PSEUDOSPECTRAL METHODS FOR DIFFERENTIAL EQUATIONS: APPLICATION TO THE SCHRÖDINGER TYPE EIGENVALUE PROBLEMS

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PSEUDOSPECTRAL METHODS FOR DIFFERENTIAL EQUATIONS: APPLICATION TO THE SCHRÖDINGER TYPE EIGENVALUE PROBLEMS

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This is to certify that we have read this thesis and that in our opinion it is fully adequate, in scope and quality, as a thesis for the degree of Master of Science.

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ABSTRACT

PSEUDOSPECTRAL METHODS FOR DIFFERENTIAL EQUATIONS: APPLICATION TO THE SCHRÖDINGER TYPE EIGENVALUE PROBLEMS

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In this thesis, a survey on pseudospectral methods for differential equations is presented. Properties of the classical orthogonal polynomials required in this context are reviewed. Differentiation matrices corresponding to Jacobi, Laguerre, and Hermite cases are constructed. A fairly detailed investigation is made for the Hermite spectral methods, which is applied to the Schrödinger eigenvalue equation with several potentials. A discussion of the numerical results and comparison with other methods are then introduced to deduce the efficiency of the method.

Keywords: Pseudospectral (collocation) Methods, Differentiation Matrices, Hermite Spectral Methods, Schrödinger Equation, Quantum Mechanical Potentials With Single and Multiminima.

ÖZ

DİFERANSİYEL DENKLEMLERDE SANKİ-SPEKTRAL YÖNTEMLER: SCHRÖDİNGER TİPİ ÖZDEĞER PROBLEMLERİNE UYGULAMA

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Bu tezde, diferansiyel denklemlerde sanki-spektral yöntemlerle ilgili bir çalışma sunulmuştur. Klasik ortogonal polinomların, bu yöntemler için gerekli özelliklerine değinilerek, Jacobi, Laguerre ve Hermite polinom sınıflarının kullanıldığı durumlara karşıgelen türevlendirme matrisleri oluşturulmuştur. Hermite spektral yöntemi derinlemesine incelenerek farklı potansiyeller altında Schrödinger özdeğer denklemine uygulanmıştır. Yöntemin duyarlılığını görmek için, diğer yöntemlerle karşılaştırmalar yapılarak sayısal sonuçlar detaylı olarak tartışılmıştır.

Anahtar Kelimeler: Sanki-spektral Yöntemler, Türevlendirme Matrisleri, Hermite Spektral Yöntemleri, Schrödinger Denklemi, Tek ve Çok kuyulu Kuantum Mekaniksel Potansiyeller.

To my family

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

Education in mathematical principals and methods typically starts with discrete systems and progresses toward continuous systems. For example, a childs initial exposure to real numbers deals exlusively with integers (and at first, only positive integers). This then develops study of fractions, decimals, and finally irrational numbers. Thus understanding of real numbers begins with a few locations on the real number axis and proceeds to include all points on the axis. In learning about calculation of the slope of a curve in (x, y) space, students initially consider straight lines for which the slope is given by the discrete expression $\Delta y/\Delta x$. Understanding of the concept of slope is completed when one is able to calculate the slope of any point on an arbitrary curve using the continuous expression $\mathrm{d}y/\mathrm{d}x$. When studying science or engineering, mathematical models for physical processes are presented in terms of algebraic expressions (e.g. $F = ma$) before they are seen in terms of differential equations [e.g. $F = \mathrm{d}(mv)/\mathrm{d}t$].

The study of numerical methods for the solution of differential equations is complex , in part , because it runs counter to the usual pattern of moving from the discrete to the continuous. Numerical methods, in brief, replace a differential description of a physical process or system with an approximate discrete analog and then solve this analog to represent the solution of the differential system. The analog should approximate the differential equation with a known and tolerable degree of accuracy.

A fundamental principle of numerical methods in the reduction of a differential equation to an approximation in terms of algebraic equations. This reduction replace a continuous differential equation, whose solution space is generally infinite dimensional, with a finite set of algebraic equations whose solution space is finite dimensional. One avenue by which this reduction can be achieved is the

finite difference method.

In broad outline form, the finite difference method proceeds by first identifying a finite number of discrete points with in the domain of interest. These points are called nodes, and it is at these locations that approximations to the true solution are computed. Definition of the node locations is called the discretization step. Next the derivatives that appear in the differential equation are replaced by discrete difference approximations. These approximations are written in terms of nodal equations of the unknown function. This step, called the approximation step, produces a set of algebraic equations with described nodal values as unknowns. If the original differential operator is linear, the resulting algebraic system is also linear; otherwise the algebraic equations may be nonlinear. The final step follows the approximation step and involves solution of the resulting algebraic system of equations. Up on completion of this step, a discrete approximation to the solution of the original differential equation is obtained.

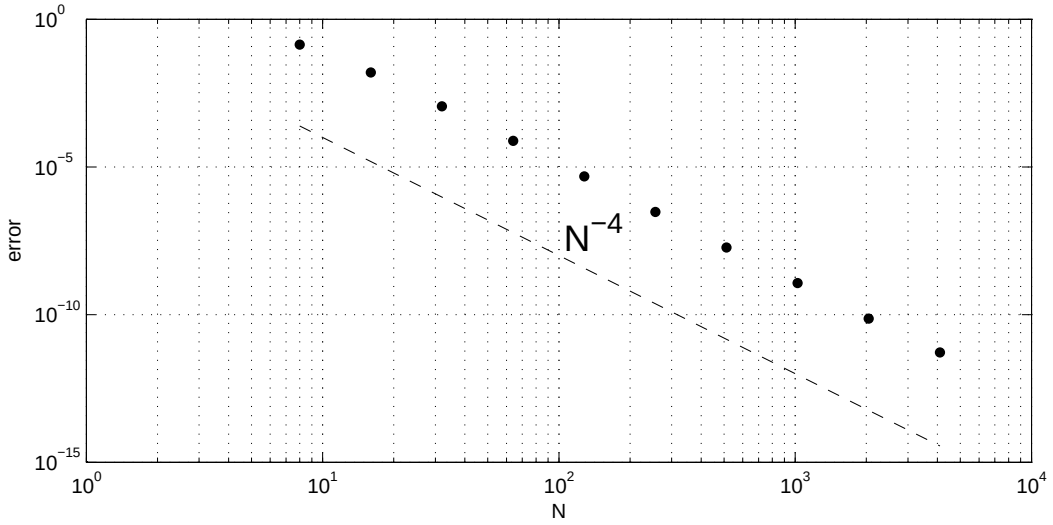

Figure 1.1: Convergence of Fourth-Order Finite Differences

Although finite difference approximation generate derivative matrices with quite good structure (i.e. they are banded with a normal bandwidth), the results are in general very poor when compared to those obtained by spectral methods.

As an illustration the function $u(x) = e^{\sin x}$ is taken to give periodic data

on $[-\pi, \pi]$ and the fourth order finite difference approximation compared with the exact derivative $u'(x_j) = \cos(x_j)e^{\sin(x_j)}$, for various values of N. The results are presented in figure (1.1), which plots the maximum error on the grid against N.[56] The fourth order accuracy is apperent.

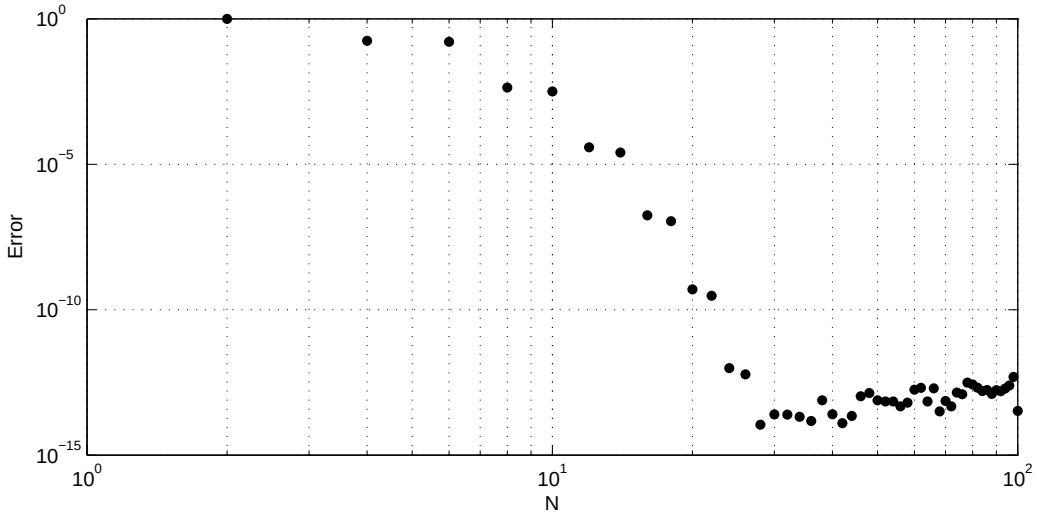

Figure 1.2: Convergence of Spectral Method

In spectral methods, for a periodic domain, the natural choice is a trigonometric polynomial on an equispaced grid. (For nonperiodic domains, algebraic polynomials on irregular grids are the right choice, which will be our concern in later chapters). Spectral approximation compared with the exact derivatives on the grid. Figure (1.2) shows the maximum error against N. The errors in figure (1.2) decrease very rapidly. This remarkable behaviour is called spectral accuracy. As N increases, the error in a finite difference scheme typically decreases like $O(N^{-m})$ for some constant m that depens on the order of approximation and the smoothness of the solution. For a spectral method, convergence at the rate $O(N^{-m})$ for every m is achieved, provided the solution is infinitely differentiable, and even faster convergence at a rate $O(c^N)$, $0 < c < 1$ is achieved if the solution is suitably analytic. The reason for this difference is that finite differences are local methods. To compute the derivative at a given point, these methods use information pertainig to a small neighbourhood of the point. In contrast, spec-

tral methods are global methods. All N points in the domain are applied in the computation.

If one wants to solve differential equations to high accuracy on a single domain and if the data defining the problem are smooth, then spectral methods are usually the best tool. They can often achieve ten digits of accuracy where a finite difference methods get two or three. At lower accuracies, they demand less computer memory then the alternatives.

The organization of the thesis is as follows: In chapter 2, we examine the properties of classical orthogonal polynomials. Chapter 3 deals with the properties of specral methods, especially spectral collocation method. Chapter 4 focuses on the Hermite spectral methods. Chapter 5 contains the application of the Hermite spectral methods to the Schrödinger type eigenvalue problem and numerical results, and in chapter 6 we discuss the numerical results of the method.

CHAPTER 2

A REVIEW OF CLASSICAL ORTHOGONAL POLYNOMIALS

Approximating functions in spectral methods are closely related to polynomial solutions of eigenvalue problems in ordinary differential equations, known as hypergeometric differntial equations. Both basic and remarkable properties of the most commonly used families of polynomials of this kind will be outlined.

2.1 Hypergeometric Differential Equations

Definition 2.1.1. The equation

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0 \tag{2.1.1}$$

where $\sigma(x)$ is a polynomial of degree at most two, $\tau(x)$ is a polynomial of degree at most one, and λ is a constant, is referred to as a differential equation of the hypergeometric type. This equation can be written in the self adjoint form

$$\big[\sigma(x)\rho(x)y'\big]' + \lambda\rho(x)y = 0 \tag{2.1.2}$$

where ρ is a function satisfying

$$\big[\rho(x)\sigma(x)\big]' = \tau(x)\rho(x). \tag{2.1.3}$$

Now let us examine the properties of solutions of (2.1.1).

Theorem 2.1.2. *All derivatives of the functions of the hypergeometric type are also functions of the hypergeometric type.*

Proof. Differentiating (2.1.1) with respect to x, we get

$$\sigma(x)y''' + \big[\sigma'(x) + \tau(x)\big]y'' + (\tau' + \lambda)y' = 0.$$

Letting $v_1 = y'$ we have

$$\sigma(x)v_1'' + \tau_1(x)v_1' + \mu_1 v_1 = 0 \tag{2.1.4}$$

where $\tau_1(x) = \sigma'(x) + \tau(x)$ is a polynomial of degree at most one, and $\mu_1 = \tau' + \lambda$ is a constant. Clearly (2.1.4) is a differential equation of the hypergeometric type in v_1, and, hence in y'. By mathematical induction, it is possible to show that an equation of the hypergeometric type for $v_n(x) = y^{(n)}(x)$,

$$\sigma(x)v_n'' + \tau_n(x)v_n' + \mu_n v_n = 0 \ , \ v_0 = y \tag{2.1.5}$$

can be obtained in which

$$\tau_n(x) = \sigma'(x) + \tau_{n-1}(x) = n\ \sigma'(x) + \tau(x) \ , \ \tau_0(x) := \tau(x) \tag{2.1.6}$$

$$\mu_n = \mu_{n-1} + \tau_{n-1}' = \lambda + n\ \tau' + \tfrac{1}{2}n(n-1)\sigma'' \ , \ \mu_0 := \lambda \tag{2.1.7}$$

for all $n = 1, 2, ...$ Notice that τ_n is linear and μ_n is constant as required. □

Theorem 2.1.3. *The differential equation (2.1.1) has polynomial solutions $p_n(x)$ of degree n for particular values of λ such that*

$$\lambda = \lambda_n = -n\ \tau' - \tfrac{1}{2}n(n-1)\sigma''$$

Proof. Obviously (2.1.5) has a constant solution $v_n = C_0$ if $\mu_n = 0$. That is, since $v_n(x) = {y_n}^{(n)}(x) = C_0$, the function $y(x)$ should be a polynomial of degree n, say $y(x) = p_n(x)$. Actually, integrating $v_n(x) = y^{(n)}(x) := p_n^{(n)}(x) = C_0$

successively, we have

$$\begin{aligned} p_n^{(n-1)}(x) &= C_0 x + C_1 \\ p_n^{(n-2)}(x) &= C_0 \frac{x^2}{2} + C_1 x + C_2 \\ \vdots & \quad \vdots \\ p_n(x) &= a_0 x^n + a_1 x^{n-1} + \cdots + a_{n-1} x + a_n \end{aligned}$$

which is clearly a polynomial in x of degree n. On the other hand, from (2.1.7), $\mu_n = 0$ implies that

$$\lambda + n\,\tau' + \tfrac{1}{2} n(n-1)\sigma'' = 0$$

which completes the proof. □

The coefficients a_j of the polynomial solution $p_n(x)$ in theorem (2.1.3) should be determined for an explicit determination of $p_n(x)$. To this end, let us consider the self adjoint forms of the hypergeometric differential equations (2.1.1) and (2.1.5),

$$\Big[\sigma(x)\,\rho(x)\,y'(x)\Big]' + \lambda\,\rho(x)\,y(x) = 0, \tag{2.1.8}$$

$$\Big[\sigma(x)\,\rho_n(x)\,{v_n}'(x)\Big]' + \mu_n\,\rho_n(x)\,v_n(x) = 0, \tag{2.1.9}$$

where

$$\Big[\sigma(x)\,\rho(x)\Big]' = \tau(x)\,\rho(x), \tag{2.1.10}$$

$$\Big[\sigma(x)\,\rho_n(x)\Big]' = \tau_n(x)\,\rho_n(x). \tag{2.1.11}$$

Note that, the equation (2.1.10) allows us to compute the explicit form of the function $\rho(x)$. Actually, integrating (2.1.10)we get

$$\rho(x) = e^{\int \frac{\tau(x)-\sigma'(x)}{\sigma(x)}\mathrm{d}x}. \tag{2.1.12}$$

In fact, there is a connection between $\rho_n(x)$ and $\rho(x) := \rho_0(x)$. From (2.1.11) we

have

$$\frac{\big[\sigma(x)\rho_n(x)\big]'}{\rho_n(x)} = \tau_n(x) = n\sigma'(x) + \tau(x)$$

which is written as

$$\frac{\big[\sigma(x)\rho_n(x)\big]'}{\rho_n(x)} = n\ \sigma'(x) + \frac{\big[\sigma(x)\rho(x)\big]'}{\rho(x)}$$

on using (2.1.10) for $\tau(x)$. The last equation is equivalent to

$$\frac{\rho_n'(x)}{\rho_n(x)} = n\ \frac{\sigma'(x)}{\sigma(x)} + \frac{\rho'(x)}{\rho(x)}$$

upon integration of which gives $\rho_n(x) = \sigma^n(x)\rho(x)$. We then see that

$$\sigma(x)\rho_n(x) = \sigma^{n+1}(x)\rho(x) = \rho_{n+1}(x). \tag{2.1.13}$$

Since $v_n'(x) = v_{n+1}(x)$ equation (2.1.9) can be written as

$$\Big[\rho_{n+1}(x)v_{n+1}(x)\Big]' + \mu_n(x)\rho_n(x)v_n(x) = 0 \tag{2.1.14}$$

so that

$$\rho_n(x)v_n(x) = -\frac{1}{\mu_n}\Big[\rho_{n+1}(x)v_{n+1}(x)\Big]'. \tag{2.1.15}$$

Therefore, for $m < n$ we obtain successively

$$\begin{aligned}
\rho_m v_m &= -\frac{1}{\mu_m}(\rho_{m+1}v_{m+1})' \\
&= -\frac{1}{\mu_m}\Big(-\frac{1}{\mu_{m+1}}\Big)(\rho_{m+2}v_{m+2})'' = (-1)^2\frac{1}{\mu_m\mu_{m+1}}(\rho_{m+2}v_{m+2})''
\end{aligned}$$

and, finally,

$$\rho_m v_m = (-1)^n\frac{1}{\mu_m\mu_{m+1}\cdots\mu_{m+n-1}}(\rho_{m+n}v_{m+n})^{(n)}.$$

Replacing n by $n-m$, we find that

$$\begin{aligned}\rho_m(x)v_m(x) &= (-1)^{n-m}\frac{1}{\mu_m\mu_{m+1}\dots\mu_{n-1}}\Big[\rho_n(x)v_n(x)\Big]^{(n-m)} \\ &= \frac{(-1)^m\mu_0\mu_1\dots\mu_{m-1}}{(-1)^n\mu_0\mu_1\dots\mu_{m-1}\mu_m\dots\mu_{n-1}}\Big[\rho_n(x)v_n(x)\Big]^{(n-m)}\end{aligned}$$

which gives

$$\rho_m v_m = \frac{\mathcal{A}_m}{\mathcal{A}_n}\,\frac{\mathrm{d}^{n-m}}{\mathrm{d}x^{n-m}}\,(\rho_n v_n) \tag{2.1.16}$$

where

$$\mathcal{A}_j(\lambda) = (-1)^j\prod_{k=0}^{j-1}\mu_k(\lambda)\ ,\ \mathcal{A}_0 = 1. \tag{2.1.17}$$

For polynomial solutions, $\lambda = \lambda_n$ and hence, we define from (2.1.17) a two dimensional array of constants

$$\mathcal{A}_{mn} := \mathcal{A}_m(\lambda_n),\quad \mathcal{A}_{0n} = 1.$$

Since, in this case, $v_n(x) = C_0$, the equation (2.1.16) takes the form

$$v_m(x) = p_n^{(m)}(x) = B_n\frac{\mathcal{A}_{mn}}{\rho_m(x)}\,\frac{\mathrm{d}^{n-m}}{\mathrm{d}x^{n-m}}\,\rho_n(x) \tag{2.1.18}$$

where $B_n = \dfrac{C_0}{\mathcal{A}_n(\lambda_n)} = \dfrac{p_n^{(n)}(x)}{\mathcal{A}_{nn}}$ is a constant. In particular, when $m = 0$ we derive an explicit represantation of polynomials of the hypergeometric type, i.e.

$$p_n(x) = B_n\frac{1}{\rho(x)}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\,\Big[\sigma^n(x)\rho(x)\Big] \tag{2.1.19}$$

for $n = 0, 1, \dots$. Here B_n may be regarded as a normalization constant and specified for historical reasons. The celebrated formula in (2.1.19) is known as the Rodriguez formula. Note that the constant $\mathcal{A}_{mn} = \mathcal{A}_m(\lambda_n)$ may be written

as

$$\mathcal{A}_{mn} = \frac{n!}{(n-m)!} \prod_{k=0}^{m-1} \left[\tau' + \tfrac{1}{2}\,(n+k-1)\sigma''\right] \tag{2.1.20}$$

by processing on $\mu_k(\lambda_n)$ in (2.1.17) [53]. Now we can obtain further properties of the polynomial solutions $p_n(x)$ of (2.1.1).

