qquad \forall x \geq d. \tag{3.3}$$

According to (MC1), we can choose $d_0 \in (d,b)$ such that (SLE)(λ_1) $\succ$ (SLE)(λ_2) on $[z_n(\lambda_1), d_0)$. This fact, the inequality given by the Equation (3.3) for $x = d_0$ and the fact that $w(\cdot;\lambda_1)$ has exactly n zeros in $[z_n(\lambda_1), d_0)$, imply, by the Sturm's First Comparison Theorem, that $w(\cdot,\lambda_2)$ has at least n zeros on $(z_n(\lambda_1), d_0)$, i.e., $z_n(\lambda_2) > z_n(\lambda_1)$.

Now, let x_0, Λ_0 be as in (ii), $\lambda_1 < \lambda_2$ in Λ_0, d as above. Since x_0 is not zero of $w(\cdot,\lambda_1)$ and $w(\cdot,\lambda_2)$, remembering the construction of the sequence $(z_n(\lambda_1))$, $(z_n(\lambda_2))$ (from the right to the left) and the fact of $z_n(\lambda_1) < z_n(\lambda_2)$, $\forall n \in \mathbb{N}$, hence, we may choose d_0, satisfying $\max\{x_0, d\} < d_0 < b$, such that, the "non-intersection" hypothesis implies $w(\cdot,\lambda_1)$ and $w(\cdot,\lambda_2)$ have the same number of zeros on $[x_0, d_0)$. This fact together the Equation (3.3) and the Second Comparison Theorem imply

$$\frac{r(x;\lambda_1)\, w'(x_0;\lambda_1)}{w(x_0;\lambda_1)} < \frac{r(x;\lambda_2)\, w'(x_0;\lambda_2)}{w(x_0;\lambda_2)}.$$

■

Before the next lemma, we will define the interface condition and the crossing of successive zero curves of w and γ.

Definition 3.3.1 — Interface Condition. For $\alpha, \beta : \Lambda \longrightarrow \mathbb{R}$, where $\alpha^2(\lambda) + \beta^2(\lambda) \neq 0$ for all $\lambda \in \Lambda$ and either $\beta \equiv 0$ or β is never zero on Λ. We called the equation

$$\alpha(\lambda) w(\gamma(\lambda);\lambda) + \beta(\lambda) w'(\gamma(\lambda);\lambda) = 0 \tag{3.4}$$

of *interface condition* for w a long a given continuous curve $\gamma : \Lambda \longrightarrow (-\infty, b)$.

Definition 3.3.2 — Crossing of Successive Zero Curves of w and γ. We say that a pair of points $\lambda_n, \lambda_{n+1} \in \Lambda$ are *crossing of successive zero curves of w with γ* if satisfies

$$z_j(\lambda_j) = \gamma(\lambda_j), \qquad \text{for } j = n, n+1,$$

where $w(z_j(\lambda_j), \lambda_j) = 0$.

Lemma 3.3.2 Suppose the conditions (a)-(c) are satisfied and let $B(\cdot)$ be as in (D) and let $w(\cdot,\cdot)$ be as in (PS). The follows statements are verified

(i) Consider that τ and ω, with $\tau < \omega$, are crossings of successive zero curves of w with γ, then $[\tau, \omega)$ contains at least one solution λ of (3.4) as well as values which are not solutions.

(ii) Assume that (MC1) holds, γ is constant equivalent to x_0 ($\gamma \equiv x_0$), and

$$\frac{r(x_0;\cdot)\alpha(\cdot)}{\beta(\cdot)}$$

is increasing (as an extended real valued function), then there is at mot one solution of (3.4) in any subinterval Λ_0 of Λ such that no zero curves of w intersect $\{x_0\} \times \Lambda_0$.

Proof. Note that the part (i) is obvious when $\beta \equiv 0$, because (3.4) becomes

$$\alpha(\lambda)w(\gamma(\lambda);\lambda) = 0 \implies w(\gamma(\lambda);\lambda) = 0$$

and this occurs if, and only if, $\gamma(\lambda) = z(\lambda)$, thus, the crossing points are themselves, the only solutions of (3.4). Now, we assume β is never zero, i.e, $\beta \neq 0$ and let $\tau = \lambda_n < \lambda_{n+1} = \omega$ be as defined in the Lemma 3.3.1. Then there are c, d such that $\lambda_n \leq c < d \leq \lambda_{n+1}$, $z_n(c) = \gamma(c)$, $z_{n+1}(d) = \gamma(d)$ and no zero curves of w cross γ between c and d, i.e. $w(\gamma(\lambda);\lambda) \neq 0$ for $c < \lambda < d$. We can constructed these points by setting

$$\begin{aligned} d &:= \inf\{\lambda \in [\lambda_n, \lambda_{n+1}] \mid z_{n+1}(\lambda) \geq \gamma(\lambda)\}, \\ c &:= \sup\{\lambda \in [\lambda_n, d] \mid z_n(\lambda) \leq \gamma(\lambda)\}. \end{aligned}$$

To ensure the existence of values c and d, we have some cases to analyses:

1° There is **not** intersection between the curves, except in the extremes, we have $d = \lambda_{n+1}$ and $c = \lambda_n$.

2° There is intersection between the curves, it's illustrated in Figure 3.3.

Using the continuity we have

$$z_{n+1}(d) \geq \gamma(d) \qquad \text{and} \qquad z_n(c) \leq \gamma(c), \tag{3.5}$$

in particular, if $c = d$, then we have the contradiction $z_{n+1}(c) \geq z_n(c)$, thus $c < d$.

For $\lambda \in (c,d)$ the definitions imply $z_{n+1}(\lambda) < \gamma(\lambda) < z_n(\lambda)$ (we also may see this in Figure 3.3), hence, $w(\gamma(\lambda);\lambda) \neq 0$ for $\lambda \in (c,d)$. From the Equation (3.4), we have

$$\frac{w'(\gamma(\lambda);\lambda)}{w(\gamma(\lambda);\lambda)} = -\frac{\alpha(\lambda)}{\beta(\lambda)}.$$

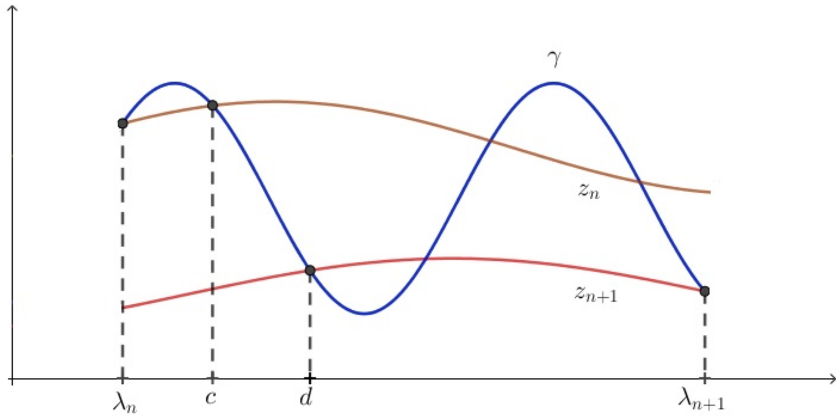

Figure 3.3: It's easy to see that there is not zero curves of w cross γ between c and d.