Theorem 2.1.4. *Let the coefficients in (2.1.1) be such that*

$$\sigma(x)\rho(x)x^k\Big|_{x=a,b} = 0 \quad for \quad k = 0, 1, \ldots \tag{2.1.21}$$

at the boundaries of x-interval (a, b). Then the polynomials of the hypergeometric type, which constitute a sequence $\{p_0(x), p_1(x), \ldots, p_m(x) \ldots, p_n(x), \ldots\}$ of real functions of the real argument x, corresponding to the different values of $\lambda = \lambda_n$, i.e. $\lambda_0, \lambda_1, \ldots, \lambda_m, \ldots, \lambda_n, \ldots$ are orthogonal on (a, b) in the sense that

$$\int_a^b \rho(x)p_m(x)p_n(x)\mathrm{d}x = 0 \tag{2.1.22}$$

for $m \neq n$, where $\rho(x)$ is now called the weighting function.

Proof. The elements $p_n(x)$ and $p_m(x)$ of the sequence satisfy the differential equations

$$\left[\sigma(x)\rho(x)p_n'(x)\right]' + \lambda_n\rho(x)p_n(x) = 0$$

and

$$\left[\sigma(x)\rho(x)p_m'(x)\right]' + \lambda_m\rho(x)p_m(x) = 0$$

respectively. Multiplying the first by p_m and the second by p_n and subtracting we get

$$p_m(x)\left[\sigma(x)\rho(x)p_n'(x)\right]' - p_n(x)\left[\sigma(x)\rho(x)p_m'(x)\right]' = (\lambda_m - \lambda_n)\rho(x)p_m(x)p_n(x) \tag{2.1.23}$$

which is equal to

$$\left[\sigma(x)\rho(x)\right]'\left[p_m(x)p_n'(x) - p_m'(x)p_n(x)\right] + \left[\sigma(x)\rho(x)\right]\left[p_m(x)p_n''(x) - p_m''(x)p_n(x)\right] = (\lambda_m - \lambda_n)\rho(x)p_m(x)p_n(x)$$

on rearranging the left hand side. A careful inspection shows that it can be written in a more compact form

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big[\sigma(x)\rho(x)W(p_m,p_n)(x)\Big] = (\lambda_m-\lambda_n)\rho(x)p_m(x)p_n(x)$$

where $W(p_m,p_n)(x) = p_m(x)p_n'(x) - p_m'(x)p_n(x)$ is the Wronsky determinant of the solutions $p_m(x)$ and $p_n(x)$. Now, integrating both sides from a to b we obtain

$$(\lambda_m-\lambda_n)\int_a^b \rho(x)p_m(x)p_n(x)\mathrm{d}x = \sigma(x)\rho(x)W(p_m,p_n)(x)\big|_{x=a,b}$$

whose right hand side is equal to zero by hypothesis. Hence, for $m \neq n$, $(\lambda_m \neq \lambda_n)$ we must have $\int_a^b \rho(x)p_m(x)p_n(x)\mathrm{d}x = 0$. More specifically, we may write

$$\int_a^b \rho(x)p_m(x)p_n(x)\mathrm{d}x = \mathcal{N}_n^2\delta_{mn} \tag{2.1.24}$$

where $\mathcal{N}_n$ is a normalization constant which is positive and δ_{mn} is Kronecker delta. □

Any polynomial $q_m(x)$ of degree m can be written as a combination of orthogonal polynomials $p_0(x), p_1(x), \ldots, p_m(x)$ of the form

$$q_m(x) = \sum_{k=0}^{m} c_{km}p_k(x).$$

To determine the combination constants, let us use the orthogonality

$$\begin{aligned}\int_a^b \rho(x)q_m(x)p_j(x)\mathrm{d}x &= \sum_{k=0}^{m} c_{km}\int_a^b \rho(x)p_k(x)p_j(x)\mathrm{d}x \\ &= c_{jm}\mathcal{N}_j^2\end{aligned}$$

from which

$$c_{km} = \frac{1}{\mathcal{N}_k^2}\int_a^b \rho(x)q_m(x)p_k(x)\mathrm{d}x, \quad k=0,1,\ldots,m. \tag{2.1.25}$$

Now, letting $q_m(x) = x^m$ with $m < n$, we have

$$x^m = \sum_{k=0}^{m} c_{km} p_k(x)$$

and

$$\int_a^b \rho(x) x^m p_n(x) \mathrm{d}x = \sum_{k=0}^{m} c_{km} \int_a^b \rho(x) p_k(x) p_n(x) \mathrm{d}x = 0.$$

since k is never equal to n. That is, the orthogonality condition (2.1.24) is equivalent to

$$\int_a^b \rho(x) x^m p_n(x) \mathrm{d}x = 0 \quad \text{if} \quad m < n,$$

which means that $p_n(x)$ is orthogonal to every polynomial of lower degree.

Theorem 2.1.5. *The following relation holds for any three consecutive orthogonal polynomials:*

$$x p_n(x) = \alpha_n p_{n+1}(x) + \beta_n p_n(x) + \gamma_n p_{n-1}(x), \quad n = 1, 2, ... \tag{2.1.26}$$

where

$$\alpha_n = \frac{a_n}{a_{n+1}}, \quad \beta_n = \frac{b_n}{a_n} - \frac{b_{n+1}}{a_{n+1}}, \quad \gamma_n = \frac{\mathcal{N}_n^2}{\mathcal{N}_{n-1}^2} \frac{a_{n-1}}{a_n}$$

and

$$p_n(x) = a_n x^n + b_n x^{n-1} + ... \ . \tag{2.1.27}$$

Proof. If we use the expansion

$$x p_n(x) = \sum_{k=0}^{n+1} c_{kn} p_k(x)$$

then by (2.1.25), we write

$$c_{kn} = \frac{1}{\mathcal{N}_n^2} \int_a^b \rho(x) p_k(x) x p_n(x) \mathrm{d}x. \tag{2.1.28}$$

However, since $x p_k(x)$ is a polynomial of degree $k+1$ we must have $c_{kn} = 0$ when

$k+1<n$. Hence, from (2.1.26), we write

$$xp_n(x) = c_{n-1,n}p_{n-1}(x) + c_{n,n}p_n(x) + c_{n+1,n}p_{n+1}(x)$$

which is nothing but the relation in (2.1.26) with

$$c_{n-1,n} = \gamma_n, \quad c_{n,n} = \beta_n, \quad c_{n+1,n} = \alpha_n.$$

To construct the relation we have to find the constants $\alpha_n, \beta_n, \gamma_n$. To this end, note that the integral in (2.1.28) is unchanged when the indices k and n are interchanged. It follows then that $\mathcal{N}_k^2 c_{kn} = \mathcal{N}_n^2 c_{nk}$. Putting $k = n-1$ we get $\mathcal{N}_{n-1}^2 c_{n-1,n} = \mathcal{N}_n^2 c_{n,n-1}$ which implies $\mathcal{N}_{n-1}^2 \gamma_n = \mathcal{N}_n^2 \alpha_{n-1}$ and finally obtain

$$\gamma_n = \frac{\mathcal{N}_n^2}{\mathcal{N}_{n-1}^2}\alpha_{n-1}. \tag{2.1.29}$$

On the other hand, since $p_n(x) = a_n x^n + b_n x^{n-1} + ...$, the equation in (2.1.26) leads to $a_n x^{n+1} + b_n x^n + ... = \alpha_n a_{n+1} x^{n+1} + (\alpha_n b_{n+1} + \beta_n a_n)x^n$ from which we get

$$\alpha_n = \frac{a_n}{a_{n+1}}, \tag{2.1.30}$$

$$\beta_n = \frac{b_n}{a_n} - \frac{b_{n+1}}{a_{n+1}}. \tag{2.1.31}$$

Therefore, (2.1.29) now reads as

$$\gamma_n = \frac{a_{n-1}}{a_n}\frac{\mathcal{N}_n^2}{\mathcal{N}_{n-1}^2}. \tag{2.1.32}$$

□

As is shown, if we know the coefficients a_n and b_n of leading order terms of $p_n(x)$ and the squared norm $\mathcal{N}_n^2$, then the orthogonal polynomials can be determined recursively from (2.1.26). To determine the coefficients a_n and b_n of highest order terms let us differentiate (2.1.27) with respect to x k times.

$$p_n^{(k)}(x) = \frac{n!}{(n-k)!}a_n x^{n-k} + \frac{(n-1)!}{(n-k-1)!}b_n x^{n-k-1} + ...$$

letting $k = n - 1$ in this equation, we have

$$p_n^{(n-1)}(x) = n! a_n x + (n-1)! b_n. \tag{2.1.33}$$

From (2.1.17), for $k = n - 1$,

$$p_n^{(n-1)}(x) = \frac{\mathcal{A}_{n-1,n} B_n}{\sigma^{n-1}(x)\rho(x)} \frac{\mathrm{d}}{\mathrm{d}x}\Big[\sigma^n(x)\rho(x)\Big]$$

or

$$p_n^{(n-1)}(x) = \mathcal{A}_{n-1,n} B_n \left[n\sigma'(x) + \sigma(x)\frac{\rho'(x)}{\rho(x)} \right].$$

Now, using (2.1.3) we write

$$p_n^{(n-1)}(x) = \mathcal{A}_{n-1,n} B_n \Big[(n-1)\sigma'(x) + \tau(x) \Big]. \tag{2.1.34}$$

On the other hand, expanding $\sigma(x)$ and $\tau(x)$ in a Taylor series about zero we get

$$\sigma(x) = \sigma(0) + \sigma'(0)x + \frac{\sigma''}{2}x^2, \tag{2.1.35}$$

$$\tau(x) = \tau(0) + \tau' x. \tag{2.1.36}$$

Plugging these series representations of $\sigma(x)$ and $\tau(x)$ into (2.1.34) yields

$$p_n^{(n-1)}(x) = \mathcal{A}_{n-1,n} B_n \Big\{ \big[(n-1)\sigma'' + \tau' \big] x + (n-1)\sigma'(0) + \tau(0) \Big\}. \tag{2.1.37}$$

Then, equating (2.1.34) and (2.1.37), we arrive at

$$a_n = \frac{1}{n!} \mathcal{A}_{n-1,n} B_n \big[(n-1)\sigma'' + \tau' \big], \tag{2.1.38}$$

$$\frac{b_n}{a_n} = n \frac{(n-1)\sigma'(0) + \tau(0)}{(n-1)\sigma'' + \tau'}. \tag{2.1.39}$$

Now, let us determine the normalization constant $\mathcal{N}_n^2$. It is known that the

derivatives of this polynomials satisfy the differential equation in (2.1.9)

$$\Big[\sigma(x)\,\rho_k(x)\,v_k{}'(x)\Big]' + \mu_{kn}\,\rho_k(x)\,v_k(x) = 0\ ,\ k = 0, 1, ..., n \tag{2.1.40}$$

where $v_k = p_n^{(k)}(x)$, $\rho_k(x) = \sigma^k(x)\rho(x)$, and, $\mu_{kn} = \lambda_n - \lambda_k$. Furthermore,

$$\sigma(x)\rho_k(x)x^k\Big|_a^b = 0 \tag{2.1.41}$$

is satisfied automatically when (2.1.21) holds. That is, the sequence

$$\{p_0^{(k)}(x), p_1^{(k)}(x), ..., p_m^{(k)}(x), ..., p_n^{(k)}(x), ...\}$$

of the $k-$ht derivatives is also orthogonal on (a, b) with respect to weight $\rho_k(x)$. Hence, we must have

$$\int_a^b \rho(x)p_m^{(k)}(x)p_n^{(k)}(x)\mathrm{d}x = \mathcal{N}_n^2\delta_{mn}\ ,\ k = 0, 1, ... \tag{2.1.42}$$

which reduces to (2.1.24) for $k = 0$, where $\mathcal{N}_n := \mathcal{N}_{0,n}$, $\rho_0(x) := \rho(x)$, and, $p_m^{(0)}(x) = p_m(x)$. From (2.1.9) and (2.1.40) we write

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big[\rho_{k+1}(x)p_n^{(k+1)}(x)\Big] + \mu_{kn}\rho_k(x)p_n^{(k)}(x) = 0$$

which leads to

$$\int_a^b p_n^{(k)}(x)\big[\rho_{k+1}(x)p_n^{(k+1)}(x)\big]'\mathrm{d}x + \mu_{kn}\int_a^b \rho_k(x)\big[p_n^{(k)}(x)\big]^2\mathrm{d}x = 0$$

on multiplying by $p_n^{(k)}(x)$ and integrating from a to b. Then, using integration by parts, we get

$$\rho_{k+1}(x)p_n^{(k+1)}(x)p_n^{(k)}(x)\Big|_a^b - \int_a^b \rho_{k+1}(x)\big[p_n^{(k+1)}(x)\big]^2\mathrm{d}x + \mu_{kn}\int_a^b \rho_k(x)\big[p_n^{(k)}(x)\big]^2\mathrm{d}x$$

in which, from (2.1.41), the first part is equal to zero. Thus, we arrive at the

relation

$$\mathcal{N}_{k+1,n} = \mu_{kn}\mathcal{N}_{kn} \ , \ k = 0, 1, ...$$

which can be solved recursively to obtain

$$\begin{aligned}
\mathcal{N}_{1,n}^2 &= \mu_{0n}\mathcal{N}_{0,n} = \mu_{0n}\mathcal{N}_n^2 \\
\mathcal{N}_{2,n}^2 &= \mu_{1n}\mathcal{N}_{1,n} = \mu_{0n}\mu_{1n}\mathcal{N}_n^2 \\
&\vdots \\
\mathcal{N}_{k,n}^2 &= \mathcal{N}_n^2 \prod_{j=0}^{k-1} \mu_{jn}
\end{aligned}$$

or by using (2.1.17), $\mathcal{N}_{k,n}^2 = \mathcal{N}_n^2(-1)^k\mathcal{A}_{kn}$ since $p_n^{(n)}(x) = n!a_n$. From (2.1.33), the relation in (2.1.42) reads as

$$\mathcal{N}_{nn}^2 = (n!a_n)^2 \int_a^b \rho_n(x)\mathrm{d}x$$

for $m = k = n$, so that the squared norm or normalization factor $\mathcal{N}_n$ is given by

$$\mathcal{N}_n^2 = \frac{(-1)^n}{\mathcal{A}_{nn}}\mathcal{N}_{nn}^2 = \frac{(-1)^n}{\mathcal{A}_{nn}}(n!a_n)^2 \int_a^b \rho_n(x)\mathrm{d}x. \tag{2.1.43}$$

Theorem 2.1.6. *Let x_j be a zero of $p_n(x)$ for $n \neq 0$. It is possible to show that there exits exactly n roots, say $x_1, x_2, ..., x_n$ of the equation $p_n(x) = 0$, which are all real and distinct lying on the interval $x \in (a, b)$.*

Proof. Let $p_n(x)$ changes sign k times on (a, b). Clearly $0 \leq k \leq n$. We have to show that $k = n$ to complete the proof. Define the polynomial

$$q_k(x) = \begin{cases} 1 & \text{for } k = 0 \\ \displaystyle\prod_{j=1}^{k}(x - x_j) & \text{for } 0 < k \leq n \end{cases}$$

in which $x_j \in (a, b)$ are the points where $p_n(x)$ changes sign. Observe that $q_k(x)p_n(x)$ is always positive on (a, b). Then the integral

$$\int_a^b \rho(x) q_k(x) p_n(x) \mathrm{d}x \neq 0 \tag{2.1.44}$$

since the integrand is positive. But from orthogonality $k = n$. Observe that the integral in (2.1.44) is zero as $p_n(x)$ is orthogonal all polynomials of degree less than n. □

There exist a finite sum formula

$$\sum_{k=0}^{n} \frac{1}{\mathcal{N}_k^2} p_k(x) p_k(y) = \frac{\mathcal{A}_n(x,y)}{y-x} \tag{2.1.45}$$

for each orthogonal polynomial, which is called Darboux-Christofel formula, where

$$\frac{\mathcal{A}_n(x,y)}{y-x} = \frac{\alpha_k}{\mathcal{N}_k^2} \det \begin{bmatrix} p_k(x) & p_k(y) \\ p_{k+1}(x) & p_{k+1}(y) \end{bmatrix}. \tag{2.1.46}$$

This result can be derived from the recurrence relation (2.1.26). Actually we have

$$\begin{aligned} \frac{1}{\mathcal{N}_k^2} x p_k(x) = & \frac{\alpha_k}{\mathcal{N}_k^2} p_{k+1}(x) + \frac{\beta_k}{\mathcal{N}_k^2} p_k(x) + \frac{\alpha_{k-1}}{\mathcal{N}_k^2} p_{k-1}(x), \\ \frac{1}{\mathcal{N}_k^2} y p_k(y) = & \frac{\alpha_k}{\mathcal{N}_k^2} p_{k+1}(y) + \frac{\beta_k}{\mathcal{N}_k^2} p_k(y) + \frac{\alpha_{k-1}}{\mathcal{N}_k^2} p_{k-1}(y). \end{aligned}$$

If we multiply the first by $p_k(y)$ and the second by $p_k(x)$ and subtract we get

$$\frac{x-y}{\mathcal{N}_k^2} p_k(x) p_k(y) = -\mathcal{A}_k(x,y) + \mathcal{A}_{k-1}(x,y).$$

Summing over k from 0 to n, we obtain

$$\begin{aligned} \sum_{k=0}^{n} \frac{1}{\mathcal{N}_k^2} p_k(x) p_k(y) = & \sum_{k=0}^{n} \frac{\mathcal{A}_k(x,y) - \mathcal{A}_{k-1}(x,y)}{y-x} \\ = & \frac{\mathcal{A}_n(x,y) - \mathcal{A}_{-1}(x,y)}{y-x} \end{aligned}$$

since the series on the right hand side is a telescoping series. Note that $\mathcal{A}_{-1}(x,y) =$

0 since $\frac{\alpha_{-1}}{\mathcal{N}_{-1}^2} = 0$ and $p_{-1}(x)p_{-1}(y) = 0$. The following theorem, which tells about the location of zeros of orthogonal polynomials, may be proved by using Darboux-Christofel formula.

Theorem 2.1.7. *The zeros of $p_n(x)$ and $p_{n+1}(x)$ are interlaced.*

Proof. Consider the limiting case of (2.1.45) or y goes to x.

$$\lim_{y\to x} \frac{\mathcal{A}_n(x,y)}{y-x}$$

which is undetermined. By using L'Hopital's rule we get

$$\begin{aligned} \lim_{y\to x} \frac{\partial}{\partial y}\mathcal{A}_n(x,y) &= \frac{\partial}{\partial y}\mathcal{A}_n(x,x) \\ &= -\frac{1}{\mathcal{N}_n^2}\frac{a_n}{a_{n+1}}\left[p_{n+1}(x)p_n'(x) - p_n(x)p_{n+1}'(x)\right] \quad (2.1.47) \end{aligned}$$

and the left hand side is equal to

$$\lim_{y\to x}\sum_{k=0}^{n}\frac{p_k(x)p_k(y)}{\mathcal{N}_k^2} = \sum_{k=0}^{n}\frac{p_k^2(x)}{\mathcal{N}_k^2}.$$

Let $x_j\ ,\ j = 1, \cdots, n+1$ be the roots of $p_{n+1}(x) = 0$. From (2.1.47), we have

$$\frac{1}{\mathcal{N}_n^2}\frac{a_n}{a_{n+1}}p_n(x_j)p_{n+1}'(x_j) = \sum_{k=0}^{n}\frac{p_k^2(x_j)}{\mathcal{N}_k^2}$$

which leads to

$$p_n(x_j)p_{n+1}'(x_j) = \mathcal{N}_n^2\frac{a_n}{a_{n+1}}\sum_{k=0}^{n}\frac{p_k^2(x_j)}{\mathcal{N}_k^2}.$$

The last equation shows that the sign of the left hand side depends only on the sign of $\frac{a_{n+1}}{a_n}$ and independent of x_j.

However, $p_{n+1}'(x)$ changes sign between x_j and x_{j+1} since $p_{n+1}(x)$ has a local extreme value there. That is, $p_n(x)$ should also change sign accordingly, which means that $p_n(x)$ has at least one zero between x_j and x_{j+1}. But since there are n-subintervals (x_j, x_{j+1}) on (a,b) and each contains at least one zero, we conclude

that there is exactly one zero between two successive zeros of $p_{n+1}(x)$. □

It is possible to compute the zeros of $p_N(x)$ by using theorem (2.1.5) and (2.1.7). Writing the recursion (2.1.26) in the form

$$\alpha_n p_{n+1}(x) - (x - \beta_n)p_n(x) + \gamma_n p_{n-1}(x) = 0,$$

for $n = 1, 2, \ldots, N$, we obtain

$$\begin{array}{llll} \alpha_0 p_1 & -(x-\beta_0)p_0 & & = 0 \\ \alpha_1 p_2 & -(x-\beta_1)p_1 & +\gamma_1 p_0 & = 0 \\ \vdots & \vdots & \vdots & \vdots \\ \alpha_{N-2} p_{N-1} & -(x-\beta_{N-2})p_{N-2} & +\gamma_{N-2} p_{N-3} & = 0 \\ \alpha_{N-1} p_N & -(x-\beta_{N-1})p_{N-1} & +\gamma_{N-1} p_{N-2} & = 0 \end{array}$$

or in matrix-vector notation we have

$$[\mathbf{A} - x\mathbf{I}]\mathbf{P} = \mathbf{Q} \tag{2.1.48}$$

where

$$\mathbf{A} = \begin{bmatrix} \beta_0 & \alpha_0 & & & 0 \\ \gamma_1 & \beta_1 & \alpha_1 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \alpha_{N-1} \\ 0 & & & \gamma_{N-1} & \beta_{N-1} \end{bmatrix}, \mathbf{P} = \begin{bmatrix} p_0 \\ p_1 \\ \vdots \\ p_{n-2} \\ p_{n-1} \end{bmatrix}, \text{and } \mathbf{Q} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ p_N \end{bmatrix}.$$

We want to find x such that $p_N(x) = 0$. Hence, (2.1.48) now reads as

$$[\mathbf{A} - x\mathbf{I}]\mathbf{P} = \mathbf{0}. \tag{2.1.49}$$

Since the zeros of $p_n(x)$ and $p_{n+1}(x)$ are interlaced, $\mathbf{P}$ can not be zero vector when $p_N(x) = 0$. Thus, (2.1.49) satisfied when $[\mathbf{A} - x\mathbf{I}] = \mathbf{0}$. But such x values are the eigenvalues of the matrix $\mathbf{A}$. Therefore, the zeros of the orthogonal polynomial $p_N(x)$ are given by the eigenvalues of the $N \times N$ three-diagonal Jacobi matrix $\mathbf{A}$.

2.2 The Gamma Function

Before starting our analysis of polynomial eigenfunctions, it is convenient to review some properties of the well-known Euler Gamma Function which, for any complex number $\mathrm{Re}(z) > 0$ is defined as

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} \mathrm{d}t. \tag{2.2.50}$$

From (2.2.50) it is straight forward after integration by parts that gamma function satisfies the recurrence relation of the form

$$\Gamma(z+1) = z\Gamma(z). \tag{2.2.51}$$

In particular when $z = n$ is an integer, we have a fundamental relation obtained from (2.2.51) by induction, i.e.,

$$\Gamma(n+1) = n!. \tag{2.2.52}$$

Another important relation is

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}, \tag{2.2.53}$$

which is known as reflection (addition) formula. From (2.2.53) one can easily obtain

$$\Gamma(\tfrac{1}{2}) = \sqrt{\pi}. \tag{2.2.54}$$

Another useful equality

$$2\Gamma(2z) = \frac{2^{2z}}{\Gamma(\frac{1}{2})}\Gamma(z)\Gamma(z+\tfrac{1}{2}) \tag{2.2.55}$$

is known as the duplication formula. In particular when $z = n$ is an integer we have

$$(2n)! = \frac{2^{2n}}{\Gamma(\frac{1}{2})} n!\Gamma(n+\tfrac{1}{2}). \tag{2.2.56}$$

From the definition of Gamma function in (2.2.50) one can easily see that $\Gamma(1) = 1$ and using the relation in (2.2.51) one obtains $\Gamma(2) = 1$.

A useful equality, which can be deduced from the definition of the beta function, is

$$B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x + y)} \tag{2.2.57}$$

where $B(x, y)$ is defined as

$$B(x, y) = \int_{-1}^{1} t^{x-1}(1 - t)^{y-1}\mathrm{d}t. \tag{2.2.58}$$

And, finally, the so called Pochhammer's symbol

$$(\beta)_n = \beta(\beta + 1) \dots (\beta + n - 1) \ , \ (\beta)_0 = 1 \tag{2.2.59}$$

can be represented as

$$(\beta)_n = \frac{\Gamma(\beta + n)}{\Gamma(\beta)} \tag{2.2.60}$$

on using the recurrence relation (2.2.51).

2.3 Classical Orthogonal Polynomials

Some special choices of $\sigma(x)$, $\tau(x)$, and λ in (2.1.1) leads to the very well-known families, such as Jacobi, Laguerre, and Hermite polynomials. Important properties of these polynomials will be introduced.

2.3.1 Jacobi Polynomials

Let $\sigma(x) = 1 - x^2$ and $\rho(x) = (1 - z)^{\alpha}(1 + z)^{\beta}$ in the differential equation (2.1.1). Then from (2.1.3), $\tau(x) = -(\alpha + \beta + 2) + \beta - \alpha$ and theorem (2.1.3), $\lambda_n = n(n + \alpha + \beta + 1)$. Corresponding polynomials are denoted and defined by the Rodriguez formula in (2.1.19)

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}(1 - x)^{-\alpha}(1 + x)^{-\beta}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\Big[(1 - x)^{n+\alpha}(1 + x)^{n+\beta}\Big] \tag{2.3.61}$$

where $B_n = \dfrac{(-1)^n}{2^n n!}$ is chosen for historical reasons. It is clear from (2.1.1) that Jacobi polynomials satisfy the differential equation

$$(1-x^2)y'' + [\beta - \alpha - (\alpha+\beta+2)x]y' + n(n+\alpha+\beta+1)y = 0. \tag{2.3.62}$$

Applying Leibniz's rule for the derivatives of a product, it can be seen from (2.3.61)

$$P_n^{(\alpha,\beta)}(x) = \frac{1}{2^n n!}\sum_{k=0}^{n}\binom{n}{k}\frac{(\alpha+1)_n}{(\alpha+1)_{n-k}}\frac{(\beta+1)_n}{(\beta+1)_k}(x-1)^{n-k}(x+1)^k$$

or equivalently, using (2.2.60) we have

$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{2^n n!}\sum_{k=0}^{n}\binom{n}{k}\frac{(x-1)^{n-k}(x+1)^k}{\Gamma(n-k+\alpha+1)\Gamma(k+\beta+1)} \tag{2.3.63}$$

and that

$$P_n^{(\alpha,\beta)}(1) = \frac{1}{n!}\frac{\Gamma(n+\alpha+1)}{\Gamma(\alpha+1)}, \tag{2.3.64}$$

$$P_n^{(\alpha,\beta)}(-1) = \frac{(-1)^n}{n!}\frac{\Gamma(n+\beta+1)}{\Gamma(\beta+1)}. \tag{2.3.65}$$

Putting $x = \mp 1$ in (2.3.62) and using (2.3.64) and (2.3.65) we get

$$\frac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}(1) = \frac{1}{2}(n+\alpha+\beta+1)\frac{\Gamma(n+\alpha+1)}{(n-1!)\Gamma(\alpha+2)}, \tag{2.3.66}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}(-1) = -(-1)^n\frac{1}{2}(n+\alpha+\beta+1)\frac{\Gamma(n+\beta+1)}{(n-1!)\Gamma(\beta+2)}. \tag{2.3.67}$$

Similarly differentiating (2.3.62) and using (2.3.66) and (2.3.67) one obtains

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_n^{(\alpha,\beta)}(1) = \frac{(n-1)(n+\alpha+\beta+2)}{2(\alpha+2)}\frac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}(1), \tag{2.3.68}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_n^{(\alpha,\beta)}(-1) = \frac{(n-1)(n+\alpha+\beta+2)}{2(\beta+2)}\frac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}(-1). \tag{2.3.69}$$

The condition (2.1.21) in theorem (2.1.4) is satisfied when $(a, b) = (-1, 1)$, provided $\alpha > -1$, $\beta > -1$. Thus, Jacobi polynomials are arthogonal on $(-1, 1)$ with respect to the weight $\rho(x) = (1-x)^\alpha(1+x)^\beta$. That is,

$$\int_{-1}^{1} P_n^{(\alpha,\beta)}(x)P_m^{(\alpha,\beta)}(x)(1-x)^\alpha(1+x)^\beta \mathrm{d}x = \mathcal{N}_n^2\delta_{mn} \tag{2.3.70}$$

where

$$\mathcal{N}_n^2 = \frac{2^{\alpha+\beta+1}}{(2n+\alpha+\beta+1)n!}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)} \tag{2.3.71}$$

is computed from (2.1.43). The leading coefficients

$$a_n = \frac{1}{2^n n!}\frac{\Gamma(2n+\alpha+\beta+1)}{\Gamma(n+\alpha+\beta+1)}, \tag{2.3.72}$$

$$\frac{b_n}{a_n} = -n\frac{\beta-\alpha}{2n+\alpha+\beta}, \tag{2.3.73}$$

are given by (2.1.38) and (2.1.39). Thus, the recurrence relation in (2.1.26) reads as,

$$\begin{aligned} 2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)P_{n+1}^{(\alpha,\beta)}(x) = \\ (n+\alpha+\beta+1)\big[(n+\alpha+\beta+2)(2n+\alpha+\beta)x+\alpha^2-\beta^2\big]P_n^{(\alpha,\beta)}(x) \\ -2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)P_{n-1}^{(\alpha,\beta)}(x) \end{aligned} \tag{2.3.74}$$

in which

$$P_0^{(\alpha,\beta)}(x) = 1, \quad P_1^{(\alpha,\beta)}(x) = \frac{1}{2}(\alpha+\beta+2)x + \frac{1}{2}(\alpha-\beta).$$

2.3.2 Chebyshev Polynomials

The Chebyshev polynomials of the first kind are related to the Jacobi polynomials with $\alpha = \beta = -\frac{1}{2}$. In fact, they are defined by

$$T_n := \delta_n P_n^{(-\frac{1}{2},-\frac{1}{2})} \ , \ n \in \mathbb{N} \tag{2.3.75}$$

where

$$\delta_n = \frac{n!\sqrt{\pi}}{\Gamma(n+\frac{1}{2})}. \tag{2.3.76}$$

Consequently, they are solutions of the differential equation

$$(1-x^2)T_n''(x) - xT_n'(x) + n^2 T_n(x) = 0. \tag{2.3.77}$$

By taking $\alpha = \beta = -\frac{1}{2}$ in (2.3.74), after appropriate scaling, we arrive at the recursion formula

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x) \tag{2.3.78}$$

where $T_0(x) = 1\ ,\ T_1(x) = x$. Using (2.3.75), (2.3.64)and (2.3.65) one can easily obtain

$$T_n(1) = 1\ ,\ T_n(-1) = (-1)^n \tag{2.3.79}$$

and similarly (2.3.66) and (2.3.67) together with (2.3.75) imply that

$$T_n'(1) = n^2\ ,\ T_n'(-1) = -(-1)^n n^2. \tag{2.3.80}$$

It is known that the functions $\{\cos n\phi\}\ ,\ n = 0, 1, ...$ form an orthogonal set over $(0, \pi)$. That is,

$$\int_0^\pi \cos m\phi\ \cos n\phi\ \mathrm{d}\phi = \begin{cases} 0 & \text{if } m \neq n \\ \pi & \text{if } m = n = 0 \\ \frac{\pi}{2} & \text{if } m = n \neq 0 \end{cases}. \tag{2.3.81}$$

If we set $\cos\phi = x$, we get another definition of the Chebyshev polynomials

$$T_n(x) = \cos n\phi = \cos(n \arccos x)\ ,\ x \in (-1, 1) \tag{2.3.82}$$

with $T_0(x) = 1\ ,\ T_1(x) = x$. Then, from (2.3.81) we see that

$$\int_{-1}^{1} T_m(x)T_n(x)\frac{1}{\sqrt{1-x^2}}\mathrm{d}x = \mathcal{N}_n^2\delta_{mn} \tag{2.3.83}$$

where

$$\mathcal{N}_n^2 = \begin{cases} \pi & , n = 0 \\ \frac{\pi}{2} & , n > 0 \end{cases} \tag{2.3.84}$$

which means that the sequence of $T_n(x)$ are orthogonal over $x \in (-1, 1)$ with respect to the weight $\rho(x) = (1 - x^2)^{-\frac{1}{2}}$.

2.3.3 Legendre Polynomials

Legendre polynomials are Jacobi polynomials with $\alpha = \beta = 0$. To simplify the notation it is standard to set $P_n := P_n^{(0,0)}$. We now review the basic properties. According to (2.3.62) we have the differential equation

$$(1 - x^2)P_n''(x) - 2xP_n'(x) + n(n + 1)P_n(x) = 0. \tag{2.3.85}$$

The recursion formula in (2.3.74) takes the form

$$(n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x) \tag{2.3.86}$$

with $P_0(x) = 1$, $P_1(x) = x$. Conditions (2.3.64) and (2.3.65) give respectively

$$P_n(1) = 1 \ , \ P_n(-1) = (-1)^n, \tag{2.3.87}$$

and similarly (2.3.66) and (2.3.67) implies that

$$P_n'(\pm 1) = (\pm 1)^{n-1}\frac{1}{2}n(n + 1). \tag{2.3.88}$$

By taking $\alpha = \beta = 0$ in (2.3.70) and (2.3.71) we get the orthogonality property for Legendre polynomials. That is,

$$\int_a^b P_n(x)P_m(x)\mathrm{d}x = \mathcal{N}_n^2\delta_{mn} \tag{2.3.89}$$

where

$$\mathcal{N}_n^2 = \frac{2}{2n + 1}. \tag{2.3.90}$$

2.3.4 Laguerre Polynomials

Now we introduce another family of polynomial solutions of the hypergeometric differential equation in (2.1.1). Let $\sigma(x) = x$ and $\rho(x) = x^{\alpha}e^{-x}$ in the differential equation (2.1.1). Then, from (2.1.3), we have $\tau(x) = \alpha + 1 - x$ and theorem (2.1.3) implies that $\lambda_n = n$. Corresponding polinomials are the generalized Laguerre polynomials denoted and defined by the Rodriguez formula (2.1.19)

$$L_n^{(\alpha)}(x) = \frac{1}{n!}e^x x^{\alpha}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\Big[x^{n+\alpha}e^{-x}\Big]. \tag{2.3.91}$$

It can be seen from (2.1.1) Laguerre polynomials satisfy the differential equation

$$xy'' + (\alpha + 1 - x)y' + ny = 0. \tag{2.3.92}$$

Applying Leibniz's rule for derivatives of a product, we have, from (2.3.91) and (2.2.60)

$$L_n^{(\alpha)}(x) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}\sum_{k=0}^{n}\binom{n}{k}\frac{\Gamma(\alpha+1)}{\Gamma(k+\alpha+1)}(-x)^k \tag{2.3.93}$$

which gives

$$L_n^{(\alpha)}(0) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}. \tag{2.3.94}$$

In (2.3.92), putting $x = 0$ we get,

$$\frac{\mathrm{d}}{\mathrm{d}x}L_n^{(\alpha)}(0) = -\frac{n}{\alpha+1}L_n^{(\alpha)}(0) = -\frac{\Gamma(n+\alpha+1)}{(n-1)!\Gamma(\alpha+2)}. \tag{2.3.95}$$

Similarly differentiating (2.3.92) in x and substituting $x = 0$ we obtain

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}L_n^{(\alpha)}(0) = -\frac{(n-1)}{\alpha+2}\frac{\mathrm{d}}{\mathrm{d}x}L_n^{(\alpha)}(0) = \frac{\Gamma(n+\alpha+1)}{(n-2)!\Gamma(\alpha+3)}. \tag{2.3.96}$$

By virtue of theorem (2.1.4) Laguerre polynomials are orthogonal on $(0, \infty)$ with respect to the weight $\rho(x) = x^{\alpha}e^{-x}$. That is,

$$\int_a^b L_n^{(\alpha)}(x)L_m^{(\alpha)}(x)x^{\alpha}e^{-x}\mathrm{d}x = \mathcal{N}_n^2\delta_{mn} \tag{2.3.97}$$

where

$$\mathcal{N}_n^2 = \frac{1}{n!}\Gamma(n+\alpha+1) \tag{2.3.98}$$

is computed from (2.1.43). The leading coefficients

$$a_n = -(n+1), \tag{2.3.99}$$

$$\frac{b_n}{a_n} = -n(n+\alpha), \tag{2.3.100}$$

are given by (2.1.38) and (2.1.39) respectively. Then, the three term recurrence relation in (2.1.26) takes the form

$$(n+1)L_{n+1}^{(\alpha)}(x) = (\alpha+2n+1-x)L_n^{(\alpha)}(x) - (\alpha+n)L_{n-1}^{(\alpha)}(x), \tag{2.3.101}$$

where $L_0^{(\alpha)}(x)1$, $L_1^{(\alpha)}(x) = \alpha + 1 - x$.