Thus, define

$$Q(\lambda) = \frac{r(\gamma(\lambda);\lambda)\; w'(\gamma(\lambda);\lambda)}{w(\gamma(\lambda);\lambda)} \qquad \text{on } (c,d) \tag{3.6}$$

and

$$H(\lambda) = -\frac{r(\gamma(\lambda);\lambda)\; \alpha(\lambda)}{\beta(\lambda)} \qquad \text{on } (c,d). \tag{3.7}$$

We want to find $\lambda_0 \in (c,d)$ such that $Q(\lambda_0) = H(\lambda_0)$, i.e., satisfy the Equation (3.4).

Note that H is continuous on $[c,d]$, consequently bounded and $w(\gamma(c);c) = w(\gamma(d),d)$, so if we will show that Ran(Q)= $\mathbb{R}$ then λ_0 will be the point of intersection between Q and H. For this it suffices to shown

$$\operatorname{sgn} w'(\gamma(c);c) = -\operatorname{sgn} w'(\gamma(d);d) \tag{3.8}$$

because $\operatorname{sgn} w(\gamma(\lambda);\lambda)$ is constant on (c,d) and $\lim_{\lambda \longrightarrow c^+} Q(\lambda) = \pm\infty$ and $\lim_{\lambda \longrightarrow d^-} Q(\lambda) = \mp\infty$. To Show (3.8), is the same, by (3.5), to prove

$$\operatorname{sgn} w'(z_n(c);c) = -\operatorname{sgn} w'(z_{n+1}(d);d). \tag{3.9}$$

Because $\lambda \longmapsto w'(z_n(\lambda);\lambda)$ is continuous and not null, its sign is constant and (3.9) follows, since $\operatorname{sgn} w'(z_n(d);d) = -\operatorname{sgn} w'(z_{n+1}(d);d)$.

Now we will prove the part (ii). If $\beta \equiv 0$, then there are obviously no solutions of (3.4) in Λ_0. For β never zero and $\gamma \equiv x_0$ let Q be defined on Λ_0. The claim follows, since the function (3.7) is decreasing and the function (3.6) is strictly increasing by the Lemma 3.3.1, Therefore them has at most one intersection, that imply the Equation (3.4) there is at most one solution.

■

REM For the special case where

(a') The x-interval is $I = (a,\infty)$.
(b') The hypotheses (D) and (PS) hold for the endpoint a of I.
(c') The following limits holds,

$$\limsup_{x\to\infty} r(x;\lambda) < \infty \qquad \text{and} \qquad \limsup_{x\to\infty} p(x;\lambda) < 0$$

for all $\lambda \in \Lambda$.

We have the exact analogues of the Lemma 3.3.1 and Lemma 3.3.2 for the solutions $v(\cdot;\lambda)$ in (PS) (principal at a). Specifically, in Lemma 3.3.1(i) we get zero curves

$$A(\cdot) \leq z_1(\cdot) < z_2(\cdot) < \cdots < z_n(\cdot) < \cdots$$

and in the part (ii) of the same lemma $\dfrac{r(x_0;\cdot)w'(x_0,\cdot)}{w(x_0;\cdot)}$ is strictly decreasing on Λ_0 if no zero curves of v intersect $\{x_0\} \times \Lambda_0$. In Lemma 3.3.2(ii) the hypothesis must be that $\dfrac{r(x_0;\cdot)\alpha(\cdot)}{\beta(\cdot)}$ is decreasing.

3.4 Main Result

The main result of this work is related to the eigenvalue of the Sturm-Liouville problem, however as we treating with a singular problem, the definition of eigenvalue is a little different.

Definition 3.4.1 — Eigenvalue. We say that a fixed λ is an eigenvalue of the Problem 3.1.2 if exist a nontrivial solution y such that

- y is principal at both endpoints a and b in case $I = (a,b)$,
- y is principal at b and satisfies (3.1) at a in case $I = [a,b)$.

Then, we called y as eigenfunction with corresponding eigenvalue λ.

Theorem 3.4.1 — Eigenvalue Accumulation. Let r, p: $I \times (\mu,\nu) \longrightarrow \mathbb{R}$ be continuous functions with $r(\cdot;\nu) > 0$ and suppose $(SLE)(\nu)$ is oscillatory on I. Then, ν is an accumulation point of (simple) eigenvalues of the parameter dependent Sturm-Liouville Problem in Λ and every left neighborhood of ν has some points which are non-eigenvalues.

Proof. We will prove this statement for two types of I. First we consider the problem for $I = (a,b)$. We will assume $A(\lambda)$ in (D) is such that (SLE)(λ) is disconjugate on $(a,A(\lambda)+\varepsilon(\lambda))$ for some $\varepsilon(\lambda) > 0$. Then the assumption implies that the solution $v(\cdot;\lambda)$ in (PS) is principal at a, by the Lemma 3.2.3, imply that $v(\cdot;\lambda)$ has no zeros on $(a;A(\lambda)+\varepsilon(\lambda))$, hence, $v(A(\lambda);\lambda) \neq 0$, $\forall \lambda \in \Lambda$.

From the Definition 3.4.1, we have that a point $\lambda \in \Lambda$ is an eigenvalue if the associated non-trivial solution is principal at both endpoints a and b. From (PS), $v(\cdot;\lambda)$ is principal at a and $w(\cdot;\lambda)$ is principal at b, thus w is equal to a v up to constant multiple, i.e.,

$$w(\cdot;\lambda) = cv(\cdot;\lambda) \implies \frac{w(\cdot;\lambda)}{v(\cdot;\lambda)} = c.$$

By differentiating with respect to λ we obtain

$$\frac{d}{d\lambda}\left(\frac{w(\cdot;\lambda)}{v(\cdot;\lambda)}\right) = 0,$$

matched at $A(\lambda)$, we obtain that the following statement: A point $\lambda \in \Lambda$ is an eigenvalue if, and only if,

$$v(A(\lambda);\lambda)w'(A(\lambda);\lambda) - v'(A(\lambda);\lambda)w(A(\lambda);\lambda) = 0.$$

We will now begin the proof. The idea of the proof is show that every left neighborhood of ν always has an eigenvalue. For this, we will show that given an any neighborhood exist an interval in this neighborhood that contains an eigenvalue.