2.3.5 Hermite Polynomials

The set of Hermite polynomials is the last family that we consider. Let $\sigma(x) = 1$ and $\rho(x) = e^{-x^2}$ in the differential equation (2.1.1). Then, (2.1.3) gives $\tau(x) = -2x$ and from theorem (2.1.3) we have $\lambda_n = 2n$. Corresponding polynomials are the Hermite polynomials defined by the Rodriguez formula in (2.1.19)

$$H_n(x) = (-1)^n e^{x^2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\Big(e^{-x^2}\Big). \tag{2.3.102}$$

Hermite polynomials satisfy the differential equation

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0. \tag{2.3.103}$$

In the light of theorem (2.1.4), we see that Hermite polynomials are orthogonal on the real line $(-\infty, \infty)$ with respect to the weight $\rho(x) = e^{-x^2}$, i.e.,

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} \mathrm{d}x = \mathcal{N}_n^2 \delta_{mn} \tag{2.3.104}$$

where

$$\mathcal{N}_n^2 = 2^n n! \Gamma(\tfrac{1}{2}) = 2^n n! \sqrt{\pi} \tag{2.3.105}$$

is obtained from (2.1.43). The leading coefficients of Hermite polynomials

$$a_n = 2^n \tag{2.3.106}$$

$$\frac{b_n}{a_n} = 0 \tag{2.3.107}$$

are given by (2.1.38) and (2.1.38) respectively. Thus, the recurrence relation in (2.1.19) reads as

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x) \tag{2.3.108}$$

with $H_0(x) = 1$, $H_1(x) = 2x$. Finally, for example, from Rodriguez formula we can obtain another useful recurrence relation

$$H_n'(x) = 2n H_{n-1}(x). \tag{2.3.109}$$

CHAPTER 3

SPECTRAL METHODS

Spectral methods, together with finite difference and finite element methods constitute the "big three" technologies for the numerical solutions of differential equations. Some general and remarkable properties of spectral methods will be investigated.

3.1 Introduction

The aim of this introductory section is to present, in a general way, the spectral methods in their various formulations: Galerkin, Tau, and collocation. By using the notion of residual, it will be shown how spectral approximation can be defined for the solution of a differential problem.

3.1.1 Generalities on The Method of Weighted Residuals

Spectral methods belong to the general class of weighted residuals method [20] for which approximations are defined in terms of a truncated series expansion, such that some quantity (error or residual) which should be exactly zero only in an approximate sense. This is done through the scalar product

$$(u, v)_\rho = \int_\alpha^\beta u(x)v(x)\rho(x)\mathrm{d}x \tag{3.1.1}$$

where $u(x)$ and $v(x)$ are two functions defined on $[\alpha, \beta]$ and $\rho(x)$ is some given weight function. Let us consider the expansion of a function $u(x)$ in the truncated series

$$u_N(x) = \sum_{k=0}^{N} \hat{u}_k \varphi_k(x), \qquad \alpha \leq x \leq \beta \tag{3.1.2}$$

where the trial (or basis) functions $\varphi_k(x)$ are given and the expansion coefficients $\hat{u}_k$ must be determined. In spectral methods the chosen trial functions are orthogonal with respect to some weight $\rho(x)$, such that

$$(\varphi_k, \varphi_l)_\rho = c_k \delta_{kl} \tag{3.1.3}$$

where c_k constant and δ_{kl} is the Kronecker delta.

Now we introduce the residual R_N which should be made equal to zero. For example, if the function $u(x)$ is given and if we look for its approximation $u_N(x)$, then the residual is

$$R_N(x) = u - u_N.$$

If $u_N(x)$ is an approximate solution to the differential equation

$$Lu - f = 0$$

then the residual $R_N(x)$ is defined by

$$R_N(x) = Lu_N - f.$$

The weighted residuals method consists in annuling R_N in an approximate sense by setting to zero the scalar product

$$(R_N, \psi_i)_{\rho_\star} = \int_\alpha^\beta R_N(x)\psi_i(x)\rho_\star(x)\mathrm{d}x = 0, \qquad i \in I_N, \tag{3.1.4}$$

where $\psi_i(x)$ are the test (or weighting functions), and the weight $\rho_\star$ is associated with the method and trial functions. The dimension of the discrete set I_N depends on the problem under consideration.

The choice of the test functions and the weight defines the method, for example:
(i) the Galerkin type method corresponds to the case where the test functions are the trial function themselves and weight $\rho_\star$ is the weight associated with the

orthogonality of the trial functions, that is,

$$\psi_i = \varphi_i \quad \text{and} \quad \rho_\star = \rho, \tag{3.1.5}$$

(ii) the collocation method corresponds to the choice

$$\psi_i = \delta(x - x_i) \quad \text{and} \quad \rho_\star = 1, \tag{3.1.6}$$

where δ is the Dirac delta-function. The collocation points x_i are selected points on $[\alpha, \beta]$. From (3.1.4) and (3.1.6) we simply get

$$R_N(x_i) = 0. \tag{3.1.7}$$

Therefore, in the collocation method, the residual is exactly zero at certain points whereas in the Galerkin-type method the residual is zero in the mean.

3.1.2 Approximation of the Solution of a Differential equation

Let us consider the approximation of the solution of the differential equation

$$Lu - f = 0, \quad \alpha < x < \beta, \tag{3.1.8}$$

where L is a differential operator assumed to be linear and of second order. To the equation (3.1.8) the following linear boundary conditions are associated

$$B_- u = g_- \quad \text{at} \quad x = \alpha, \quad B_+ u = g_+ \quad \text{at} \quad x = \beta, \tag{3.1.9}$$

where B_- and B_+ correspond to Dirichlet, Neumann or Robin conditions.

The Traditional Galerkin Method

The traditional Galerkin method applies when the trial functions φ_k in the expansion (3.1.2) satisfy the homogeneous boundary conditions associated with

(3.1.9), let

$$B_-\varphi = 0 \quad \text{at} \quad x = \alpha, \quad B_+\varphi = 0 \quad \text{at} \quad x = \beta. \tag{3.1.10}$$

In this case, the solution u of Eqs. (3.1.8)-(3.1.9) can be sought as the combination

$$u = \tilde{u} + v,$$

where $\tilde{u}$ is any function satisfying the boundary conditions (3.1.8). The resulting problem for v is then

$$\begin{aligned} Lv - h &= 0, \quad \alpha < x < \beta, \\ B_-v &= 0 \quad \text{at} \quad x = \alpha, \\ B_+v &= 0 \quad \text{at} \quad x = \beta, \end{aligned}$$

where $h = f - L\tilde{u}$. The fact that the trial functions φ_k satisfies the homogeneous boundary conditions guarantees that the approximation $u_N(x)$, defined by

$$v_N(x) = \sum_{k=0}^{N} \tilde{v}_k \varphi_k(x), \tag{3.1.11}$$

satisfies the boundary conditions whatever the values of the expansion coefficients $\tilde{v}_k$ are. Now the residual $R_N(x)$ is

$$R_N(x) = Lv_N - h. \tag{3.1.12}$$

Then, according to the general formulation (3.1.4) with $I_N = 0, ..., N$ and (3.1.5), the Galerkin equations are

$$(R_N, \varphi_i)_\rho = (Lv_N - h, \varphi_i)_\rho = 0, \quad i = 0, ..., N, \tag{3.1.13}$$

or else, by replacing v_n by its expansion (3.1.11),

$$\sum_{k=0}^{N} \hat{v}_k (L\varphi_k, \varphi_i)_\rho = (h, \varphi_i)_\rho, \quad i = 0, ..., N. \tag{3.1.14}$$

The scalar product $(L\varphi_k, \varphi_i)_\rho$ is evaluated using the properties of the trial functions, in particular their orthogonality. The scalar product $(h, \varphi_i)_\rho$ is equal to $c_i\hat{h}_i$ where $\hat{h}_i$, $i = 0, ..., N$, is the expansion coefficient of h. System (3.1.14) furnishes $N + 1$ equations for determining the $N + 1$ coefficients $v_k\, k = 0, ..., N$.

Note that, in the present case, the number of Galerkin equations (3.1.13) of the general type (3.1.4) is exactly $N + 1$. This is because the boundary conditions are satisfied by the trial functions. When this latter property does not hold, the method may be applied by constructing, from the basis φ_k, a new basis ψ_k satisfying the boundary conditions; this can be done generally by defining ψ_k as a linear combination of some φ_k's. But the new basis may not be orthogonal, so that this approach is not much used and generally one prefers a simple method called the "Tau method" which is described in the following subsection.

The Tau Method

The so called Tau method, introduced by Lanczos [32] in 1938 , is a modification of the Galerkin method allowing the use of trial functions not satisfying the homogeneous boundary conditions in (3.1.10). The solution of Eqs. (3.1.8)-(3.1.9) is sought in the form

$$u_N(x) = \sum_{k=0}^{N} \hat{u}_k \varphi_k(x). \tag{3.1.15}$$

The equations determining the $N+1$ coefficients $\hat{u}_k$, $k = 0, ..., N+1$, are obtained by considering the Galerkin equations of type (3.1.4) with $R_N(x) = Lu_N - f$, $\psi_i = \varphi_i$, $\rho_\star = \rho$ and $I_N = 0, ..., N-2$, therefore,

$$\sum_{k=0}^{N} \hat{u}_k (L\varphi_k, \varphi_i)_\rho = (f, \varphi_i)_\rho, \quad i = 0, ..., N-2, \tag{3.1.16}$$

these equations being completed with the boundary conditions

$$B_- u_N(\alpha) = g_-, \quad B_+ u_N(\beta) = g_+. \tag{3.1.17}$$

System (3.1.16)-(3.1.17) permits the calculation of the $N+1$ coefficients of $\hat{u}_k$, $k = 0, ..., N$. The non-consideration of the Galerkin equations for $i = N-1$ and $i = N-2$ introduces a supplementary error, the "Tau error" which has given its name to the method. For a detailed discussion see Gottlieb and Orszag [25] and Canuto et al. [11].

The Collocation Method

Following the general description made in section 1.1, the collocation equations are obtained by considering the expansion (3.1.15) and by making the associated residual $R_N = Lu_N - f$ zero at the inner collocation points $x_i \in I_N = 1, ..., N-2$, let

$$Lu_N(x_i) = f(x_i), \quad i = 1, ..., N-1. \tag{3.1.18}$$

Equations (3.1.16)-(3.1.17) give a system of $N+1$ equations for the $N+1$ coefficients $\hat{u}_k$, $k = 0, ..., N$. An equivalent formulation is, however, generally preferred. It consists of considering the values $u_N(x_i)$ at the collocation points x_i, $i = 0, ..., N$, as unknowns rather than the coefficients $\hat{u}_k$. This is possible since the $\hat{u}_k$, $k = 0, ..., N$, can be expressed in terms of the $u_N(x_i)$, $i = 0, ..., N$. Therefore, one can consruct differentiation formulas expressing the derivative, of any order, at a given collocation point in terms of the values of the function itself at all collocation points, that is,

$$u_N^{(p)}(x_i) = \sum_{j=0}^{N} d_{i,j}^{(p)} u_N(x_j). \tag{3.1.19}$$

If D is the differentiation matrix defined by $D = [d_{i,j}^{(p)}]$, $i, j = 0, ..., N$, and $p > 0$, and if we denote by U the vector whose components are the values of u_N at the collocation points, and by $u^{(p)}$ the vector of the values of the pth derivative of U, we have $U^{(p)} = D^p U$. This construction will be made more precise in the following section.

3.2 Pseudospectral Methods

Pseudospectral methods, also known as spectral collocation method, for solving differential equations is based on weighted interpolants of the form

$$f(x) = P_{N-1}(x) = \sum_{j=1}^{N} \frac{\rho(x)}{\rho(x_j)} \ \phi_j(x) f_j \tag{3.2.20}$$

where $x_j \ , \ j = 1, ..., N$ is a set of distinct interpolant nodes, $\rho(x)$ is a weight function which is positive and at least p times differentiable, $\phi_j(x) \ , \ j = 1, ..., N$ satisfies $\phi_j(x_k) = \delta_{jk} \ , \ k = 1, ..., N$ and $f_j = f(x_j)$. This means that $P_{N-1}(x)$ defined by (3.2.20) is an interpolant of the function $f(x)$ in the sense that

$$f(x_j) = P_{N-1}(x_j) \ , \ j = 1, ..., N.$$

Derivative operator is generated by taking the p-th derivatives of (3.2.20) and evaluating the result at the nodes $x_i \ , \ i = 1, ..., N$

$$f^{(p)}(x_j) = \sum_{j=1}^{N} \frac{\mathrm{d}^p}{\mathrm{d}x^p} . \left[\frac{\rho(x)}{\rho(x_j)} \ \phi_j(x) \right]_{x=x_j} f_j.$$

The derivative operator can be represented by a matrix $D^{(p)}$, the differentiation matrix, with entries

$$d_{ij}^{(p)} = \sum_{j=1}^{N} \frac{\mathrm{d}^p}{\mathrm{d}x^p} \left[\frac{\rho(x)}{\rho(x_j)} \ \phi_j(x) \right]_{x=x_j} \qquad i, j = 1, ..., N. \tag{3.2.21}$$

The numerical differentiation process may therefore be performed as a matrix vector product

$$f^{(p)} = D^{(p)} f \tag{3.2.22}$$

where f (respectively $f^{(p)}$) is the vector of function values (respectively approximate derivative values) at the nodes.

When solving differential equations, the derivatives are approximated by the discrete derivative operators (3.2.22). A linear two point boundary value problem

may thus be converted to a linear system. A differential eigenvalue problem may likewise be converted to a matrix eigenvalue problem.

Now, we will introduce the concept of a differentiation matrix that has been proven to be very useful tool in the numerical solutions of differential equations.

Differentiation matrices are derived from pseudospectral method. In this method the unknown solution to the differential equation is expanded as a global interpolant, such as a trigonometric or polynomial. The latter, in which the set of interpolating functions $\phi_j(x)\ ,\ j = 1, ..., N$ consist of polynomials of degree $N-1$, will be our concern. The interpolant (3.2.20) is given by

$$P_{N-1}(x) = \sum_{j=1}^{N} \varphi_{N-1,j}(x) f_j,$$

where

$$\varphi_{N-1,j}(x) = \frac{\rho(x)}{\rho(x_j)}\ \phi_j(x)\ ,\ j = 1, ..., N, \tag{3.2.23}$$

and $\phi_j(x)\ ,\ j = 1, ..., N$ are the Lagrangian interpolating polynomials defined by

$$\phi_j(x) = \prod_{\substack{m=1 \\ m \neq j}}^{N} \left(\frac{x - x_m}{x_j - x_m} \right)\ ,\ j = 1, ..., N. \tag{3.2.24}$$

The function $\rho(x)$, as mentioned before, is an arbitrary, positive weight, with at least p continuous derivatives.

Lagrangian interpolating functions in (3.2.24) may be written in an equivalent form,

$$\phi_j(x) = \frac{S_N(x)}{S'_N(x_j)(x - x_j)}, \tag{3.2.25}$$

where

$$S_N(x) = \prod_{m=1}^{N} (x - x_m). \tag{3.2.26}$$

Then (3.2.23) takes the form

$$\varphi_{N-1,j}(x) = \frac{1}{c_j} \rho(x) \frac{S_N(x)}{(x - x_j)} \tag{3.2.27}$$

with

$$c_j = \rho(x_j) S'_N(x_j). \tag{3.2.28}$$

Then the derivative operator (3.2.24) reads as

$$d_{ij}^{(p)} = \frac{\mathrm{d}^p}{\mathrm{d}x^p}\Big[\varphi_{N-1,j}(x)\Big]_{x=x_i} \ , \ i = 1, ..., N \tag{3.2.29}$$

or, equivalently

$$d_{ij}^{(p)} = \frac{1}{c_j}\frac{\mathrm{d}^p}{\mathrm{d}x^p}\left[\rho(x)\frac{S_N(x)}{(x-x_j)}\right]_{x=x_i} \ , \ i = 1, ..., N. \tag{3.2.30}$$

Now, we present a result, which form the core of the computational method for computing $D^{(p)}$ recursively, in the following theorem.

Theorem 3.2.1 (Welfert). *For $p \geq 0$ and $i \geq 0$, $j \leq N$ we have*

$$d_{ij}^{(p+1)} = \begin{cases} \dfrac{1}{c_j}\dfrac{(\rho S_N)^{p+2}(x_j)}{p+2} & \text{, if } i = j \\ \\ \dfrac{p+1}{x_i - x_j}\left(\dfrac{c_i}{c_j} d_{ii}^{(p)} - d_{ij}^{(p)}\right) & \text{, if } i \neq j \end{cases} \tag{3.2.31}$$

where c_i is defined by (3.2.28) for $i = 1, ..., N$.