Let $u(\cdot;\lambda)$ be the solution of (SLE)(λ) on I determined by the initial conditions

$$\begin{cases} u(x_0;\lambda)=1 \\ u'(x_0;\lambda)=0 \end{cases}$$

at some fixed point $x_0 \in I$. Since $u(\cdot;\lambda) \longrightarrow u(\cdot;\nu)$ and $u'(\cdot;\lambda) \longrightarrow u'(\cdot;\nu)$ locally uniformly on I as $\lambda \longrightarrow \nu$ and $u(\cdot;\nu)$ must have infinity many zeros on I, because (SLE)(ν) is oscillatory on I. It follows that the number of zeros of $u(\cdot;\lambda)$ on I goes to ∞ as $\lambda \longrightarrow \nu$. Hence, by the Separation Theorem (observe that SLE_1=SLE_2), between two zeros of a solution u there exist a zero of w and since the number of zeros go to infinity, w also has infinity zeros as λ .

Since (SLE)(λ) is disconjugate on $(a,A(\lambda))$ for any λ, $w(\cdot;\lambda)$ may have at most one zero on $(a,A(\lambda)]$. Thus, fix $\mu_0 \in \Lambda$, let $0 \le n < \infty$ be the number of zeros of $w(\cdot;\mu_0)$ on $[A(\mu_0),b)$, and choose $\lambda_0 \in (\mu_0,\nu)$ such that $w(\cdot;\lambda_0)$ has at least $n+2$ zeros on $[A(\lambda_0),b)$. Now fix any x_0 with

$$a < x_0 < \min\{A(\lambda) \mid \mu_0 \le \lambda \le \lambda_0\} \tag{3.10}$$

and consider, for the λ-interval $[\mu_0,\lambda_0]$, the *auxiliary equation*

$$-(\tilde{r}(x;\lambda)f'(x))' + \tilde{p}(x;\lambda)f(x) = 0 \tag{3.11}$$

with continuous coefficients $\tilde{r}$, $\tilde{p}$ on $(-\infty,b)\times[\mu_0,\lambda_0]$ defined by

$$\tilde{r}(x;\lambda) := \begin{cases} r(x;\lambda) & x_0 \le x < b \\ r(x_0;\lambda) & -\infty < x < x_0 \end{cases}$$

and

$$\tilde{p}(x;\lambda) := \begin{cases} p(x;\lambda) & x_0 \le x < b \\ p(x_0;\lambda)+(x-x_0) & -\infty < x < x_0. \end{cases}$$

The term $(x-x_0)$ in $\tilde{p}(x;\lambda)$ above is due to the condition (c).

Let $\tilde{w}(\cdot;\lambda)$ be the extension of $w(\cdot;\lambda)$ from $[x_0,b)$ onto $(-\infty,b)$ as a solution this auxiliary equation, in this way, $\tilde{w}$ and w are identical on $[x_0,b)\times[\mu_0,\lambda_0]$. From the comments above at least the $(n+1)$'st and $(n+2)$'ns zero curves of $\tilde{w}$ must cross $A(\cdot)$ on $[\mu_0,\lambda_0]$ which will be denoted by ξ and η in the Figure 3.4. Setting $\alpha(\lambda) = -v'(A(\lambda);\lambda)$ and $\beta(\lambda) = v(A(\lambda);\lambda)$ in the Equation (3.4) and applying the Lemma 3.3.2(i) to the auxiliary equation it follows that there is at least on eigenvalue in $[\mu_0,\lambda_0]$. Thus, by the previous construction we can choose a arbitrary μ_0 so close of ν and repeating the same arguments above, we guarantees the existence of an eigenvalue λ between μ_0 and ν, concluding that ν is a accumulation point for λ.

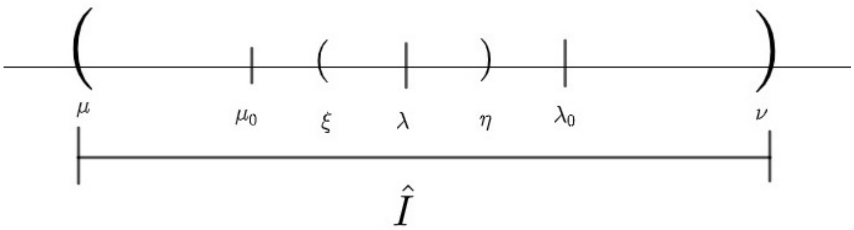

Figure 3.4: The figure illustrates the accumulation of the eigenvalue in ν.

The proof for $I=[a,b)$ is a special case of the arguments above. We must apply the above consideration to the auxiliary equation (3.11) with $x_0 = a\ \forall\lambda \in \Lambda$. Another consideration that we apply the Lemma (3.3.2) with $\gamma \equiv a$ on Λ. ■

Theorem 3.4.2 — Non-accumulation. Consider that (MC1,MC2) hold, $r(\cdot;\nu)$ and $p(\cdot;\nu)$ are continuous with $r(\cdot;\nu)$ on I, except at finitely many points $a_1,\dots,a_m$ and let (SLE)(λ) be non-oscillatory on each component of $I\backslash\{a_1,\dots,a_m\}$. Then, the eigenvalues do not accumulate at any point of Λ nor at the endpoint μ either.

Proof. We will prove this statement for two type of I. First we consider $I=(a,b)$. We assume, without loss of generality that $A(\lambda)$ above is decreasing. Due to the non-oscillation hypothesis, on each component of $I\backslash\{a_1,\dots,a_m\}$,we have a bound on the number of zeros of any nontrivial solution of (SLE)(ν). By the Sturm condition in (MC1) and the Sturm's Separation Theorem we also obtain such bounds on the number of zeros of nontrivial solutions of (SLE)(λ) on the corresponding components independent of λ. Taking into account the possibility of zeros at the points $a_1,\dots,a_m$ we get a bound M on the number of zeros for any nontrivial solution of (SLE)(λ) on I independent of λ,in this way , the solutions $w(\cdot;\lambda)$ has a bound M on the number of zeros.

Note that there are only finitely many zeros of $w(\cdot;\lambda)$ on $A(\cdot)$. Indeed, we will show this claim by contradiction. If there were infinitely many zeros we could choose $[\hat{\mu},\hat{\lambda}]\subset\Lambda$ such that there are at least $M+1$ zeros of w on $A|_{[\hat{\mu},\hat{\lambda}]}$ and we can define x_0 and the auxiliary equations like at the Equations (3.10) and (3.11), respectively. From the monotonicity of zero curves of $\tilde{w}$ by hypothesis, there are at least $M+1$ crossing of *different* zero curves of w with A, as shown in the Figure 3.5.