Proof. Let $0 \leq j \leq N$ and $p \geq 0$. From (3.2.27) we write

$$\frac{1}{c_j}\rho(x) S_N(x) = (x - x_j)\varphi_{N-1,j}(x).$$

Now taking the $(p+2)nd$ derivative of both sides we write

$$\begin{aligned} \frac{1}{c_j}(\rho S_N)^{(p+2)}(x) &= \sum_{k=0}^{p+2} \binom{p+2}{k} (x - x_j)^{(k)} \varphi_{N-1,j}^{p+2-k}(x) \\ &= (x - x_j)\varphi_{N-1,j}^{p+2}(x) + (p+2)\varphi_{N-1,j}^{p+1}(x). \end{aligned} \tag{3.2.32}$$

For $x = x_j$ we obtain

$$\frac{1}{c_j}(\rho S_N)^{(p+2)}(x_j) = (p+2)\varphi^{p+1}_{N-1,j}(x_j) = (p+2)d^{(p+1)}_{jj} \tag{3.2.33}$$

thereby proving the theorem for all diagonal elements of $D^{(p+1)}$. On the other hand, if we apply (3.2.32) with $p+1$, (instead $p+2$), and $x = x_i$ with $i \neq j$ we get

$$\begin{aligned}\frac{1}{c_j}(\rho S_N)^{(p+1)}(x_i) &= (x_i - x_j)\varphi^{(p+1)}_{N-1,j}(x_i) + (p+1)\varphi^{(p)}_{N-1,j}(x_i) \\ &= (x_i - x_j)d^{(p+1)}_{ij} + (p+1)d^{(p)}_{ij}\end{aligned}$$

by (3.2.33), this yields

$$(p+1)\frac{c_i}{c_j}d^{(p)}_{ii} = (x_i - x_j)d^{(p+1)}_{ij} + (p+1)d^{(p)}_{ij},$$

which proves the theorm for $i \neq j$. □

A number of well known differentiation matrices can be constructed by using theorem (3.2.1); for example $\rho(x) = 1$ corresponds to polynomial interpolation (Jacobi, Chebyshev, Legendre, etc.), $\rho(x) = e^{-x^2/2}$ to Hermite collocation, and $\rho(x) = e^{-x/2}$ to the Laguerre collocation method. If $\rho(x)$ is a rational function, the method obtained is simply a rational collocation method.

Theorem (3.2.1) allows us to easily compute the off-diagonal entries of $D^{(p+1)}$ from the off-diagonal and diagonal entries of $D^{(p)}$. The diagonal elements of $D^{(p+1)}$ are more difficult to obtain recursively from theorem (3.2.1) directly. When the function $\rho(x)S_N(x)$ is the solution of a known differential equation (such as singular Sturm-Liouville problems), it is relatively easy to compute the diagonal entries of $D^{(p+1)}$. For general functions $\rho(x)$ and collocation points x_j, however, this is not feasible. There are two approaches for computing the diagonal entries. First one is to note that the diagonal entries are uniquely determined by the off-diagonal ones. In particular, the differentiation matrices should at least

differentiate the weight function $\rho(x)$ perfectly (in exact arithmetic). Therefore

$$D^{(p+1)}\rho = \rho^{(p+1)}$$

where ρ is the vector of function values $\rho(x_j)$, and $\rho^{(p+1)}$ is the vector of values $\rho^{(p+1)}(x_j)$. Once the off-diagonal entries have been computed by theorem (3.2.1), everything in this equation is known but the main diagonal of $D^{(p+1)}$. Hence the diagonal entries may be solved for. This approach is ill-conditioned, however, when $\rho(x)$ is a function for which $max_j\ \rho(x_j)/min_j\ \rho(x_j)$ is large. This occurs, for example, in the Hermite case $\left[\rho(x) = e^{-x^2/2}\right]$, as well as the Laguerre case $\left[\rho(x) = e^{-x/2}\right]$.

Alternative is the recursive procedure of Welfert [60] given in the following theorem.

Theorem 3.2.2 (Welfert). *For $p \geq 0$ and $1 \leq i \neq j \leq N$ we have*

$$d_{ii}^{(p+1)} = \frac{p+1}{x_i - x_j}\ \hat{d}_{\bar{i}\bar{i}}^{(p)} + \hat{d}_{\bar{i}\bar{i}}^{(p+1)}$$

where $\hat{d}^{(p)}$ and $\hat{d}^{(p+1)}$ are $(N-1)\times(N-1)$ differentiation matrices of order p and $p+1$, respectively, based on $x_1, ..., x_{j-1}, x_{j+1}, ..., x_N$ and $\bar{i} = i$ if $i < j$, $\bar{i} = i+1$ if $i > j$.

Proof. Without loss of generality we can suppose that $j = N$. Then,

$$S_N(x) = (x - x_N)S_{N-1}(x),$$

and thus

$$S'_N(x) = (x - x_N)S'_{N-1}(x) + S_{N-1}(x).$$

For $1 \leq i < N$ we obtain

$$S'_N(x_i) = (x_i - x_N)S'_{N-1}(x_i)$$

so that

$$\varphi_{N,i}(x)\frac{\rho(x)(x-x_N)S_{N-1}(x)}{\rho(x_i)(x_i-x_N)S_{N-1}(x_i)}\frac{1}{x-x_i}=\frac{x-x_N}{x_i-x_N}\varphi_{N-1,i}(x)\ ,\ \varphi_{1,i}(x)=\frac{\rho(x)}{\rho(x_i)}. \tag{3.2.34}$$

Since ρ is analytic in $\mathbb{R}$, $\varphi_{N-1,i}$ is too, and can be expanded as

$$\varphi_{N,i}(x)=\sum_{p\geq 0}\frac{\psi_{N,i}^{(p)}}{p!}(x-x_i)^p \tag{3.2.35}$$

with

$$\psi_{N,i}^{(p)}=\varphi_{N,i}^{(p)}(x_i)=d_{ii}^{(p)}. \tag{3.2.36}$$

Plugging (3.2.35) into (3.2.34) yields

$$\begin{aligned}\sum_{p\geq 0}\frac{\psi_{N,i}^{(p)}}{p!}(x-x_i)^p &= \frac{x-x_N}{x_i-x_N}\sum_{p\geq 0}\frac{\psi_{N-1,i}^{(p)}}{p!}(x-x_i)^p\\ &= \frac{1}{x_i-x_N}\sum_{p\geq 0}\frac{\psi_{N-1,i}^{(p)}}{p!}(x-x_i)^{p+1}+\sum_{p\geq 0}\frac{\psi_{N-1,i}^{(p)}}{p!}(x-x_i)^p\end{aligned}$$

and by comparing the coefficients of $(x-x_i)^m\ ,\ m>0$, we get

$$\psi_{N,i}^{(m)}=\frac{m}{x_i-x_N}\psi_{N-1,i}^{(m-1)}+\psi_{N-1,i}^{(m)} \tag{3.2.37}$$

which proves the result. □

Now let us examine (3.2.37) more closely. Applying (3.2.37) to the term $\psi_{N-1,i}^{(m)}$ in (3.2.37), and continuing this procedure we get

$$\begin{aligned}\psi_{N,i}^{(m)} &= \frac{m}{x_i-x_N}\psi_{N-1,i}^{(m-1)}+\frac{m}{x_i-x_{N-1}}\psi_{N-2,i}^{(m-1)}+...+\\ &\quad +\frac{m}{x_i-x_{i+1}}\psi_{i,i}^{(m-1)}+\frac{m}{x_i-x_{i-1}}\psi_{i-2,i}^{(m-1)}+...+\psi_{1,i}^{(m)}\end{aligned}$$

or in an equivalent form

$$\psi_{N,i}^{(m)} = \psi_{1,i}^{(m)} + m \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\psi_{j-1,i}^{(m-1)}}{x_i - x_j} \tag{3.2.38}$$

where

$$\psi_{1,i}^{(m)} = \frac{\rho^{(m)}(x_i)}{\rho(x_i)}$$

and from (3.2.36) the quantities $\psi_{N,i}^{(m)}$ are the $d_{ii}^{(m)}$ diagonal entries of $D^{(m)}, m > 0$.

Theorem (3.2.1) and theorem (3.2.2) gives the entries of $D^{(p)}$ recursively. As for the stability of these recursions following investigation conducted by Weideman and Reddy [59]. Differentiation matrices $D^{(p)}$ constructed in double and quadruple precision arithmetic respectively. The relative error computed in the Frobenius norm,

$$\text{R.E.} = \frac{\| \tilde{D}^{(p)} - D^{(p)} \|_F}{\| \tilde{D}^{(p)} \|_F} \ , \ p = 1, 2, ... \tag{3.2.39}$$

where the tilde refers to the matrices computed in quadruple precision. The relative error for the Chebyshev, Laguerre, and Hermite differentiation matrices is less then 10^{-13}. Increase in the matrix size has not much effect on the relative error.

Results confirm that the recursions are stable. But when p gets larger, error starts to increase, especially for larger values of N. This is due to the accumulation of roundoff errors in the (double precision) computation of $D^{(p)}$. Also the repeated division by $x_i - x_j$ in $D^{(p)}$, like the repeated multiplication of numbers of size $O\big((x_i - x_j)^{-1}\big)$ in $D^{(p)}$, increases the roundoff errors substantially when x_i is close to x_j.

As a result the algoritm is stable and provides accurate matrices $D^{(p)}$ for the values of p used most in practice.

3.3 Generation of First Order Differentation Matrices

In this section a number of well-known (Chebyshev, Legendre, Laguerre) first order differentation matrices will be constructed.

Definition 3.3.1. The $N+1$ points η_j , $j = 1, ..., N+1$ consisting of zeros of $\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x)$ plus the two points -1 and 1 are referred to as Gauss-Lobatto collocation points.

Definition 3.3.2. The N points ξ_j , $j = 1, ..., N$ consisting of zeros of $\frac{\mathrm{d}}{\mathrm{d}x}L_N^{(\alpha)}(x)$ plus the point 0 are referred to as Gauss-Radau collocation points.

Definition 3.3.3. The N points x_j , $j = 1, ..., N$ consisting of zeros of the orthogonal polynomial $p_N(x)$ are referred to as Gauss collocation points.

If one wants to solve boundary value problems on finite interval $[a, b]$, it is natural to construct the differentiation matrices by using Gauss-Lobatto points. Note that the interval $[a, b]$ can be mapped to the interval $[-1, 1]$ through the change of variables $\tilde{x} \to \frac{1}{2}[(b-a)x + (a+b)]$. Similarly, boundary value problems on semi-infinite domain $[0, \infty)$ and infinite domain $(-\infty, \infty)$ can be approximated by using Gauss-Radau and Gauss points redpectively.

For polynomial interpolation the weight function $\rho(x)$ is taken to be 1. Thus (3.2.23) takes the form

$$\varphi_{N,j}(x) = \phi_j(x) \ , \ j = 1, ..., N+1. \tag{3.3.40}$$

Note that the points η_j in definition (3.3.1) are the roots of $(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x)$. If the polynomial basis is taken as $S_N(x) = (1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x)$, then (3.2.25) implies that the interpolant is

$$\phi_j(x) = \frac{(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x)}{c_j(x-\eta_j)} \ , \quad j = 1, ..., N+1 \tag{3.3.41}$$

where

$$c_j = S_N'(\eta_j) = -d_j N(N+\alpha+\beta+1)P_N^{(\alpha,\beta)}(\eta_j) \tag{3.3.42}$$

and

$$d_1 = \frac{1}{\alpha+1}\ ,\ d_{N+1} = \frac{1}{\beta+1}\ ,\ d_j = 1 \text{ for } j = 2, ..., N$$

so that $\phi_j(\eta_j) = 1$. The c_j are obtained using the differential equation (2.3.62). Then the derivative operator in (3.2.29) together with (3.2.23) imply that

$$d_{ij}^{(1)} = \frac{1}{c_j}\frac{\mathrm{d}}{\mathrm{d}x}\Big[\phi_j(x)\Big]_{x=\eta_j}\ ,\ i,j = 1, ..., N+1. \tag{3.3.43}$$

That is, evaluation of the derivatives of Lagrangian interpolating polynomials at the collocation points η_j gives the first Jacobi differentiation matrix. Note that, the boundaries -1 and 1 are taken into account by the factor $(1-x^2)$. Differentiation of (3.3.41) in x gives

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}\phi_j(x) &= \frac{1}{c_j}\frac{1}{(x-\eta_j)^2}\Big\{\big[-2x\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x) + (1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(x)\big](x-\eta_j)\\ &\quad -(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x)\Big\}\ ,\ j = 1, ..., N+1\end{aligned} \tag{3.3.44}$$

For the off-diagonal entries, replacing $x = \eta_j$ in (3.3.44) we get

$$d_{ij}^{(1)} = \frac{1}{c_j}\frac{1}{\eta_i - \eta_j}(1-\eta_i^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(\eta_i). \tag{3.3.45}$$

Note that the values $(1-\eta_i^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(\eta_i)$ can be expressed in terms of $P_N^{(\alpha,\beta)}(\eta_i)$. Actually, the differential equation (2.3.62) gives

$$(1-\eta_i^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(\eta_i) = -N(N+\alpha+\beta+1)P_N^{(\alpha,\beta)}(\eta_i) \tag{3.3.46}$$

which is nothing but the c_i. Therefore (3.3.45) now reads as

$$d_{ij}^{(1)} = \frac{c_i}{c_j}\frac{1}{\eta_i - \eta_j} = \frac{d_i}{d_j}\frac{P_N^{(\alpha,\beta)}(\eta_i)}{P_N^{(\alpha,\beta)}(\eta_j)}\frac{1}{\eta_i - \eta_j}\ ,\ i,j = 1, ..., N+1\ ,\ i \neq j. \tag{3.3.47}$$

Computation of the diagonal entries is a little bit complicated, but it is not hard to manage. Taking limit as x goes to η_j in (3.3.44) and using L'Hopital's

rule we get

$$d_{jj}^{(1)} = \lim_{x\to\eta_j} \frac{-1}{2c_j}\left[\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x) + 4x\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(x) - (1-x^2)\frac{\mathrm{d}^3}{\mathrm{d}x^3}P_N^{(\alpha,\beta)}(x)\right]. \quad (3.3.48)$$

For $i = j = 1$, we have $\eta_1 = 1$ and the limit in (3.3.48) leads to

$$\begin{aligned} d_{11}^{(1)} &= \frac{-1}{2c_j}\left[\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(1) + 4\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(1)\right] \\ &= \frac{N(N\alpha+\beta+1)-\beta}{2(\alpha+2)}. \end{aligned} \quad (3.3.49)$$

To check (3.3.49), one should remember that c_1 is as in (3.3.42) while $\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(1)$ and $\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(1)$ are respectively given by (2.3.66) and (2.3.68). Similarly, for $i = j = N+1$, one obtains

$$d_{N+1,N+1}^{(1)} = \frac{N(N+\alpha+\beta+1)-\alpha}{2(\beta+2)} \quad (3.3.50)$$

this time recalling c_{N+1}, $\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(-1)$, $\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(-1)$. Taking derivative in x in (2.3.62) we have the following expression

$$\begin{aligned} -(1-x^2)\frac{\mathrm{d}^3}{\mathrm{d}x^3}P_N^{(\alpha,\beta)}(x) = \quad & \Big[\beta-\alpha-(\alpha+\beta+4)x\Big]\tfrac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(x) \\ & +(N-1)(N+\alpha+\beta+2)\tfrac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta)}(x). \end{aligned}$$

Inserting this equation into (3.3.48) we obtain

$$d_{jj}^{(1)} = \frac{-1}{c_j}\frac{1}{1-\eta_j^2}\Big[(\beta-\alpha)-(\alpha+\beta)\eta_j\Big]\frac{\mathrm{d}^2}{\mathrm{d}x^2}P_N^{(\alpha,\beta)}(\eta_j).$$

Now, the identity in (3.3.46) yields

$$d_{jj}^{(1)} = \frac{(\alpha+\beta)\eta_j+\alpha-\beta}{2(1-\eta_j^2)}\ ,\ j = 2,...,N.$$

Hence, the first order Jacobi pseudospectral differentiation matrix is

$$d_{ij}^{(1)} = \begin{cases} \dfrac{N(N+\alpha+\beta+1)-\beta}{2(\alpha+2)} & , \ i=j=1 \\ \dfrac{d_i}{d_j}\dfrac{P_N^{(\alpha,\beta)}(\eta_i)}{P_N^{(\alpha,\beta)}(\eta_j)}\dfrac{1}{\eta_i-\eta_j} & , \ i,j=1,...,N+1 \ , \ i\neq j \\ \dfrac{(\alpha+\beta)\eta_j+\alpha-\beta}{2(1-\eta_j^2)} & , \ 1<i=j<N+1 \\ \dfrac{N(N+\alpha+\beta+1)-\alpha}{2(\beta+2)} & , \ i=j=N+1 \end{cases} \tag{3.3.51}$$

where the d_i are as defined in (3.3.42). See also Funaro [22].

The differentiation matrix in (3.3.51) make sense when α and β are properly chosen real numbers. For example, the choice $\alpha=\beta=-\frac{1}{2}$ leads to the Chebyshev differentiation matrix. Note that the zeros of $(1-x^2)T_N'(x)$ are $\eta_j=\cos\frac{(j-1)\pi}{N}$, $j=1,...,N+1$ which are the Gauss-Lobatto Chebyshev collocation points. For these values we have from (2.3.82)

$$T_N(\eta_j)=(-1)^{j-1}. \tag{3.3.52}$$

Using (2.3.75) and (3.3.52), from (3.3.51), the first Chebyshev pseudospectral differentiation matrix can be obtained

$$d_{ij}^{(1)} = \begin{cases} \frac{1}{6}(2N^2+1) & , \ i=j=1 \\ \dfrac{d_i}{d_j}\dfrac{(-1)^{i+j}}{\eta_i-\eta_j} & , \ i,j=1,...,N+1 \ , \ i\neq j \\ \dfrac{-\eta_j}{2(1-\eta_j^2)} & , \ 1<i=j<N+1 \\ -\frac{1}{6}(2N^2+1) & , \ i=j=1 \end{cases} \tag{3.3.53}$$

where $d_1=d_{N+1}=2$, and $d_j=1$ for $j=2,...,N$. See also Funaro [22].