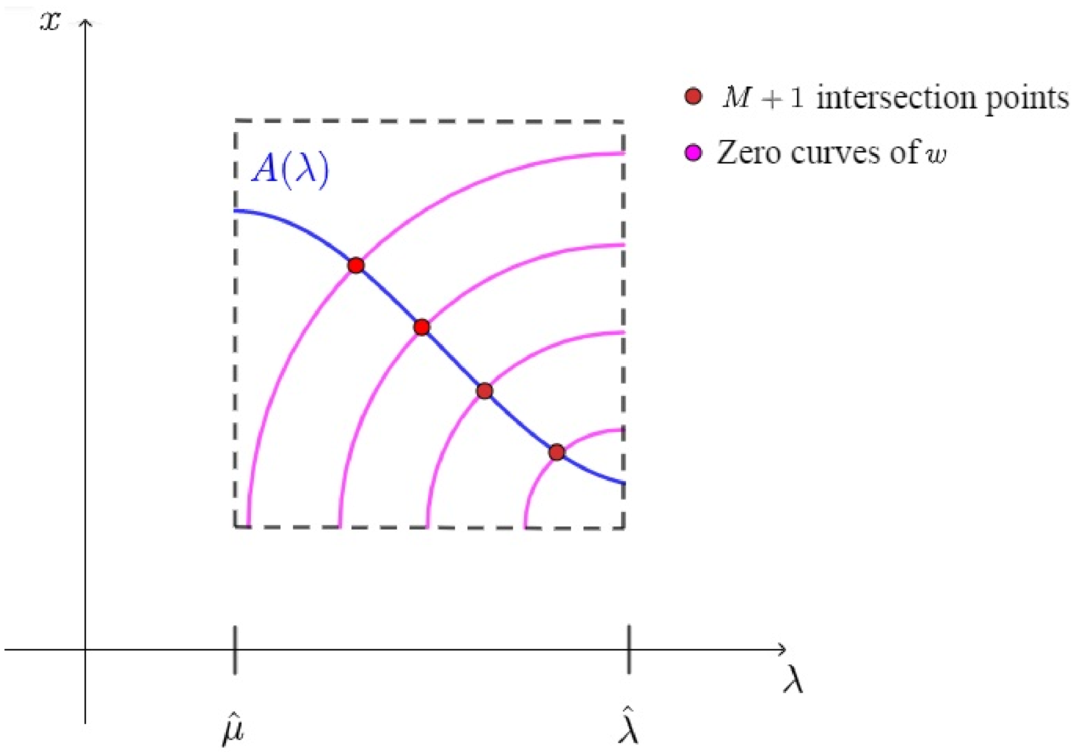

Figure 3.5: The figure illustrates the level curves of zero curves of w crossing with $A(\lambda)$ in at least $M+1$ points.

Since $\tilde{w}$ and w coincide on this interval, $w(\cdot;\lambda)$ has at least $M+1$ zeros on (a,b) for some $\lambda\in[\hat{\mu},\hat{\lambda}]$ and that is a contradiction.

Therefore, we can choose μ_0 such that there are no zeros of w on $A|_{[\mu_0,\nu)}$. Let $\lambda_0 \in (\mu_0, \nu)$ be arbitrary and we will observe the auxiliary equation (3.11) and the segment $\{x_0\} \times [\mu_0, \lambda_0]$ for $x_0 := A(\lambda_0)$, then the zero curves of $\tilde{w}$ (also w) cannot intersect this segment for the choose of μ_0. The eigenvalues in $[\mu_0, \lambda_0]$ are the points where v and w can be "matched" along the segment $\{x_0\} \times [\mu_0, \lambda_0]$, as shown the Figure 3.6.

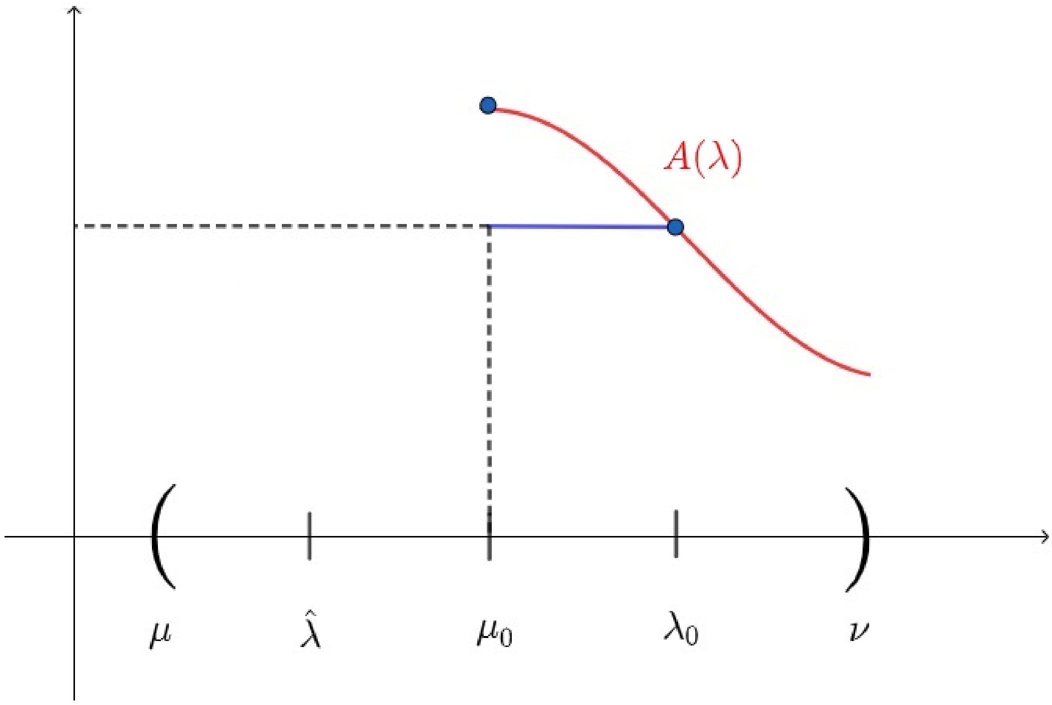

Figure 3.6: The figure illustrates the construction of μ_0, λ_0 and the segment $\{x_0\} \times [\mu_0, \lambda_0]$ (the segment blue) where we can calculated the eigenvalues.

Now, consider an analogous auxiliary equation with coefficients $\tilde{r}$, $\tilde{p}$ defined on $(a,\infty) \times [\mu_0, \lambda_0]$ by $(-\infty, b) \times [\mu_0, \lambda_0]$ defined by

$$\tilde{r}(x;\lambda) := \begin{cases} r(x;\lambda) & a \leq x < x_0 \\ r(x_0;\lambda) & x_0 < x \leq \infty, \end{cases}$$

and

$$\tilde{p}(x;\lambda) := \begin{cases} p(x;\lambda) & a < x \leq x_0 \\ p(x_0;\lambda) - (x - x_0) & x_0 < x < \infty. \end{cases}$$

Similar to the Theorem 3.4.1, the term $-(x-x_0)$ in $\tilde{p}(x;\lambda)$ above is due to the condition (c).

Let $\tilde{v}(\cdot;\lambda)$ be the extension of $v(\cdot;\lambda)$ from $(a,x_0]$ onto (a,∞) as a solution this auxiliary equation. Setting $\alpha(\lambda) = -v'(x_0;\lambda)$ and $\beta(\lambda) = v(x_0;\lambda)$ in the Equation (3.4) and applying the Lemma 3.3.2(i) to the auxiliary equation it follows that there is at most one eigenvalue in $[\mu_0, \lambda_0]$. Since the choose of μ_0 is arbitrary, the non-accumulation at ν is proved by the same argument utilized in the Theorem 3.4.1.

To finish the proof, we will show the non-accumulation of the eigenvalue at μ, and for this we do not need any information about the limit-equation. Let $\mu_0 \in \Lambda$ be fixed and observe that there is a finite bound M for the number of zeros of any nontrivial solution of (SLE)(μ_0) on (a,b). Thus, since (SLE)(λ) $\succeq$ (SLE)(μ_0), due to the Separation's Theorem, we get that a nontrivial solution of (SLE)(λ) has at most $M+1$ zero. Arguing in the same way as the non accumulation at ν above, we obtain that μ is not an accumulation point to the eigenvalues. Since the eigenvalue non accumulation on the interval neither (μ, λ_0) non (λ_0, ν), we get that the has not an accumulation point to the eigenvalues.

The proof for $I = [a,b)$ is a special case of the argument utilized above. We must do the same considerations as the Theorem 3.4.1 (in the end of the proof), but in this case we have that the λ-dependent boundary condition is given (as an interface condition on $\tilde{w}$ along the line x=a) instead of being generated by the family of solutions v.

■

CHAPTER

4 Application to Schrödinger Equation

Emmy Noether[1], in 1918, proved the following theorem [45], [14].

> "Every conservation law is consequence of a particular symmetry in the laws of physics that govern the universe."

Hence, if the potential energy is rotationally invariant (i.e., symmetric to rotations about a point), then it dependent only on the distance r from a center of force, chosen as the coordinate origin, therefore, the orbital angular momentum is conserved. This constant enables us to reduce three-dimensional Schrödinger Equation to an ordinary differential equation, the radial equation.

In this chapter, firstly, we will deduce the Schrödinger Equation like Ervin Schrödinger make and we will give a physical support about the Schrödinger Equation based in [8] [29] [35], and in the end, we will apply the Theorem about the Eigenvalue Accumulation of the previous chapter for this physical application.

4.1 Deduction of The Schrödinger Equation

In this section we will deduce the Schrödinger Equation in the same way that Ervin Schrödinger make in his papers [37], [38].

The beginning of this deduction is the Hamilton-Jacobi Equation. We may obtain it at least two ways. The first is applying a canonical transformation (a change of coordinates where the equation (Lagrange, Hamilton, etc.) are invariants) on the Hamiltonian, where the new Hamiltonian is identically null. This transformation is

$$p \longrightarrow \frac{\partial S}{\partial q} \qquad E \longrightarrow -\frac{\partial S}{\partial t}$$

where obtain

$$H(q,p,t) = E \longrightarrow H(q, \frac{\partial S}{\partial q}, t) = -\frac{\partial S}{\partial t}$$

that is the Hamilton-Jacobi Equation.

[1]NOETHER, Emmy (1882-1935), studied in Gödttingen and Erlangen, becoming associate professor in Göttingen in 1922. After her emigration to the United States in 1933, she obtained a guest professorship at the small college of Bryn Mawr. N. has deeply influenced various branches of algebra by her work. It may be ascribed to her influence that structural theoretical thinking became a dominant principle of modern mathematics. [14]

REM The Hamilton-Jacobi is a formalism to study the motion, like the Hamiltonian H and the Lagrangian L but the equations of motion are the same of the Hamiltonian, just to this transformations.

The function S that appears in Hamilton-Jacobi Equation is known as *action* and given by

$$S = \int dtL. \tag{4.1}$$

This functional is extremely important in the Physics because the minimization of action S implies in the equation of motion (Principle of Least Action). Feynman [11], based on the work of Dirac [10], concluded that the classical trajectory, is nothing more than the function, among all the possible function, that minimize the functional action.

The another way to obtain the Hamilton-Jacobi is due to A. Small and K. S. Lam [39]. Consider the functional action, given by the Equation (4.1). Since the Lagrangian L and the Hamiltonian H are related by the equation

$$p\frac{dq}{dt} - H(p,q,t) = L$$

where p and q are the generalized coordinates and the generalized conjugate momentum, we obtain

$$S = \int_{t_0}^{t} dt \left(p\frac{dq}{dt} - H(p,q,t) \right)$$

and can be rewrite in the form

$$S(q,t) = \int_{q_0}^{q} pdq - \int_{t_0}^{t} Hdt \tag{4.2}$$

where $q_0 = q(t_0)$.

Furthermore, since S is a function of q and p, we may write it as

$$S(q,t) = \int_{q_0}^{q} \frac{\partial S}{\partial q} dq + \int_{t_0}^{t} \frac{\partial S}{\partial t} dt. \tag{4.3}$$

Comparing terms in Equations (4.2) and (4.3), we conclude that

$$p = \frac{\partial S}{\partial q}, \tag{4.4}$$

and

$$\frac{\partial S}{\partial t} = -H(p,q,t). \tag{4.5}$$

Replacing (4.4) into (4.5)

$$H\left(\frac{\partial S}{\partial q}, q, t\right) = -\frac{\partial S}{\partial t} \tag{4.6}$$

where (4.6) is the Hamilton-Jacobi Equation.

Now we will begin the deduction of Schrödinger Equation. In the conservative case (without explicit temporal dependency) the function S is separable in the form

$$S = W - Et$$

where E is the energy of the system. Then, the Hamilton-Jacobi Equation becomes

$$H\left(q, \frac{\partial W}{\partial q}\right) = E. \tag{4.7}$$

Studying analogies between this equation and the wave theory, Schrödinger do the transformation

$$W = K \ln \psi, \tag{4.8}$$

where the constant K must be introduced from consideration of dimensions, being dimension of action.

REM In his paper, Schrödinger not explain the reason for this transformation, but he do as analogy with the entropy's expression in statistic Physics [31] [36] [21].

Consider a non-relativistic particle submitted to Keplerian motion, thus, the Hamiltonian is given by

$$H(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q})$$

where V is the potential.

The choice of coordinates can be arbitrary, then let us take rectangular Cartesian. Thus $\mathbf{q} = \mathbf{r}$ and $\mathbf{r} = x\hat{i} + y\hat{j} + z\hat{k}$. Hence, the Equation (4.7) becomes

$$\frac{1}{2m}\left[\left(\frac{\partial W}{\partial x}\right)^2 + \left(\frac{\partial W}{\partial y}\right)^2 + \left(\frac{\partial W}{\partial z}\right)^2\right] + V(\mathbf{r}) = E$$

and make the substitution (4.8), we obtain

$$R := \left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 + \frac{2m}{K^2}(V(\mathbf{r}) - E)\psi = 0. \tag{4.9}$$

Schrödinger postulate that in Quantum Mechanics, R must be non-null and the integral

$$\iiint dx\, dy\, dz\, R\left(\psi, \frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}, x, y, z\right) \tag{4.10}$$

assume the smallest value. In the Schrödinger words

> We now seek a function ψ, such that for any arbitrary variation of it the integral of the said quadratic form, taken over the whole coordinate space, is stationary, ψ being everywhere real single-valued finite, and continuously differentiable up to the second order. (SCHRÖDINGER,1926).