Similarly taking $\alpha = \beta = 0$ in (3.3.51), we recover the entries of the first Legendre pseudospectral differentiation matrix,

$$d_{ij}^{(1)} = \begin{cases} \frac{1}{4}N(N+1) & , \ i = j = 1 \\ \\ \frac{P_N(\eta_i)}{P_N(\eta_j)} \frac{1}{\eta_i - \eta_j} & , \ i, j = 1, ..., N+1 \ , \ i \neq j \\ \\ 0 & , \ 1 < i = j < N+1 \\ \\ -\frac{1}{4}N(N+1) & , \ i = j = 1 \end{cases} \tag{3.3.54}$$

See also Funaro [22]. Application of a similar procedure to the case of Laguerre polynomials is referred to as Laguerre collocation method which is a useful tool for solving boundary value problems on $[0, \infty)$. The basis function is

$$S_N(x) = e^{-x/2} x \frac{\mathrm{d}}{\mathrm{d}x} L_N^{(\alpha)}(x) \ , \ x \in [0, \infty) \ , \ N \in \mathbb{N}$$

in which the boundary $x = 0$ is included in the collocation points. In most problems it is required that the solution tends to zero as x goes to infinity. This requirement is taken care of by the weight function $\rho(x) = e^{-x/2}$. Note that, the nodes are Gauss-Radau collocation points. Now, (3.2.25) implies that the interpolant is

$$S_N(x) = \frac{1}{c_j} \frac{e^{-x/2} x \frac{\mathrm{d}}{\mathrm{d}x} L_N^{(\alpha)}(x)}{x - \xi_j} \ , \ j = 1, ..., N$$

where

$$c_j = S_N'(\xi_j) = d_j e^{-\xi/2} \xi_j \frac{\mathrm{d}}{\mathrm{d}x} L_N^{(\alpha)}(\xi_j) = -d_j N e^{-\xi/2} \xi_j L_N^{(\alpha)}(\xi_j)$$

and

$$d_1 = \frac{1}{\alpha + 1} \ , \text{ and } d_j = 1 \ , \text{for } j = 2, ..., N$$

so that $\psi_{N-1,j}(\xi_j) = 1$. Similar to Jacobi case,differentiating the interpolant and evaluating at the nodes ξ_i, the first generalized (associated) Laguerre pseudospec-

tral differentiation matrix

$$d_{ij}^{(1)} = \begin{cases} -\frac{1}{2}\frac{\alpha+2N}{\alpha+2} & , \ i=j=1 \\ \\ \frac{d_i}{d_j}\frac{e^{-\xi_i/2}L_N^{(\alpha)}(\xi_i)}{e^{-\xi_j/2}L_N^{(\alpha)}(\xi_j)}\frac{1}{\xi_i-\xi_j} & , \ i,j=1,...,N+1 \ , \ i\neq j \\ \\ -\frac{\alpha}{2\xi_j} & , \ 1<i=j<N+1 \end{cases} \tag{3.3.55}$$

is obtained, see also Funaro [22].

CHAPTER 4

HERMITE SPECTRAL METHODS

In this chapter a fairly detailed investigation of Hermite spectral (Galerkin and collocatin) methods will be given.

4.1 Eigenvalues of Hermite Spectral Methods

The Hermite spectral method is based on expansions in normalized Hermite functions

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} e^{-\frac{1}{2}x^2} H_n(x) \tag{4.1.1}$$

where $H_n(x)$ is the Hermite polynomial of degree n. For theoretical purposes the scaling factor $\frac{1}{\sqrt{2^n n!}}$ is redundant, but it is essential for computation. Without it, the max-norm of $\psi_n(x)$ grows explosively with n and overflow may occur [6]. The scaling also leads to the symmetric matrices, as will become apparent below. The functions $\psi_n(x)$ satisfy the orthogonality condition (2.3.104)

$$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x)\mathrm{d}x = \sqrt{\pi}\delta_{mn}, \tag{4.1.2}$$

where δ_{mn} is Kronecker delta. Galerkin spectral method may be based on the truncated series

$$f(x) = \sum_{n=0}^{N} a_n \psi_n(x), \tag{4.1.3}$$

where the coefficients are given by

$$a_n = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(x)\psi_n(x)\mathrm{d}x. \tag{4.1.4}$$

The nodes are choosen as the roots of $H_{N+1}(x)$, allowing one to compute the integrals with Hermite quadrature formulas. When solving differential equations we need to relate the coefficients of the derivative to those of the original function, as given by

$$f^{(k)}(x) = \sum_{n=0}^{N} a_n \psi_n(x) = \sum_{n=0}^{N} a_n^{(k)} \psi_n(x). \tag{4.1.5}$$

To do this, we use the recurrence formulas (2.3.108) and (2.3.109) to obtain

$$\begin{aligned} \psi_n'(x) &= \frac{1}{\sqrt{2^n n!}} e^{-\frac{1}{2}x^2} \big[-\frac{1}{2} H_{n+1}(x) + n H_{n-1}(x) \big] \\ &= \frac{1}{\sqrt{2}} \big[-\sqrt{n+1}\psi_{n+1}(x) + \sqrt{n}\psi_{n-1}(x) \big]. \end{aligned} \tag{4.1.6}$$

Inserting this expression in (4.1.5) yields,

$$a_n^{(1)} = \frac{1}{\sqrt{2}} \big[-\sqrt{n} a_{n-1} + \sqrt{n+1} a_{n+1} \big]. \tag{4.1.7}$$

Similarly, one more diferentiation of (4.1.6) gives,

$$a_n^{(2)} = \frac{1}{2} \big[\sqrt{(n-1)n} a_{n-2} + (2n+1) a_n + \sqrt{(n+1)(n+2)} a_{n+2} \big], \tag{4.1.8}$$

set $a_n = 0$ whenever $n < 0$ or $n > N$. We summarize these differentiation formulas as the matrix vector products

$$a^{(p)} = D^{(p)} a, \tag{4.1.9}$$

where $a = (a_1, ..., a_{N+1})^T$. Observe that $D^{(2)}$ is almost the square of $D^{(1)}$; only the truncation prevents this from being truly the case. The matrices $D^{(k)}$ have nice properties for efficient computation. First, they are banded. Second, the first and second derivative matrices are skew-symmetric and symmetric respectively.

Collocation (pseudospectral) derivatives can also be represented by matrices $D^{(p)}$ according to $f^{(p)} = D^{(p)} f$. The idea of last section implies that the inter-

polant is

$$\psi_{N,j}(x) = \frac{1}{c_j} \frac{e^{-x^2/2} H_{N+1}(x)}{x - x_j} \ , \ j = 0, 1, ..., N \tag{4.1.10}$$

where

$$c_j = e^{-x_j^2/2} H'_{N+1}(x_j) \tag{4.1.11}$$

so that $\psi_{N,j}(x_i) = \delta_{ij}$. Differentiating and evaluating at the collocation points (zeros of $H_{N+1}(x)$) yields

$$d_{ij}^{(1)} = \begin{cases} \frac{c_i}{c_j} \frac{1}{x_i - x_j} & , \ i \neq j \\ \\ 0 & , \ i = j \end{cases} \tag{4.1.12}$$

and similarly, one more differentiation of interpolant gives

$$d_{ij}^{(2)} = \begin{cases} -\frac{c_i}{c_j} \frac{2}{(x_i - x_j)^2} & , i \neq j \\ \\ \frac{1}{3}(x_i^2 - 2N - 1) & , i = j \end{cases} \tag{4.1.13}$$

where c_j is defined by (4.1.11).

However, simpler approach, which will be helpful to prove some results on Hermite pseudospectral differentiation matrices, given by [58]. Define $g(x)$ as

$$g(x) = e^{x^2/2} f(x). \tag{4.1.14}$$

The new function $g(x)$ is differentiated with polynomial spectral differentiation using the roots $x_1 < x_2 < ... < x_{N+1}$ of $H_{N+1}(x)$ as collocation points. Specifically given the function values $g(x_j)$, we interpolate them with a polynomial of degree N, the Lagrangian form of which is

$$\phi_N(x) = \sum_{j=0}^{N} \frac{H_{N+1}(x)}{H'_{N+1}(x_j)(x - x_j)} g(x_j).$$

Differentiation of this polynomial at the collocation points x_i provides an approx-

imation to $g^{(k)}(x_i)$. The process can be summarized as a matrix-vector product

$$g^{(k)} = D^k g,$$

where $g = \big(g(x_1), ..., g(x_{N+1})\big)^T$, and $g^{(k)} = \big(\phi_N^{(k)}(x_1), ..., \phi_N^{(k)}(x_{N+1})\big)^T$. In this expression D^k denotes the power. The matrix D has entries

$$d_{ij} = \frac{\mathrm{d}}{\mathrm{d}x}\Big[\frac{H_{N+1}(x)}{H'_{N+1}(x_j)(x-x_j)}\Big]_x = x_i.$$

Up on using the recurrence (2.3.109) and L'Hopital's rule for the diagonal elements, this simplifies to

$$D = HQH^{-1},$$

where

$$H = \mathrm{diag}(H_N(x_i)) \quad \text{and} \quad q_{ij} = \begin{cases} \dfrac{1}{x_i - x_j} & , \ i \neq j \\ x_i & , \ i = j. \end{cases}$$

The matrix D differentiates the function $g(x)$. To obtain the differentiation matrices for the original function $f(x)$ we differentiate (4.1.14)

$$\begin{aligned} f'(x) &= e^{-x^2/2}[g'(x) - xg(x)], \\ f''(x) &= e^{-x^2/2}[g''(x) - 2xg'(x) + (x^2-1)g(x)]. \end{aligned} \tag{4.1.15}$$

Collocation derivative may therefore be computed by

$$\begin{aligned} f'(x) &= E[D - X]E^{-1}f, \\ f''(x) &= E[D^2 - 2XD + (X^2 - I)]E^{-1}f, \end{aligned} \tag{4.1.16}$$

where $X = \mathrm{diag}(x_j)$, $E = \mathrm{diag}(e^{-x_j^2/2})$, $f = \big(f(x_1), ..., f(x_{N+1})\big)^T$ and I is the identity matrix. Collocation matrices in (4.1.16) and (4.1.12)-(4.1.13) are the same. Unlike the Galerkin counterparts, the collocation matrices are neither skew-symmetric nor symmetric. But even so, we will show that first derivatives have purely imaginary eigenvalues, and second derivatives have real and negative eigenvalues. Moreover, they are given by the roots of Hermite polynomials. Here

we normalize $H_n(x)$ such that its leading coefficient is $(-1)^n$, which differs from the scaling used in (4.1.1). The reason for this is that we define the characteristic polynomial of an $(N \times N)$ matrix D as $p_n(\lambda) = \det(D - \lambda I)$, which also has a leading coefficient $(-1)^n$. In terms of this normalization we have the recurrrence relations

$$H_{n+1}(x) = -xH_n(x) - \frac{1}{2}nH_{n-1}(x) \ , \ H_0(x) = 1 \ , \ H_1(x) = x, \tag{4.1.17}$$

and

$$H_n'(x) = -nH_{n-1}(x), \tag{4.1.18}$$

as well as the Darboux-Christofel formula in (2.1.45)

$$\sum_{n=0}^{N} \frac{H_n(x)H_n(y)}{2^{-n}n!} = \frac{H_N(x)H_{N+1}(y) - H_{N+1}(x)H_N(y)}{2^{-N}N!(x-y)}. \tag{4.1.19}$$

We start with the Galerkin first derivative matrix $D^{(1)}$ defined by (4.1.7) A similarity transformation with

$$J = \text{diag}(i^0, i^1, ..., i^N) \tag{4.1.20}$$

brings it to symmetric form

$$D^{(1)} = iJ\tilde{D}^{(1)}J^{-1}$$

where

$$\tilde{\mathbf{D}}^{(\mathbf{1})} = \begin{bmatrix} 0 & \sqrt{1} & & & \\ \sqrt{1} & 0 & \sqrt{2} & & \\ & \sqrt{2} & 0 & \ddots & \\ & & \ddots & \ddots & \sqrt{N} \\ & & & \sqrt{N} & 0 \end{bmatrix}. \tag{4.1.21}$$

The characteristic polynomial $P_{N+1}(\lambda)$ of $\tilde{D}^{(1)}$ is developed in the usual manner, leading to (4.1.18), and thus we conclude that $P_{N+1}(\lambda) = H_{N+1}(\lambda)$. Hence we

obtain the following theorem.

Theorem 4.1.1 (Weideman). *The eigenvalues of the matrix $D^{(1)}$, as determined by (4.1.7), are distinct, purely imaginary, and given by $\lambda_j = i\mu_j$, where μ_j are the roots of $H_{N+1}(\mu)$.*

Turning the second derivatives, closer inspection of (4.1.7) and (4.1.8) reveals that the second derivative matrix is almost the square of the first derivative, with a slight adjustment due to the truncation

$$D^{(2)} = {D^{(1)}}^2 - \frac{1}{2}(N+1)Z \tag{4.1.22}$$

where Z is the matrix consisting of zeros everywhere, except for its bottom right hand element which is 1.

Theorem 4.1.2 (Weideman). *The eigenvalues of the matrix $D^{(2)}$, as determined by (4.1.8), are real, negative, and distinct, and given by $\lambda_j = -\mu_j^2$, where μ_j are the $N+1$ positive roots of the polynomial $H_{N+1}(\mu)H_{N+2}(\mu)$.*

Proof. From (4.1.22),

$$-J^{-1}D^{(2)}J = \tilde{D}^{(1)^2} + \frac{1}{2}(N+1)Z$$

where J and $\tilde{D}^{(1)}$ are defined by (4.1.20) and (4.1.21). We prove the theorem by explicitly constructing the characteristic polynomial of the matrix on the right-hand side.

Let $p_n(\lambda)$ and $q_n(\lambda)$ be the characteristic polynomials of the $(n \times n)$ submatrices consisting of the first n rows and columns of $\tilde{D^{(1)}}^2 + \frac{1}{2}(N+1)Z$ and $\tilde{D^{(1)}}^2$, respectively. We have shown above that the characteristic polynomial of $\tilde{D}^{(1)}$ is $H_{N+1}(\lambda)$, for all N, therefore

$$q_n(\lambda) = H_n(-\sqrt{\lambda})H_n(\sqrt{\lambda}). \tag{4.1.23}$$

Since $\tilde{D^{(1)}}^2 + \frac{1}{2}(N+1)Z$ and $\tilde{D^{(1)}}$ differ only in their last elements, we develop the characteristic polynomial of the former matrix starting with its final column

and thus find that for all $n = 1, 2, ..., N+1$

$$p_n(\lambda) = q_n(\lambda) + \frac{1}{2} n p_{n-1}(\lambda) \ , \ p_0 = 1.$$

Applying this formula recursively yields

$$p_{N+1}(\lambda) = \frac{(N+1)!}{2^{N+1}} \sum_{n=0}^{N+1} \frac{q_n(\lambda)}{2^{-n} n!}.$$

Inserting (4.1.23) into above equation gives

$$p_{N+1}(\lambda) = \frac{(N+1)!}{2^{N+1}} \sum_{n=0}^{N+1} \frac{H_n(-\sqrt{\lambda}) H_n(\sqrt{\lambda})}{2^{-n} n!}.$$

Now, using Darboux-Christofel formula in (4.1.19), we get

$$p_{N+1}(\lambda) = \frac{H_{N+1}(\sqrt{\lambda}) H_{N+2}(-\sqrt{\lambda}) - H_{N+2}(\sqrt{\lambda}) H_{N+1}(-\sqrt{\lambda})}{2\sqrt{\lambda}}.$$

Finally, using the fact that $H_n(x)$ is an even (resp. odd) for n even (resp. odd), we have,

$$p_{N+1}(\lambda) = (-1)^N \frac{H_{N+1}(\sqrt{\lambda}) H_{N+2}(\sqrt{\lambda})}{\sqrt{\lambda}} \tag{4.1.24}$$

which is a characteristic polynomial of $-J^{-1} D^{(2)} J$, and theorem follows. □

The above theorem applies to the Galerkin differentiation matrices. The eigenvalues of the collocation matrices are very similar. In fact, we start by proving that first derivatives, collocation and Galerkin have identical eigenvalues.

Theorem 4.1.3 (Weideman). *The eigenvalues of the Hermite collocation differentiation matrix $E(D-X)E^{-1}$, as determined by (4.1.16), are distinct, purely imaginary, and given by $\lambda_j = i\mu_j$, where the μ_j are the roots of $H_{N+1}(\mu)$.*

Proof. Consider the eigenvalue equation

$$(D - X)g = \lambda g,$$

and let $P_N(x)$ be the polynomial interpolant of the data values $g = (g_0, g_1, ..., g_N)^T$. Then, since D differentiates $P_N(x)$ exactly, this equation is equivalent to

$$P'_N(x_j) - x_j P_N(x_j) = \lambda P_N(x_j) \ , \ j = 0, ..., N.$$

Now, consider the residual

$$R_{N+1}(x) = P'_N(x) - xP_N(x) - \lambda P_N(x),$$

which is a polynomial of degree $N+1$ with roots $x_0, x_1, ..., x_N$. Therefore, we have $R_{N+1}(x) = cH_{N+1}(x)$ with c a constant, and so

$$P'_N(x) - xP_N(x) = \lambda P_N(x) + cH_{N+1}(x). \tag{4.1.25}$$

Expand $P_N(x)$ as a Hermite series

$$P_N(x) = \sum_{n=0}^{N} a_n H_n(x)$$

and insert in (4.1.25). Using recurrence relations (4.1.17) and (4.1.18), and adjusting indices, gives

$$\sum_{n=1}^{N+1} a_{n-1} H_n(x) - \frac{1}{2} \sum_{n=0}^{N-1} (n+1) a_{n+1} H_n(x) = \lambda \sum_{n=0}^{N} a_n H_n(x) + cH_{N+1}(x) \tag{4.1.26}$$

Comparing coefficients for $n = N+1$ gives, $c = a_N$. And for $n = 0, ..., N$ we obtain

$$\hat{D}^{(1)} = \lambda a,$$

where $a = (a_0, a_1, ..., a_N)^T$, and

$$\hat{\mathbf{D}}^{(\mathbf{1})} = \begin{bmatrix} 0 & -\frac{1}{2} & & & \\ 1 & 0 & -\frac{2}{2} & & \\ & 1 & 0 & \ddots & \\ & & \ddots & \ddots & -\frac{N}{2} \\ & & & 1 & 0 \end{bmatrix}. \tag{4.1.27}$$

Symmetrizing the above matrix, we find $\hat{D}^{(1)} = iT\tilde{D}^{(1)}T^{-1}$, where the matrix $T = \mathrm{diag}\big((-i)^n 2^{n/2}/\sqrt{n!}\big)$ and $\tilde{D}^{(1)}$ is given by (4.1.21). Since $\tilde{D}^{(1)}$ has characteristic polynomial $p_{N+1}(\lambda) = H_{N+1}(\lambda)$, the theorem is proved. □

The fact that the collocation and Galerkin matrices share the same eigenvalues doesn't carry over the second derivatives, as shown in the next theorem.