Thus, the quantum condition are replaced by a variation problem.

The Equation (4.10) is minimized when the following Euler equation for three independent variables [2]

$$\frac{\partial R}{\partial \psi} - \frac{\partial}{\partial x}\frac{\partial R}{\partial \psi_x} - \frac{\partial}{\partial y}\frac{\partial R}{\partial \psi_y} - \frac{\partial}{\partial z}\frac{\partial R}{\partial \psi_z} = 0 \tag{4.11}$$

is satisfied. Therefore, replacing Equation (4.9) into (4.11), we get

$$\frac{-K^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

that is the Famous Schrödinger Equation.

Due to the Balmer Series to the hydrogen atom, we have that the constant K must have the value $h/2\pi$.

As a consequence of choosing $R \neq 0$, we get the concept of trajectory does not exist and the wave function ψ stores all the information about to dynamics of the system.

4.2 Stationary Schrödinger Equation

Consider a particle of mass m moving in a central-force field. The Hamiltonian for this particle is given by

$$H = \frac{\mathbf{P}^2}{2m} + V(r) \tag{4.12}$$

where p is the momentum.

The Schrödinger Equation in the position representation to the Hamiltonian above is given by

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r},t) + V(r)\psi(\mathbf{r},t) \tag{4.13}$$

where ψ is known as wave function.

Since the potential does not depend on the time, we can try to find solutions of this equation of the form

$$\psi(\mathbf{r},t) = \varphi(\mathbf{r})\tau(t). \tag{4.14}$$

Substituting (4.14) into (4.13), we obtain

$$i\hbar\varphi(\mathbf{r})\frac{d\tau(t)}{dt} = -\tau(t)\left[\frac{\hbar^2}{2m}\Delta\varphi(\mathbf{r})\right] + V(r)\tau(t)\varphi(\mathbf{r}). \tag{4.15}$$

Dividing both sides of the Equation (4.15) by $\varphi(\mathbf{r})\tau(t)$.

$$\frac{i\hbar}{\tau(t)}\frac{d\tau(t)}{dt} = -\frac{1}{\varphi}\left[\frac{\hbar^2}{2m}\Delta\varphi(\mathbf{r})\right] + V(r). \tag{4.16}$$

Since the left side of the Equation (4.16) depends only on t, and the right side depends of $\mathbf{r}$, then both the sides must be equal to a constant, which we shall set equal to E, where we will see that this E is the energy of the system. Thus we obtain two ODE's.

$$\begin{cases} i\hbar\dfrac{d\tau(t)}{dt} = E\tau(t), & (4.17) \\ -\dfrac{\hbar^2}{2m}\Delta\varphi(\mathbf{r}) + V(r)\varphi(\mathbf{r}) = E\varphi(\mathbf{r}). & (4.18) \end{cases}$$

Solving the Equation (4.17), we have that the solution of the Schrödinger Equation is

$$\psi(\mathbf{r},t) = \varphi(\mathbf{r})e^{-iEt}$$

called *stationary solution of the Schrödinger Equation* due to time-independent probability density $|\psi(\mathbf{r},t)|^2 = |\varphi(\mathbf{r})|^2$.

Therefore, the interest is in to study the Equation (4.18), that can be written

$$\left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\varphi(\mathbf{r}) = E\varphi(\mathbf{r}). \tag{4.19}$$

Replacing the Equation (4.12) into the Equation (4.19), we obtain

$$H\varphi(\mathbf{r}) = E\varphi(\mathbf{r})$$

Thus, $\varphi(\mathbf{r})$ is an eigenfunction associated to the eigenvalue E.

REM The Equation (4.19) is also known as *time-independent Schrödinger Equation*, as opposed to *time-dependent Schrödinger Equation*, name given to Equation (4.13).

4.3 Schrödinger Equation for Central Force

Consider the same system of the Section 4.2, where a particle of mass m is moving in a central force field. The fundamental importance of this type of Hamiltonian, given by the Equation (4.12), lies in the fact that it is spherically symmetrical.

We saw, by Noither's Theorem, that the orbital angular momentum is conserved. Another way to show this, is to check that $[H,\mathbf{L}] = 0$, and this occurs since $[\mathbf{L},\mathbf{P}^2] = [\mathbf{L},V(r)] = 0$, where $\mathbf{L}$ is the orbital angular momentum operator, given by

$$\mathbf{L} = L_x\hat{\mathbf{x}} + L_y\hat{\mathbf{y}} + L_z\hat{\mathbf{z}}.$$

From the eigenvalue equation of H, in the position representation

$$\left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\varphi(\mathbf{r}) = E\varphi(\mathbf{r}).$$

In spherical coordinates, we can express the Laplacian Δ as

$$\Delta = \frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

and now the eigenfunction $\varphi(\mathbf{r})$ is a function of the variables r,θ,ϕ.

Furthermore, we known the operator $\mathbf{L}^2$ is given by

$$\mathbf{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

Thus, the Equation (4.19) becomes

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{2mr^2}\mathbf{L}^2 + V(r)\right]\varphi(r,\theta,\phi) = E\varphi(r,\theta,\phi). \tag{4.20}$$

Since the operator H, L_z and $\mathbf{L}^2$ all commute with each other, i.e.,

$$[H,L_z] = [H,\mathbf{L}^2] = [L_z,\mathbf{L}^2] = 0$$

we have that the basis of the state space of the particle is composed of eigenfunctions commons to these three observables, i.e., the energy eigenfunctions are also eigenfunctions of L_z and $\mathbf{L}^2$. Thus, the function $\varphi(r,\theta,\phi)$, that is a solution of (4.20) and eigenfunction of $\mathbf{L}^2$ and L_z, must satisfy

$$H\varphi(r,\theta,\phi) = E\varphi(r,\theta,\phi), \tag{4.21a}$$

$$\mathbf{L}^2\varphi(r,\theta,\phi) = l(l+1)\hbar^2\varphi(r,\theta,\phi), \tag{4.21b}$$

$$L_z\varphi(r,\theta,\phi) = \mu\hbar\varphi(r,\theta,\phi). \tag{4.21c}$$

However we already know that the common eigenfunction of $\mathbf{L}^2$ and L_z is the spherical harmonics $Y_l^{\mu}(\theta,\phi)$ that depends only the coordinates θ and ϕ.

Therefore, we may concluded that $\varphi(\mathbf{r})$ is a products of a function of r, that we called $R(r)$, and the spherical harmonics $Y_l^{\mu}(\theta,\phi)$ where l and μ are fixed values because the angular orbital to be conserved. Thus,

$$\varphi(\mathbf{r}) = R(r)Y_l^{\mu}(\theta,\phi)$$

is a solution of the Equation (4.21). Replacing this equation into (4.20) we obtain

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{2mr^2}\mathbf{L}^2 + V(r)\right]R(r)Y_l^{\mu}(\theta,\phi) = ER(r)Y_l^{\mu}(\theta,\phi).$$

From the Equation (4.21b), we have that $\varphi(\mathbf{r})$ is an eigenfunction of $\mathbf{L}^2$ with the eigenvalue $l(l+1)\hbar^2$, then

$$\left[-\frac{\hbar^2}{2mr}\frac{d^2}{dr^2}r + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]R(r) = ER(r). \tag{4.22}$$

REM Our procedure is entirely equivalent to the method of separation of variables [42], [12], [26] in spherical coordinates, however we emphasize the physical meaning of the method.

Introducing another radial wave function by the substitution

$$y(r) = rR(r),$$

we obtain, multiplying both sides of the Equation (4.22) and making this substitution

$$-\frac{\hbar^2}{2m}\frac{d^2y(r)}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]y(r) = Ey(r) \tag{4.23}$$

We can interpret y as a wave function in one dimension for a particle moving in an effective potential

$$V_{eff}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2}.$$

In the case where the potential energy $V(r)$ is not too singular at the origin, then the Equation above shows that there is an angular momentum barrier for all states with $l \neq 0$, as shown in Figure 4.1, which makes it very improbable for a particle to located near the origin.

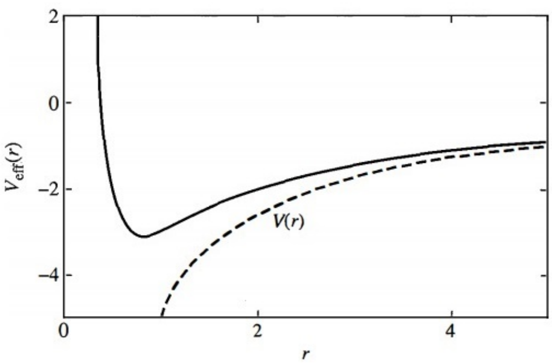

Figure 4.1: The V_{eff} that governs the behavior of the "radial wave function" $y(r)$. [35]

4.4 Accumulation of the Energy

Consider the radial Schrödinger Equation with symmetric potential, given by the Equation (4.23), with the boundary conditions

$$\begin{cases} -\frac{1}{2}y''(r) + \left[\frac{l(l+1)}{2r^2} + V(r) - E\right] y(r) = 0, \\ r \in (0,\infty) \\ y(0) = 0 \end{cases} \tag{4.24}$$

where units have been chosen such that $\hbar^2/m = 1$ and $l \in \mathbb{N}$ is the quantum number for orbital angular momentum.

We assume some conditions about the potential $V(r)$:

- $V(r)$ is continuous on $(0,\infty)$
- $\lim_{r\longrightarrow\infty} \inf V(r) = 0$
- $V(r) \geq \frac{l}{r} - \frac{l(l+1)}{2r^2}$ on $(0,x_0]$ for some constant $l, x_0 > 0$.
- $\lim_{r\longrightarrow\infty} \sup \frac{l(l+1)}{2r^2} + V(r) < \infty$

We consider $E \in (-\infty,0)$ and wish to determine if 0 is an accumulation point of eigenvalue from the left.

REM In this case, $\lambda = E$ is defined to be an eigenvalue if, and only if, there is a nontrivial solution $y \in L^2(0,\infty)$ of (4.24).

Observe that the second hypothesis about $V(r)$ and Lemma 3.2.3 imply hypothesis (D) and the second and third hypothesis on $V(r)$ together with Lemma 3.2.5 ensure (PS). Furthermore, (MC1) obviously holds and since the solutions which satisfy $y(0) = 0$ are just those which are principal at 0, then (MC2) is not verified.

At last, as the term

$$\frac{l(l+1)}{2r^2} + V(r)$$

is bounded, then we have the limit point case at ∞ for each E. By the Lemma 3.2.4, holds that E is an eigenvalue in the sense of the Main Theorem (Theorems 3.4.1 and 3.4.2) and if and only if E is an eigenvalue in the sense defined here.

By the Theorem 3.4.1, the negative eigenvalues of (18) are discrete and bounded in $(-\infty,0)$, and they accumulate at 0 if and only if the limit-equation

$$-\frac{1}{2}y''(r) + \left[\frac{l(l+1)}{2r^2} + V(r)\right] y(r) = 0$$

is oscillatory near $+\infty$.

Consider potentials "behaving like"

$$\boxed{V(r) \propto -cr^{-\gamma} \quad \text{near } \infty,}$$

in another words, suppose $-V(x)r^{\gamma} \longrightarrow c$ as $r \longrightarrow \infty$ for some constants $c, \gamma > 0$. Applying Hille-Kneaser Oscillation Criteria give:

$$\boxed{\begin{array}{l} \left.\begin{array}{c}\gamma < 2 \\ \text{or} \\ \gamma = 2,\ c > 1/8 + \dfrac{l(l+1)}{2}\end{array}\right\} \Longrightarrow \text{accumulation at } 0 \\ \\ \left.\begin{array}{c}\gamma > 2 \\ \text{or} \\ \gamma = 2,\ c < 1/8 + \dfrac{l(l+1)}{2}\end{array}\right\} \Longrightarrow \text{no accumulation at } 0 \end{array}} \tag{4.25}$$

We can check our result in the physics, on the particular case where $\gamma = 1$. In this situation we obtain the Hydrogen atom problem, where consider the potential being the Coulomb potential. The energy of this system is given by

$$E_n = -\frac{13,6}{n^2}, \qquad n \in \mathbb{N}^* \tag{4.26}$$

Thus, we can see through the Equation (4.26) that 0 is an accumulation point.

Another point to emphasize is that physically, our result is coherent. In the case where $\gamma < 2$ we have that the term $\dfrac{l(l+1)}{2r^2}$ is more dominant than the potential V, i.e., near infinitely, $\dfrac{l(l+1)}{2r^2} > V$. Thus, the effective potential behaves like the Figure 4.2.