Theorem 4.1.4 (Weideman). *The eigenvalues of the Hermite collocation differentiation matrix $E[D^2 - 2XD + (X^2 - I)]E^{-1}$, as determined by (4.1.16), are real, negative, and distinct, and given by $\lambda_j = -\mu_j^2$, where μ_j are the $\lfloor (N+1)/2 \rfloor$ positive roots of the polynomial $H_{N+1}(\mu)$, together with the interlacing $\lfloor (N+2)/2 \rfloor$ positive roots of $H'_{N+1}(\mu) - \mu H_{N+1}(\mu)$. The symbol $\lfloor\ \rfloor$ denotes the integer part.*

Proof. Reasoning as in the previous theorem, we obtain the second derivatives analogues of (4.1.25) and (4.1.26)

$$P''_N(x) - 2xP'_N(x) + (x^2 - 1)P_N(x) = \lambda P_N(x) + (c + dx)H_{N+1}(x),$$

and

$$\begin{aligned} &\sum_{n=2}^{N+2} a_{n-1}H_n(x) - \frac{1}{2}\sum_{n=0}^{N}(2n+1)a_nH_n(x) + \frac{1}{4}\sum_{n=0}^{N-2}(n+1)(n+2)a_nH_n(x) \\ &= \lambda\sum_{n=0}^{N} a_nH_n(x) + cH_{N+1}(x) - dH_{N+2}(x) - \frac{1}{2}d(N+1)H_N(x). \end{aligned}$$

Comparing coefficients for $n = N+1, N+2$ gives respectively $c = a_{N-1}$, and

$d = -a_N$. And for $n = 0, ..., N$ we obtain

$$\hat{D}^{(2)} = \lambda a$$

with

$$\hat{D}^{(2)} = \hat{D}^{(1)^2} - (N+1)Z$$

in which $\hat{D}^{(1)}$ is defined in the previous theorem, and Z is as defined before. Thus

$$-T^{-1}\hat{D}^{(2)}T = \tilde{D}^{(1)^2} + (N+1)Z,$$

where T is the matrix used in the previous theorem. We determine the eigenvalues by explicitly constructing the characteristic polynomial $r_{N+1}(x)$ of the matrix on the right hand side. First we write it as

$$\tilde{D}^{(1)^2} + (N+1)Z = \big[\tilde{D}^{(1)^2} + \frac{1}{2}(N+1)Z\big] + \frac{1}{2}(N+1)Z.$$

Then we expand its characteristic polynomial starting with the final column as in previous theorem, and use the fact that the characteristic polynomial $p_{N+1}(\lambda)$ of $\tilde{D}^{(1)^2} + \frac{1}{2}(N+1)Z$ is given by (4.1.24). This gives

$$\begin{aligned} r_{N+1}(\lambda) &= p_{N+1}(\lambda) + \frac{1}{2}(N+1)p_N(\lambda) \\ &= (-1)^N \frac{H_{N+1}(\sqrt{\lambda})}{\sqrt{\lambda}}\Big[H_{N+2}(\sqrt{\lambda}) - \frac{1}{2}(N+1)H_N(\sqrt{\lambda})\Big] \\ &= (-1)^N \frac{H_{N+1}(\sqrt{\lambda})}{\sqrt{\lambda}}\Big[H'_{N+1}(\sqrt{\lambda}) - \sqrt{\lambda}H_{N+1}(\sqrt{\lambda})\Big] \end{aligned}$$

where we have used (4.1.17) and (4.1.18).

By evaluating the polinomial $H'_{N+1}(\mu) - \mu H_{N+1}(\mu)$ at consecutive roots of $H_{N+1}(\mu)$, one concludes that it has $|(N+2)/2|$ real and positive roots, and that they interlace those of $H_{N+1}(\mu)$, thus proving the theorem. □

4.2 Spectral Radii of Hermite Differentiation Matrices

For numerical stability the important quantities are the spectral radii of the differentiation matrices defined respectively as

$$\rho(D) = \max_j |\lambda_j|,$$

where the λ_j are the eigenvalues of the differentiation matrix D. For our differentiation matrices the extreme eigenvalues are given by the roots of Hermite polynomials, the properties of which can be found in, for example, [45] or [1].

For the first derivative Hermite Galerkin matrix determined by (4.1.7), as well as its collocation counterpart given by (4.1.15), we have the following bound on the spectral radius

$$\rho(D^{(1)}) < (2N+3)^{1/2}\Big[1 - \frac{\mathcal{A}}{2^{1/3}(2N+3)^{2/3}}\Big] \cong O(\sqrt{N}),$$

here $\mathcal{A} = 2,3381...$ is the eabsolute value of the smallest zero of the Airy function. Likewise, theorem (3.3.23) states that the spectral radius of the Hermite Galerkin second derivative matrix is given by the square of the largest root of $H_{N+2}(\mu)$

$$\rho(D^{(2)}) < (2N+5)\Big[1 - \frac{\mathcal{A}}{2^{1/3}(2N+5)^{2/3}}\Big]^2.$$

For the Hermite collocation second derivative, we need the largest root of

$$H'_{N+1}(\mu) - \mu H_{N+1}(\mu)$$

which can be obtained by asymptotics. But a simple application of the inequality $\rho(\hat{D}^{(2)}) \leq \| \hat{D}^{(2)} \|_\infty$ to the matrix $\hat{D}^{(2)}$ as defined in theorem (4.1.4) provides an upper bound

$$\rho(D^{(2)}) < 2N+1 \cong O(N).$$

Thus, we have seen that the spectral radii for the first and second hermite dif-

ferentiation matrices are $O(\sqrt{N})$ and $O(N)$, respectively, where $N+1$ is the number of truncated terms used. This places rather weak stability restrictions on the Hermite method. For example, consider the standard heat equation

$$u_t = u_{xx}, \quad x \in (-\infty, \infty).$$

When an explicit method is used to integrate in time, the eigenvalues determine the maximum absolute time step. Specifically, it is necessary that

$$\triangle t < c/\rho(D^{(2)})$$

to ensure a bounded solution as $t \to \infty$, $\triangle t$ is fixed. The constant c depends on the intgration method. For Hermite method a maximum step size in the time direction is of order $O(N^{-1})$ whereas for Chebyshev method it is of order $O(N^{-4})$ [57]. In practise this means that one need not even consider implicit time integration methods with Hermite method.

The real line can be mapped to itself by a change of variable $x = \alpha\tilde{x}$, where α is any finite positive real number. This freedom does not exist for a finite interval, but after a change of scale in x, an infinite domain is still an infinite domain. In general optimum value of α depends on N in a manner determined by the properties of the solution. Allowing α to vary with N will change the effective spectral radius. it was pointed out by Boyd [6] that α should increase with the truncated terms used.

CHAPTER 5

APPLICATION TO THE SCHRÖDINGER EQUATION AND NUMERICAL RESULTS

In this chapter, we will use spectral collocation method to solve one-dimensional Schrödinger equation numerically with respect to a wide range of potential types. We deal with the symmetric

$$V(x) = v_2x^2 + v_{2m}x^{2m}, \quad \text{(generalized anharmonic oscillator)} \quad (5.0.1)$$

$$V(x) = -v_2x^2 + v_4x^4, \quad \text{(symmetric double well oscillator)} \quad (5.0.2)$$

$$V(x) = -e^{-\beta x^2}, \quad \text{(Gaussian potential)} \quad (5.0.3)$$

and asymmetric potentials of the form

$$V(x) = v_2x^2 + v_3x^3 + v_4x^4, \quad \text{(asymmetric double well oscillator)} \quad (5.0.4)$$

$$V(x) = (e^{-\beta x} - 1)^2, \quad \text{(Morse like potential)} \quad (5.0.5)$$

to test the method. The important point is that we not only restrict ourselves to polynomial potentials but also consider non-polynomial ones like Gaussian and Morse potentials. Numerical computations employ quadruple precision arithmetic and the eigenvalues of the well potentials are exact up to the last figure.

In numerical tables, n shows the quantum number of the state, and N stands for the truncation size to obtain the desired accuracy. Numerical results are obtained systematically with respect to different values of the scaling parameter α for all eigenvalue problems considered in this study.

5.1 Generalized Anharmonic Oscillators

The quantum mechanical problem of the generalized anharmonic oscillators described in the one-dimensional case by the potential

$$V(x) = v_2 x^2 + v_{2m} x^{2m}, \quad m = 2, 3, ... \tag{5.1.6}$$

continues to attract an appreciple amount of interest.This is due to the analogy between this model and one-dimensional quantum field teories, both of which yield divergent perturbation expansions. Furthermore, anharmonic oscillators are also directly relevant to the study of various atomic and molecular problems of quantum chemistry.

The potential (5.1.6) can be investigated in the form $V(x) = x^2 + \beta x^{2m}$. By making a transformation of variable from x to $v_2^{1/4} x$, we reduce the number of parameters to one and it is defined by

$$\beta = v_2^{-\frac{m+1}{2}} v_{2m}. \tag{5.1.7}$$

As an example to polynomials of this type, we choose quartic and sextic anharmonic oscillators.

5.1.1 Quartic Anharmonic Oscillator

Several approximation methods have consequently been used to calculate eigenvalues of quartic oscillator $V(x) = x^2 + \beta x^{2m}$. Among these we can recall WKB methods [30], [28], [2], [39], Rayleigh-Ritz variational method [52], Hill's determinant [17], perturbation techniques [29], [33], and finite difference approach [19]. Distinctively Banerjee et. al. [3] derived a method involving the use of an appropriately scaled basis for the determination of each eigenvalue. An integration-free method, namely Wronskian approach to solve anharmonic oscillators was devised by Demiralp [15]. A fairly detailed numerical application made in [52] to the quartic anharmonic oscillator, and it was suggested that the method could be extended to arbitrary polynomial potentials.

At the numerical side of this work, the result are compared with those of Taşeli and Erseçen [55], who have published extremely accurate results for the infinite interval. Tables (5.1), (5.2), (5.3) are for the ground state and the first two even excited states of the quartic oscillator respectively as functions of β and the parameter α_{opt}. Tables (5.4),(5.5), (5.6) give information about the convergence properties for $\beta = 0.001, 1.100000$ with respect to α.

Table 5.1: Ground state eigenvalues of the quartic oscillator $V(x) = x^2 + \beta x^4$, as a function of β.

β	E_0	N	α_{opt}
0.0001	1.000 074 986 880 200 111 122 834 155 30	15	1
0.01	1.007 373 672 081 382 460 533 843 905 98	32	1
1	1.392 351 641 530 291 855 657 507 876 61	51	2.1
10	2.449 174 072 118 386 918 268 793 906 19	53	3.1
1000	10.639 788 711 328 046 063 622 042 669 43	56	6.5
10000	22.861 608 870 272 468 891 759 867 963 52	55	10
100000	49.225 447 584 229 625 157 076 387 001 12	56	14

Table 5.2: Second state eigenvalues of the quartic oscillator $V(x) = x^2 + \beta x^4$, as a function of β.

β	E_2	N	α_{opt}
0.0001	5.000 974 615 938 385 599 377 851 129 58	18	1
0.01	5.093 939 132 742 309 225 377 304 880 22	37	1.1
1	8.655 049 957 759 309 688 116 539 457 38	54	2.2
10	16.635 921 492 413 757 783 361 917 932 19	57	3.1
1000	74.681 404 200 164 813 260 852 269 799 06	60	6.5
10000	160.685 912 611 711 511 059 174 059 116 9	60	9.5
100000	346.089 659 044 305 888 651 336 244 698 9	61	13.5

Table 5.3: Fourth state eigenvalues of the quartic oscillator $V(x) = x^2 + \beta x^4$, as a function of β.

β	E_4	N	α_{opt}
0.0001	9.003 072 972 044 612 550 295 311 892 34	21	1
0.01	9.289 479 816 311 885 668 219 161 173 62	40	1.1
1	18.057 557 436 303 252 894 771 239 646 52	59	2.3
10	35.885 171 222 253 873 712 281 269 098 19	62	3.2
1000	162.802 374 196 975 230 178 579 711 888 7	62	6.5
10000	350.435 896 215 566 009 349 619 220 592 44	65	9.5
100000	754.846 776 429 477 520 329 034 132 304 8	67	13

Table 5.4: Convergence rate of E_0 for $V(x) = x^2 + 0.0001x^4$ as a function of α.

α	N
0.5	138
0.7	66
0.9	31
0.95	24
1	15
1.1	30
1.3	51
1.5	73
2	137

Table 5.5: Convergence rate of E_0 for $V(x) = x^2 + x^4$ as a function of α.

α	N
1.5	88
1.8	57
1.9	51
2.1	51
2.2	55
2.3	59
2.5	61
2.9	80
3.3	107

Table 5.6: Convergence rate of E_0 for $V(x) = x^2 + 100000x^4$ as a function of α.

α	N
10	81
11	71
12	62
13	57
14	56
15	56
16	56
17	59
18	64
20	83

5.1.2 Sextic Anharmonic Oscillator

Like the quartic anharmonic oscillator, similar numerical methods have been applied to sextic anharmonic oscillator, $V(x) = x^2 + \beta x^6$. This potential has been studied by WKB approximation [28], Rayleigh-Ritz method [63], [52], [55] and Wronskian approach [15]. Numerical results are tabulated in Tables (5.7), (5.8), (5.9) for the ground state and the first two even excited states of the sextic oscillator respectively due to various values for $\beta = 0.001, 1, 100000$ with respect to α.

Table 5.7: Ground state eigenvalues of the sextic oscillator $V(x) = x^2 + \beta x^6$, as a function of β.

β	E_0	N	α_{opt}
0.0001	1.000 187 228 153 680 768 286 355 665 62	30	1
0.01	1.016 741 363 754 732 031 671 817 981 51	70	1.8
1	1.435 624 619 003 392 315 761 272 220 54	78	3.2
10	2.205 723 269 595 632 351 009 973 387 17	78	4.2
1000	6.492 350 132 329 671 550 549 557 845 3	79	7.5
10000	11.478 798 042 264 543 961 289 816 038 6	78	10
100000	20.375 098 656 309 660 844 567 287 513 5	78	12.9

Table 5.8: Second state eigenvalues of the sextic oscillator $V(x) = x^2 + \beta x^6$, as a function of β.

β	E_2	N	α_{opt}
0.0001	5.004 664 711 299 977 247 236 965 159 06	37	1
0.01	5.347 420 351 008 538 697 020 820 798 845	75	1.8
1	9.966 621 999 718 110 281 520 795 353 93	83	3.2
10	16.641 218 108 251 080 173 659 025 662 6	82	4.2
1000	51.182 480 106 305 690 884 693 028 921 5	84	7.1
10000	90.821 278 911 708 845 698 836 999 923 1	83	9.5
100000	161.395 652 930 207 952 854 887 264 588 16	92	12.3

Table 5.9: Second state eigenvalues of the sextic oscillator $V(x) = x^2 + \beta x^6$, as a function of β.

β	E_4	N	α_{opt}
0.0001	9.023 907 201 408 495 110 395 496 369 884	44	1
0.01	10.408 337 508 093 468 885 090 647 944 98	76	1.8
1	22.910 180 430 728 544 504 095 956 817 7	83	3.3
10	39.289 330 657 370 355 991 128 134 360 7	85	4.2
1000	122.321 705 320 204 002 373 196 508 244	85	7.4
10000	217.261 999 779 374 805 291 563 665 596	83	10.3
100000	386.206 210 872 676 914 710 823 857 436	86	13

Table 5.10: Convergence rate of E_0 for $V(x) = x^2 + 0.0001x^6$ as a function of α.

α	N
0.6	100
0.7	70
0.8	52
0.9	38
1	30
1.1	34
1.3	44
1.5	66
2	130

Table 5.11: Convergence rate of E_0 for $V(x) = x^2 + x^6$ as a function of α.

α	N
2	120
2.4	94
2.8	81
3.2	78
3.6	80
4	96
4.4	102
4.8	120

Table 5.12: Convergence rate of E_0 for $V(x) = x^2 + 100000x^6$ as a function of α.

α	N
8.5	124
9	114
9.8	102
11.5	84
12.2	82
12.9	78
13.6	79
14.5	80

5.2 Symmetric Double Well Oscillator

The double well oscillator $V(x) = -v_2x^2 + v_4x^4$ has attrached the attention of scientists for a long time. This oscillator has two minima when both $v_2 > 0$ and $v_4 > 0$. The very interesting property of its energy spectrum is that the lower eigenvalues are closely bunched in pairs if the wells are sufficiently seperated. This situation occurs for weak coupling when $v_4/v_2 \ll 1$, and means that the potential has nearly degenerate minima. Thus the determination of the shift in energy levels due to tunneling through a potential barrier becomes more important. In such a case, the gap between the nearly degenerate eigenvalues has been investigated by the WKB approximation [14], by finite difference calculation [62], by the path-integral approach [24] and by the perturbation theory at large orders [9]. On the other hand, accurate results for the eigenvalues by using an appropriately scaled expansion basis and a recursive series method presented in [4]. A two step approach and JWKB approximation have been proposed by Hsue and Chern [27] and Sanchez and Bejarano [39], respectively and applied to the double well oscillator. More recently, Taşeli and Erseçen [55] have been published extremely accurate results on the symmetric double well potential.

The potential $V(x) = -v_2x^2 + v_4x^4$ may be investigated in the form $V(x) = -x^2 + \beta x^4$. With the transformation of variable from x to $v_2^{1/4}x$, we have $\beta = v_2^{-3/2}v_4$. Moreover, the operator shifted by $1/(4\beta)$ is now positive definite. So the eigenvalues are given in terms of $E + 1/(4\beta)$.

In Table (5.14), the nearly degenerate eigenvalues for the case of $\beta = 0.01$ are presented. The ground and the first four excited states of the symmetric double well oscillator for larger couplings are reported in Table (5.13).

Table 5.13: Eigenvalues of the symmetric double-well oscillators, as a function of β.

β	α_{opt}	n	N	E_n
0.05	1.3	0	76	1.358 422 103 747 795 462 828 858 001 13
	1.3	1	77	1.360 133 597 773 303 266 049 420 318 88
	1.3	2	76	3.746 917 080 727 930 707 382 042 658 90
	1.3	3	76	3.848 838 300 057 397 949 123 848 305 50
	1.3	4	76	5.369 059 360 284 711 606 322 475 533 06
0.1705	1.6	0	60	1.005 907 534 732 669 494 259 934 270 98
	1.6	1	61	1.465 359 922 207 691 593 693 811 222 26
	1.6	2	63	3.120 683 690 166 030 901 005 016 518 38
	1.6	3	64	4.822 552 955 752 771 227 915 786 027 28
	1.6	4	65	6.876 623 854 334 680 478 308 869 928 85
1	2.1	0	58	0.907 653 005 180 715 123 059 021 723 111
	2.1	1	58	3.084 536 202 119 304 214 654 676 208 749
	2.1	2	58	6.413 901 256 963 068 240 915 237 315 023
	2.1	3	62	10.288 646 120 711 576 043 356 901 150 295
	2.1	4	63	14.622 406 504 677 868 955 906 567 619 672
10	3.1	0	54	2.137 877 898 050 259 289 303 800 668 73
	3.1	1	56	7.786 789 928 304 487 098 125 425 821 37
	3.1	2	58	15.505 390 136 564 835 078 358 830 039 90
	3.1	3	60	24.384 990 424 717 251 665 235 908 096 38
	3.1	4	62	34.200 530 589 304 058 305 960 711 826 09
100	4.4	0	53	4.845 921 891 362 033 319 865 475 050 73
	4.4	1	55	17.444 197 413 120 973 381 603 569 928 96
	4.4	2	57	34.340 152 315 559 552 006 178 212 246 22
	4.4	3	59	53.716 507 749 978 459 831 972 443 757 69
	4.5	4	62	71.085 977 797 358 526 304 872 975 386 82

Table 5.14: Nearly degenerate states of the symmetric double-well oscillator for $\beta = 0.01$.

n	N	α_{opt}	E_n
1	100	1	1.404 048 605 297 706 882 425 707 570 82
2	100	1	1.404 048 605 297 706 882 602 566 280 56
3	105	1	4.170 193 605 999 310 127 833 875 071 30
4	105	1	4.170 193 605 999 310 219 613 291 198 73
5	109	1	6.870 088 833 714 024 612 172 315 168 49
6	109	1	6.870 088 833 714 046 802 425 995 681 89
7	110	1	9.498 578 387 187 870 055 194 418 356 55
8	110	1	9.498 578 387 191 178 212 320 856 961 14
9	116	1.1	12.049 309 486 334 092 592 332 880 171 60
10	116	1.1	12.049 309 486 673 006 847 573 312 477 88
11	119	1.1	14.514 205 022 981 239 103 429 421 443 86
12	119	1.1	14.514 205 048 121 017 338 991 612 415 80

5.3 Asymmetric Double Well Potential

Next we considered, the asymmetrical double well potential of the form

$$V(x) = v_2x^2 + v_3x^3 + v_4x^4 \tag{5.3.8}$$

which has two minima located asymmetrically around the origin, if the parameters satisfy the inequalities $v_4 > 0$ and $9v_3^2 - 32v_2v_4 > 0$. Here we take into account the alternative form

$$V(x) = c_1x^2(x + c_2)(x - 1), \quad 0 < c_2 < 1, \quad c_1 > 0 \tag{5.3.9}$$

of the ADWPs proposed by Taşeli [49].

These potentials are of practical interest for the protonic movement of hydrogen-bonded systems [43]. Znojil [64] constructed Hill's determinant of the problem by matching two power series valid for negative and positive values of the argument, respectively. Some numerical results were introduced by Diaz at. al. [16], but a

more systematic numerical study ADWPs may be found in [49] and [55].

The numerical results are reported in Table (5.15)-(5.24) for c_1 values of 0.01, 1, and 100 respectively, as afunction of c_2. The range of c_2 is covered by choosing $c_2 = 0.25$, $c_2 = 0.5$, $c_2 = 0.75$. It is clear that the lefthand limiting value of c_2, $c_2 = 0$, does not represent a double well oscillator anymore where the potential has an inflection point at $x = 0$. On the other hand, $c_2 = 1$ corresponds to a symmetrical two well potential which was examined extensively in [48]. Table (5.18) and (5.19) demonstrates the rate of convergence of the method as the optimization parameter α varies.

Table 5.15: Eigenvalues of asymmetrical double-well oscillators for $c_1 = 0.01$, as a function of c_2.

c_2	α_{opt}	N	n	E_n
0.25	1	52	0	0.220 496 933 551 383 181 180 584 101 238
		56	1	0.799 076 156 134 041 042 756 335 888 802
		58	2	1.579 425 872 715 042 186 839 788 277 334
		61	3	2.475 227 126 276 957 997 940 355 211 699
0.50	1	54	0	0.218 255 536 797 065 407 353 982 485 211
		56	1	0.793 475 852 449 351 300 718 466 956 319
		58	2	1.571 726 799 166 984 751 587 449 207 978
		60	3	2.465 596 537 785 138 574 857 695 511 215
0.75	1	51	0	0.215 207 254 047 971 748 843 624 710 39
		53	1	0.785 867 870 008 598 255 331 395 933 43
		55	2	1.561 286 635 695 375 110 776 021 304 72
		57	3	2.452 542 721 464 178 763 806 091 811 26

Table 5.16: Eigenvalues of asymmetrical double-well oscillators for $c_1 = 1$, as a function of c_2.

c_2	α_{opt}	N	n	E_n
0.25	2	59	0	0.869 694 617 647 318 773 345 709 020 35
		59	1	3.358 793 828 433 288 053 701 048 464 78
		61	2	6.859 073 162 056 196 233 256 933 927 90
		63	3	10.903 704 068 138 317 871 260 599 290 63
0.50	2	58	0	0.820 154 510 028 224 184 518 349 604 83
		58	1	3.234 414 126 319 227 742 294 069 206 91
		59	2	6.691 150 275 295 513 627 696 545 335 53
		62	3	10.694 056 898 461 014 997 542 820 263 34
0.75	2	57	0	0.752 313 748 218 290 226 508 186 964 66
		57	1	3.062 371 804 064 220 085 319 934 596 33
		59	2	6.461 681 817 708 838 046 691 399 198 93
		61	3	10.408 002 113 532 361 485 956 111 209 75

Table 5.17: Eigenvalues of asymmetrical double-well oscillators for $c_1 = 100$, as a function of c_2.

c_2	α_{opt}	N	n	E_n
0.25	4.4	69	0	−4.277 344 849 182 474 166 847 348 848 02
		69	1	7.080 517 391 364 158 656 090 710 350 21
		72	2	19.817 761 502 618 821 399 175 325 525 15
		73	3	36.209 337 296 287 706 584 558 242 608 56
0.50	4.4	58	0	−6.816 052 047 536 736 982 561 430 365 98
		58	1	4.675 693 930 558 290 057 997 135 848 24
		59	2	15.973 204 136 317 836 561 600 922 534 71
		62	3	31.505 546 630 519 551 260 800 075 872 05
0.75	4.4	57	0	−9.459 479 212 224 512 858 546 562 584 43
		57	1	0.010 560 072 717 619 621 379 801 416 92
		59	2	10.866 977 233 476 768 562 653 506 503 66
		61	3	24.888 991 175 519 381 797 134 001 071 93

Table 5.18: Convergence rate of E_0 for asymmetrical double-well oscillator w.r.t. α when $N = 54$, $c_1 = 0.01$ and $c_2 = 0.25$.

α	E_0
2	0.220 619
1.8	0.220 502
1.6	0.220 496 631
1.4	0.220 496 933 553
1.2	0.220 496 933 551 383 181 180 602
1.1	0.220 496 933 551 383 181 180 584 101
1	0.220 496 933 551 383 181 180 584 101 238
0.8	0.220 496 933 551 383 181 180 584
0.6	0.220 496 933 551 383 181

Table 5.19: Convergence rate of E_0 for asymmetrical double-well oscillator w.r.t. α when $N = 69$, $c_1 = 100$ and $c_2 = 0.25$.

α	E_0
2.8	−4.277 344 849 182 474 166
3.2	−4.277 344 849 182 474 166 847 347
3.6	−4.277 344 849 182 474 166 847 348
4.0	−4.277 344 849 182 474 166 847 348 847
4.4	−4.277 344 849 182 474 166 847 348 848 02
4.8	−4.277 344 849 182 474 166 847 348 848 02
5.2	−4.277 344 849 182 474 166 847 348 847
5.6	−4.277 344 849 182
6.4	−4.277 344 848
6.8	−4.277 344

5.4 Gaussian Potential

In the literature, generally radial form of the Gaussian potential

$$V(r) = -Ae^{-\beta r^2} \tag{5.4.10}$$

is preferred to work with as it is of importance in nuclear physics. It has been used as potential model in the theory of nucleon-nucleon scattering [10] using direct numerical integration and by Stephenson [44] using the Liouville-Green asymptotic method. Bessis et. al. [5] have obtained the bound state energies of the Gaussian potential for $\beta = 1$ using the perturbational and also a variational treatment on a conveniently chosen basis of transformed Jacobi functions. It is shown that the traditional Rayleigh- Schrödinger method on the chosen basis can yield fairly accurate results. Cohen [13] has proposed a simple method to calculate the bonud state energies of the Gaussian potential from a first-order perturbation theory based on a scaled harmonic oscillator model. more recently, Taşeli and Erseçen [55] have published extremely accurate results for the eigenvalues of the Gaussian potential using scaled Hermite-Weber basis.

Here, we are interested in finding the eigenvalues of the one dimensional Schrödinger equation, therefore we will take

$$V(r) = -e^{-\beta x^2} \tag{5.4.11}$$

as the Gaussian potential which differs from the previous problems, since it is a non-polynomial one.

The ground-state and first three even numbered excited states of the original Gaussian potential (5.4.11) are presented in Table (5.20) when $\beta = 0.001,\ 0.01,\ 0.1$. Finally, Table (5.21) and (5.22) gives the convergence rate of the Gaussian potential with respect to the optimization parameter α.

Table 5.20: Eigenvalues of the Gaussian potential $V(x) = -e^{-\beta x^2}$.

β	α_{opt}	N	n	E_n
0.001	0.2	56	0	−0.968 752 703 034 398 668 606 599 656 91
		70	2	−0.846 820 196 725 804 118 603 225 951 44
		85	4	−0.731 125 549 125 734 739 132 375 767 29
		103	6	−0.621 888 650 443 182 657 155 148 987 66
0.01	0.3	81	0	−0.903 763 987 980 773 054 539 687 567 95
		128	2	−0.550 801 670 798 557 886 254 842 935 81
		128	4	−0.267 463 693 629 351 027
		128	6	−0.068 692 251
0.1	0.2	148	0	−0.721 530 628 487 107 638 685 036 884 81
			2	−0.007 90

Table 5.21: Convergence rate of E_0 for Gaussian potential w.r.t. α when $\beta = 0.001$, $N = 56$.

α	E_0
1	−0.965
0.8	−0.968 104
0.6	−0.968 737
0.4	−0.968 752 702
0.3	−0.968 752 703 034 398 373
0.2	−0.968 752 703 034 398 668 606 599 656 913
0.1	−0.968 752 703 034 396

Table 5.22: Convergence rate of E_0 for Gaussian potential w.r.t. α when $\beta = 0.01$, $N = 81$.

α	E_0
1	−0.903 762
0.8	−0.903 763 983
0.6	−0.903 763 987 980 564
0.4	−0.903 763 987 980 773 054 539 413
0.3	−0.903 763 987 980 773 054 539 687 567 952
0.2	−0.903 763 987 980 773 054 547
0.1	−0.903 764

5.5 A Morse Like Potential

The last potential that we considered in this study

$$V(x) = (e^{-\beta x} - 1)^2 \tag{5.5.12}$$

is a Morse like potential. It gives us the possibility of testing Hermite collocation method for a non-polynomial, asymmetric potential. It is used to determine vibrational energy levels of diatomic molecules [34], [50], [54]. This singular eigenvalue problem over $-\infty < x < \infty$ has finite number of eigenvalues lying between $0 < E < 1$, and a continuous spectrum for all $E \geq 1$. As in the case of harmonic oscillator, Morse potential problem [54] has an analytic solution as well. The solutions for the bound states are expressible as

$$\varphi_n = B_n(2/\beta)^{\nu_n} e^{-\beta\nu_n x} L_n^{2\nu_n}(2e^{-\beta x}/\beta), \quad E_n = k_n(2 - k_n) \tag{5.5.13}$$

for

$$n = 0, 1, ..., K \tag{5.5.14}$$

where

$$k_n = \frac{1}{2}\beta(2n + 1), \qquad \nu_n = \frac{1}{\beta}(1 - k_n) > 0, \tag{5.5.15}$$

and K, B_n and $L_n^{(m)}(x)$ are, respectively, the integer part of the parameter $\frac{1}{\beta} - \frac{1}{2}$, a normalization constant and the generalized Laguerre polynomials. It is also have shown that the problem has no bound states if $\beta > 2$.

Numerical results are given in Tables (5.23)-(5.25). The ground state and the first four excited states of the Morse potential (5.5.12) is presented in Table (5.23) when $\beta = 0.02,\ 0.2$. Also, the convergence rate of the Morse potential with respect to the optimization parameter α given in Tables (5.24) and (5.25) respectively.

Table 5.23: Eigenvalues of the Morse potential $V(x) = (e^{-\gamma x} - 1)^2$, when $\gamma = 0.02$ and 0.2.

γ	α_{opt}	N	n	E_n	E_{exact}
0.02	0.1	84	0	0.019 900 000 000 000 000 000 000 000 000	199×10^{-4}
		90	1	0.059 100 000 000 000 000 000 000 000 000	591×10^{-4}
		94	2	0.097 500 000 000 000 000 000 000 000 000	975×10^{-4}
		98	3	0.135 100 000 000 000 000 000 000 000 000	1351×10^{-4}
		100	4	0.171 900 000 000 000 000 000 000 000 000	1719×10^{-4}
0.2	0.4	102	0	0.190 000 000 000 000 000 000 000 7	19×10^{-2}
			1	0.510 000 000 000 000 005	51×10^{-2}
			2	0.750 000 000 005	75×10^{-2}
			3	0.910 000 5	91×10^{-2}

Table 5.24: Convergence rate of E_0 for Morse potential w.r.t. α when $\gamma = 0.02$, $N = 100$.

α	E_0
0.4	0.019 900 000 3
0.3	0.019 900 000 000 000 6
0.2	0.019 900 000 000 000 000 000 000 000 003
0.1	0.019 900 000 000 000 000 000 000 000 000
0.08	0.019 900 000 000 000 000 000 000
0.06	0.019 9

Table 5.25: Convergence rate of E_0 for Morse potential w.r.t. α when $\gamma = 0.2$, $N = 100$.

α	E_0
1	0.190 000 04
0.8	0.190 000 000 09
0.6	0.190 000 000 000 003
0.5	0.190 000 000 000 000 000 5
0.4	0.190 000 000 000 000 000 000 001
0.3	0.190 000 000 000 000 000 02
0.2	0.190 000 000 004
0.1	0.189

CHAPTER 6

CONCLUSIONS

In this thesis, spectral collocation method is used to calculate the energy eigenvalues of the one dimensional Schrödinger equation to thirty digits for single and double-well oscillators corresponding to polynomial and non-polynomial potentials. Since Hermite functions are the solutions of the harmonic oscillator problem, it is natural to use Hermite spectral collocation method. The roots of Hermite polynomials are found by diagonalizing the three diagonal Jacobi matrix **A** in (2.1.49). Then, differentiation matrices are constructed by using Welfert's [60] algorithm. After adding potential matrices to the second order Hermite differentiation matrix, eigenvalues are determined by the standard routines ORTHES, which brings the matrix to upper Hessenberg form and HQR, which finds the eigenvalues of the reduced matrix by using the QR method. For these computations quadruple precision arithmetic is used.

A scaling parameter α is inserted in the structure of the Hermite collocation basis, so as to improve the accuracy. This is possible since after a change of scale in x, an infinite domain still an infinite domain. The spectra of various potentials are obtained by way of determining the optimum value for parameter α.

First of all, Hermite spectral method applied to polynomial potentials like quartic and sextic anharmonic oscillators. The numerical results show that the method converges to the eigenvalues of the problem up to thirty digits with acceptable matrix dimensions. For example, for finding the ground state eigenvalues of $V(x) = x^2 + 0.0001x^4$ the method requires only a matrix of order 15, and the optimization parameter has no effect on the solution, i.e. $\alpha = 1$.(Table 5.1). This is because when β is very small potential behaves like the harmonic oscillator. However, as β grows i.e., in the pure anharmonic regime, the contribution of the optimization parameter α becomes significant. For example, when $\beta = 100000$,

α_{opt} becomes 14 for which the desired accuracy is reached with a truncation size of 56.

A similar discussion is also valid for sextic anharmonic oscillators. Although the sextic anharmonic oscillator has a stronger anharmonic behaviour than the quartic oscillator, especially when β is large, there is small increase in the matrix dimensions.

In the case of symmetric double-well potentials, it is seen from (Table 5.13) that for $\beta \geq 0.1705$ eigenvalues stabilize when $N = 53 - 63$ and the variation of β affects the optimization parameter α. As an exceptional case, a slowing down of convergence is seen for small couplings whenever there are four classical turning points in certain cases of the quantum number n. In the regime of $\beta < 0.1705$ the lower eigenvalues are closed to each other in pairs due to tunelling through the potential barrier and therefore there exist nearly degenerate states of eigenvalues (Table 5.14). When $\beta = 1705$, there exits four classical turning points only for the ground and the first excited states. So $\beta = 1705$ is a treshold value [48] after which the number of turning points reduces to two and the probability of tunelling approaches zero.

If one recalls the fact that many methods fail for potentials with degenerate minima [24],[30], the power of Hermite collocation method in obtaining the nearly degenerate eigenvalues with such an accuracy is quite impressive.

It may be checked through comparison that the eigenvalues calculated by Taşeli [48], and also Taşeli and Erseçen [55] agree with our results to the accuracy quoted. However, since we didn't seperate the eigenlevels as even and odd parity states, in the symmetric cases, truncation size N is doubled.

In the asymmetrical polynomial potentials, truncation size N is more reasonable as compared with the symmetric cases. In this case, the optimization parameter α increases together with the parameter c_1. Still even in the asymmetric potential case the method works well.

Testing the method for only polynomial type potentials is not enough. To make a comparison, Gaussian and a Morse like potential are chosen as a non-polynomial potential types. Gaussian potential has both continuous and discrete spectrum. The discrete eigenlevel occurs for $E < 1$. As β gets larger, i.e.,

at the border of the continuous spectrum, there is a decrease in the number of discrete eigenvalues and the method fails to give the desired accuracy. For example, when $\beta = 0.1$ only two discrete eigenvalues has been obtained, and although the truncation size $N = 148$, the convergence gets worse (Table 5.21). In Table (5.22) the contribution of α to the convergence of E_0 is observed. The optimization parameter α always gets values between 0 and 1.

In Morse potential luckily exact solution of the problem exists. Therefore, it is easy to check the accuracy of the eigenvalues. In this potential, the discrete eigenlevel occurs for $0 < E < 1$. Table (5.23) shows that when β is small we obtain the exact solution, but as β gets larger, i.e., at the border of the continuous spectrum, the method fails to give 30 digits, especially in higher energy levels. Like the Gaussian potential α_{opt} is smaller than 1.

As compared to the variational Rayleigh-Ritz method using Hermite-Weber basis [55], Hermite collocation method has some computational advantages. In the former, construction of the variational matrices is not so easy that one has to evaluate the integrals containing Hermite functions. Fortunately, these integrals can be computed by hand so that numerical integration is not needed. If this was not the case, then additional erros would arise and the accuracy of the method decreases. But for the latter case construction of the differentiation matrices is easier and less time consuming process than the former one.

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