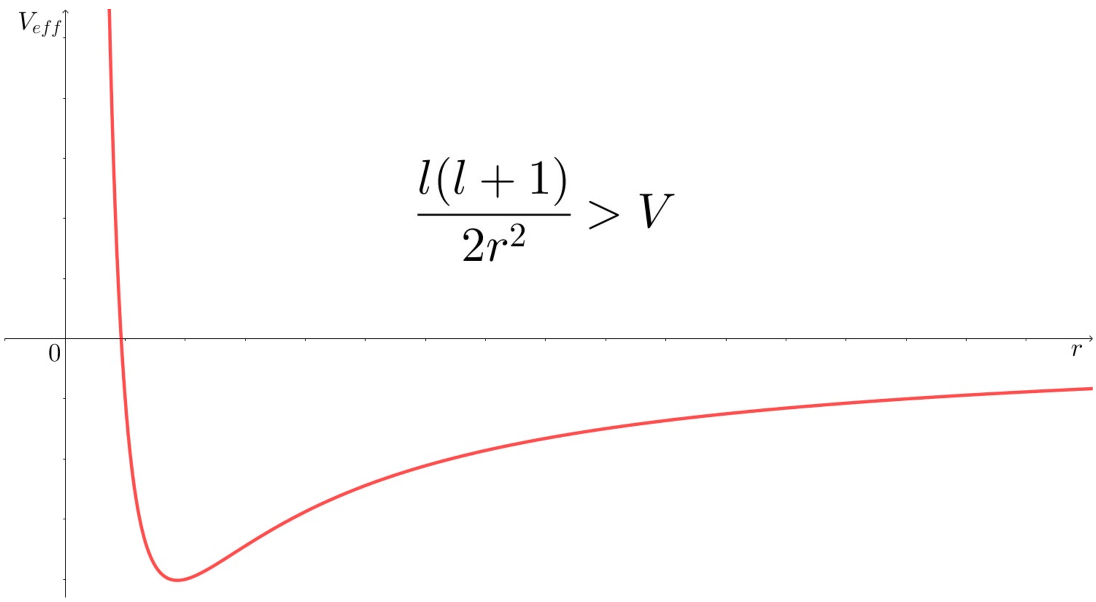

Figure 4.2: The figure illustrates the solution of 4.24 in the case where $\dfrac{l(l+1)}{2r^2} > V$.

Hence, we have discrete eigenvalue which accumulate in 0. For energy above of the value 0, the spectrum is continuous.

Furthermore, in the case $\gamma > 2$ we have $\dfrac{l(l+1)}{2r^2} < V$ near infinity, the potential V is dominant. The effective potential behaves like the Figure 4.3.

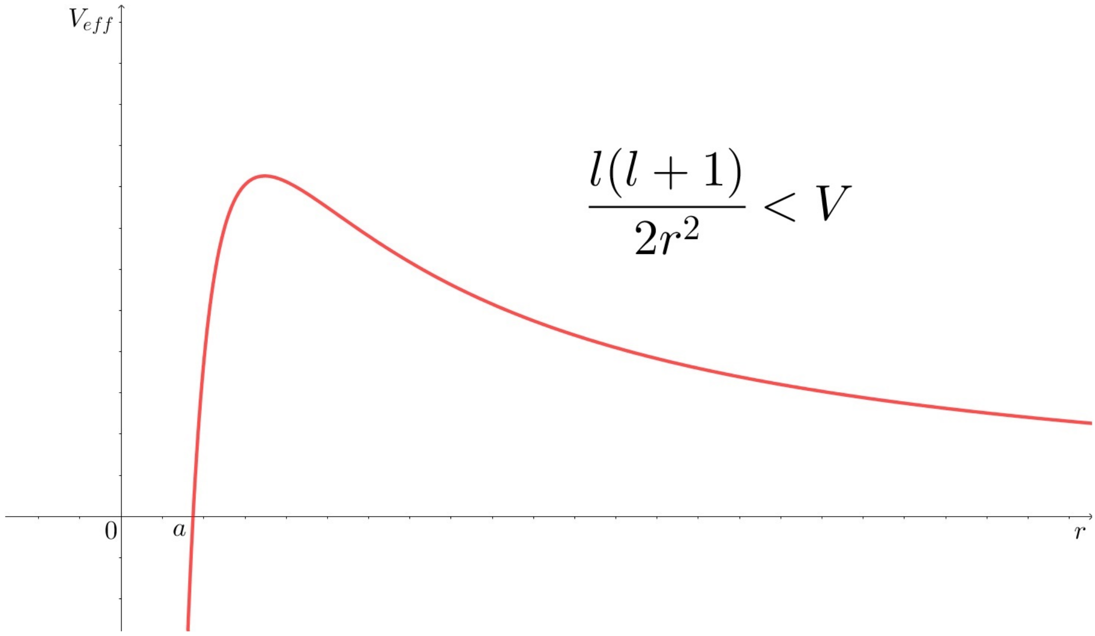

Figure 4.3: The figure illustrates the solution of 4.24 in the case where $\frac{l(l+1)}{2r^2} < V$.

We may even have discrete eigenvalue on the interval $(0,a)$, however, when the energy is "high", occurs the phenomenon called *tunneling*. In addition, when we have "lower" energy the electron go to collide with the nucleus, and this case the atom not is stable. Thus, the energy not accumulate.

APPENDIX A

Hille-Kneaser Oscillation Criteria

In the Main Theorem of this Undergraduate Thesis, we need the hypothesis of the equation being oscillatory. In this section, we will provide some criteria of oscillation which will utilize in our application, see [43].

Theorem A.0.1 — Hille-Kneaser Criteria. Let

$$\omega^* = \lim_{x\longrightarrow\infty} \sup x^2 c(x), \qquad \omega_* = \lim_{x\longrightarrow\infty} \inf x^2 c(x).$$

where c is a real-valued continuous function. Then, the equation

$$u'' + c(x)u = 0 \tag{A.1}$$

is:

- Nonoscillatory if $\omega^* < \dfrac{1}{4}$.
- Oscillatory if $\omega_* > \dfrac{1}{4}$.
- No information about the oscillation if either ω_* or ω^* is equal to $1/4$.

Proof. In the case where $\omega^* < \dfrac{1}{4}$, there exists a number $\gamma < 1/4$ and a number $x_0 > 0$ such that $c(x) - \gamma x^{-2} < 0$ for $x \geq x_0$. Suppose that the solution of (A.1) had arbitrary large zeros, then, by the Sturm's Comparison Theorem, every solution of the Euler equation $v'' + \gamma x^{-2} v = 0$ would have arbitrarily large zero for $\gamma < 1/4$. However, we know that the Euler Equation is nonoscillatory for $\gamma > 1/4$. Hence, the contradiction show that (A.1) is nonoscillatory.

Now, when $\omega_* > \dfrac{1}{4}$, the idea of the proof is analogous to the first case.

Finally, to prove the last statement of theorem, consider the equation (A.1) with

$$c(x) = \frac{1}{4x^2} + \frac{\delta}{(x\log x)^2},$$

where we have as general solution

$$u(x) = x^{1/2}\left[k_1(\log x)^{\xi} + k_2(\log x)^{(1-\xi)}\right]$$

where, we choose

$$\xi = \frac{1 \pm \sqrt{1-4\delta}}{2}$$

for the Equation (A.1) to be satisfied. Notice that,

- if $\delta \leq 1/4$ then $\xi \in \mathbb{R}_+$ and we got $u(x)$ is nonoscillatory because $(\log x)^{\xi} \longrightarrow +\infty$ and $(\log x)^{1-\xi} \longrightarrow +\infty$ as $x \longrightarrow \infty$.
- if $\delta > 1/4$ then $\xi = \alpha + \beta i$ and

$$(\log x)^{\beta i} = \left(e^{\log x}\right)^{\beta i} = \cos(\beta \log x) + i \sin(\beta \log x).$$

  Thus, the solutions are oscillatory.

■

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